

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

Gas phase species [ppb]	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 ₂	4.5		1.5		0.4	0.1
HNO ₃	1		0.3		0.15	
CH ₄	1700		1700		1700	
H ₂ O ₂	1		0.001	1	0.001	1
H ₂	2000	500	2000	500	2000	500
CO	200	300	150		140	
O ₃	90		60	40	40	30
HCl	6	0.2	0.7	0.1	0.5	
NH ₃	25	5	1.5		0.05	
CO ₂	5 · 10 ⁵	3.57 · 10 ⁵	3.3 · 10 ⁵	3.57 · 10 ⁵	3.3 · 10 ⁵	3.57 · 10 ⁵
SO ₂	10	5	1		0.1	
HCHO	0.1	1	0.1	0.5	0.01	0.5
C ₂ H ₆	2		1.5		1	0.5
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		1		1	
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		0.5		0	
HC8: Alkanes with OH rate constant greater than 6.8 · 10 ⁻¹² cm ³ s ⁻¹ (298 K, 1 atm)	0.1		0		0	
C ₂ H ₄	1		0.5		0.1	
OLT: Terminal alkenes	0.1		0.1		0.1	
Isoprene	0.1	0	0.1	1	0.1	0
TOL: Toluene and less reactive aromatics	0.1		0.01		0	
CSL: Cresol and other OH-substituted aromatics	0.001		0.001		0	
XYL: Xylene and more reactive aromatics	0.1		0.01		0	

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 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 [M]								
O _{2(aq)}	3 · 10 ⁻⁴		b	3 · 10 ⁻⁴		b	3 · 10 ⁻⁴	b
OH ⁻	3.16 · 10 ⁻¹⁰			3.16 · 10 ⁻¹⁰			1.6 · 10 ⁻⁹	
pH	4.5		b	4.5		b	5.2	i
Cl ⁻	1 · 10 ⁻⁴		h	1 · 10 ⁻⁴		h	5.6 · 10 ⁻⁴	j
Br ⁻	3 · 10 ⁻⁶		h	3 · 10 ⁻⁷		h	1.8 · 10 ⁻⁶	j
Fe ³⁺	5 · 10 ⁻⁶		d	5 · 10 ⁻⁷		d	5 · 10 ⁻⁸	d
Mn ³⁺	2.5 · 10 ⁻⁷		d	2.5 · 10 ⁻⁸		d	1 · 10 ⁻⁹	d
Cu ⁺	2.5 · 10 ⁻⁷	0	d	2.5 · 10 ⁻⁸	0	d	1 · 10 ⁻⁹	d
Cu ²⁺	0	2.5 · 10 ⁻⁷		0	2.5 · 10 ⁻⁸		0	1 · 10 ⁻⁹
HSO ₄ ⁻	3 · 10 ⁻⁷			3 · 10 ⁻⁷			3 · 10 ⁻⁸	
SO ₄ ²⁻	5.97 · 10 ⁻⁵		e	5.97 · 10 ⁻⁵		e	5.97 · 10 ⁻⁶	i
C ₂ O ₄ ²⁻	5 · 10 ⁻⁶		k	5 · 10 ⁻⁷		k	5 · 10 ⁻⁸	k

Constant concentrations
during simulation time

H ₂ O _(g)	2 · 10 ⁷	3 · 10 ⁷	3 · 10 ⁷
O _{2(g)}	2 · 10 ⁸	2 · 10 ⁸	2 · 10 ⁸
N _{2(g)}	7.8 · 10 ⁸	7.8 · 10 ⁸	7.8 · 10 ⁸
H ₂ O _(aq)	55.5	55.5	55.5

^{a)} 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 [C₂O₄]²⁻ = [Fe³⁺], Sedlak and Hoigné, 1992; ^l Rohrer and Brüning, 1992

Table 2: Emissions and Depositions**Table 2a: Emissions**

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

	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	1.01·10 ⁷		2.86·10 ⁵		2.8·10 ⁴	
CO	8.99·10 ⁷		3.7·10 ⁶		8.53·10 ⁵	
NH ₃	3.03·10 ⁶		9.06·10 ⁵		4.57·10 ⁵	
SO ₂	3.27·10 ⁷	3.27·10 ⁶	2.91·10 ⁵		7.92·10 ⁴	
HCHO	2.58·10 ⁵		3028		17.8	
ethane (ETH)	1.54·10 ⁶		1.5·10 ⁴		8.91	
HC3: Alkanes with OH rate constant between 2.7·10 ⁻¹³ and 3.4·10 ⁻¹² cm ³ s ⁻¹ (298 K, 1 atm)	2.76·10 ⁶		1.53·10 ⁴		1.73	
HC5: Alkanes with OH rate constant between 3.4·10 ⁻¹² and 6.8·10 ⁻¹² cm ³ s ⁻¹ (298 K, 1 atm)	4.9·10 ⁶		6.31·10 ⁴		2.653	0
HC8: Alkanes with OH rate constant greater than 6.8·10 ⁻¹² cm ³ s ⁻¹ (298 K, 1 atm)	3.19·10 ⁶		4.044·10 ⁴		11.72	0
ethene (OL2)	2.61·10 ⁶		4.54·10 ⁴		45.0	
terminale alkenes (OLT)	4.94·10 ⁵		7950		7.28	0
dienes (DIEN)	1.24·10 ⁶		1.55·10 ⁴		11.7	
isoprene (ISO)	0	1.54·10 ⁵	0	1.5·10 ⁶		
TOL: Toluene and less reactive aromatics	1.7·10 ⁶		2.108·10 ⁴		5.81	
CSL: Cresol and other OH-substituted aromatics	1.82·10 ⁶		2.88·10 ⁴		7.78	0
XYL: Xylene and more reactive aromatics	9.88·10 ⁵		1.13·10 ⁴		0.721	0
acetaldehyde and higher aldehydes	5.93·10 ⁵		3171		10.41	
ketones (KET)	9.9·10 ⁵		8920		1.59	
CH ₃ COOH	8.44·10 ⁴		3350		810	
CH ₃ OH	1.16·10 ⁶		1.07·10 ⁴		0.59	
Ethanol	4.03·10 ⁶		3736		0.415	
α-Pinene (API)	1.88·10 ⁵	1.93·10 ⁴	1.93·10 ⁴	1.88·10 ⁵	8987	0
Limonene (LIM)	1.88·10 ⁵	1.93·10 ⁴	1.93·10 ⁴	1.88·10 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] / (10⁵ cm height of layer) = [s⁻¹]

	urban = remote	marine
NO ₂	4·10 ⁻⁶	1·10 ⁻⁶
HNO ₃	2·10 ⁻⁵	5·10 ⁻⁶
N ₂ O ₅	2·10 ⁻⁵	5·10 ⁻⁶
H ₂ O ₂	1·10 ⁻⁵	5·10 ⁻⁶
CO	1·10 ⁻⁶	1·10 ⁻⁶
O ₃	4·10 ⁻⁶	4·10 ⁻⁷
HCl	1·10 ⁻⁵	5·10 ⁻⁶
NH ₃	1·10 ⁻⁵	1·10 ⁻⁵
SO ₂	1·10 ⁻⁵	5·10 ⁻⁶
H ₂ SO ₄	2·10 ⁻⁵	5·10 ⁻⁶
HCHO	1·10 ⁻⁵	5·10 ⁻⁶
CH ₃ OOH	5·10 ⁻⁶	5·10 ⁻⁶
HCOOH	1·10 ⁻⁵	5·10 ⁻⁶
CH ₃ OH	1·10 ⁻⁵	1·10 ⁻⁵
EtOH	5·10 ⁻⁶	5·10 ⁻⁶
HOBr	2·10 ⁻⁶	2·10 ⁻⁶
HOCl	2·10 ⁻⁶	2·10 ⁻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	$\Delta H / R$, 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 <i>et al.</i> , 1985b National Bureau of Standards, 1971	
	7	7	H ₂ O 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 <i>et al.</i> , 1996	
	10	10	N ₂ O ₅	1.4		<i>estimated equal as N₂O₄</i> Schwartz and White, 1983	value for N ₂ O 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 <i>et al.</i> , 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 measurement, not estimate
	16	16	CH ₃ OOH	6 310	-5607	<i>Jacob, 1986</i> Lind and Kok, 1994	
*	17	17	CH ₃ C(O)OOH	669	-5890	Lind and Kok, 1994	
	18	18	CH ₃ OH	220	-5390	Betterton, 1992	
	19	19	C ₂ H ₅ OH	190	-6290	Betterton, 1992	
	20	20	CH ₃ CHO	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 ₃ COOH	5500	-5890	Khan and Brimblecombe, 1992	
	23	23	CH ₃ O ₂	6 310	-5607	<i>Jacob, 1986</i> $K_H(CH_3O_2) = K_H(CH_3OOH)$	

24	24	ETHP	6 340	-87	$K_H(CH_3O_2) = K_H(ETHP)$ estimated equal as CH_3CH_2OOH	better estimate O'Sullivan et al., 1996
25	25	Cl ₂	$9.15 \cdot 10^{-2}$	20.7	Wilhelm <i>et al.</i> , 1977	
26	26	Br ₂	0.758	31.6	Loomis, 1928	better estimate
27	27	H ₂ SO ₄	$2.1 \cdot 10^5$ $8.7 \cdot 10^{11}$		$K_H(H_2SO_4) = K_H^{eff}(MSA)/K_A(MSA)$ Brimblecombe and Clegg, 1988 $K_H(H_2SO_4) = K_H(HNO_3)$ $K_H(ACO_3) = K_H(CH_3C(O)OOH)$	
28	28	ACO ₃	669	1263 -5893		
29		GLY	1.4		Betterton and Hoffmann, 1988a	
30		O ₂	$1.3 \cdot 10^{-3}$	-1700	Loomis, 1928	
31		CINO ₂	0.024		Behnke <i>et al.</i> , 1997	
32		BrNO ₂	0.3		Frenzel <i>et al.</i> , 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 [$10^5 \text{ m}^2 \text{ s}^{-1}$]	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 <i>et al.</i> , 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 ₂ O ₂	0.11	Davidovits <i>et al.</i> , 1995	0.1532	1.46	McElroy, 1997	
	8	8	HNO ₃	0.054	Davidovits <i>et al.</i> , 1995	0.0868	1.32	Kirchner, 1990	
	9	9	NO ₃	$4 \cdot 10^{-3}$	Kirchner, 1990 Rudich, 1996	$4 \cdot 10^{-3}$	1.00	Thomas, 1998	
	10	10	N ₂ O ₅	$3.7 \cdot 10^{-3}$	George <i>et al.</i> , 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 ₂ NO ₂	0.1	Jacob, 1986	0.1	1.30	Schweitzer, 1998	
	14	14	SO ₂	$3.5 \cdot 10^{-2}$	Tang and Lee, 1987 Gardner, 1987	0.11	1.28	McElroy, 1997	
	15	15	HCHO	0.02	estimated	0.02	1.64	Fuller, 1986 ^{a)}	
	16	16	CH ₃ OOH	$3.8 \cdot 10^{-3}$	Davidovits <i>et al.</i> , 1995	$6.758 \cdot 10^{-3}$	1.31	Fuller, 1986 ^{a)}	

*	17	17	CH ₃ C(O)OOH	0.019	$\alpha_{17} = \alpha_{31}$	0.019	1.02	Fuller, 1986 ^{a)}	
	18	18	CH ₃ OH	$1.5 \cdot 10^{-2}$	Davidovits <i>et al.</i> , 1995	0.0271	1.16	Schwartz, 1986	
	19	19	C ₂ H ₅ OH	$8.2 \cdot 10^{-3}$	Davidovits <i>et al.</i> , 1995	0.0176	0.95	Schwartz, 1986	
	20	20	CH ₃ CHO	0.03	estimated	0.03	1.22	Fuller, 1986 ^{a)}	
	21	21	HCOOH	0.012	Davidovits <i>et al.</i> , 1995	0.0229	1.53	Schwartz, 1986	
	22	22	CH ₃ COOH	0.019	Davidovits <i>et al.</i> , 1995	0.0322	1.24	Schwartz, 1986	
	23	23	CH ₃ O ₂	$3.8 \cdot 10^{-3}$	$\alpha = \alpha_{\text{CH}_3\text{OOH}}$	$6.7581 \cdot 10^{-3}$	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 ₂ SO ₄	0.07	Davidovits <i>et al.</i> , 1995	0.12	1.30	Schwartz, 1986	
	28	28	ACO ₃	0.019	$\alpha = \alpha_{\text{CH}_3\text{COOH}}$	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 <i>et al.</i> , ?	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 ₂ H ₆	$1 \cdot 10^{-4}$	estimated		0.95	Fuller, 1986 ^{a)}	"
		31	C ₂ H 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 ₂ O ₂ + Fe ²⁺ → OH + OH ⁻ + Fe ³⁺	76		Walling, 1975	
				50		Barb <i>et al.</i> , 1950	
*	2		Mn(OH) ²⁺ + H ₂ O ₂ → MnO ₂ ⁺ + H ⁺ + H ₂ O	$2.8 \cdot 10^3$		Jacobsen <i>et al.</i> , 1997	several studies confirm this value
*	3		Mn ⁴⁺ + H ₂ O ₂ → Mn ²⁺ + 2 H ⁺ + O ₂	$1 \cdot 10^6$		Jacobsen <i>et al.</i> , 1997	new data available (MnO ₂ ⁺)
	4	2	H ₂ O ₂ + Cu ⁺ → OH + OH ⁻ + Cu ²⁺	$7.0 \cdot 10^3$		Berdnikov, 1973	new data available
*	5	3	H ₂ O ₂ + Mn ³⁺ → HO ₂ + H ⁺ + Mn ²⁺	$7.3 \cdot 10^4$		Davies <i>et al.</i> , 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 <i>et al.</i> , 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 <i>et al.</i> , 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 <i>et al.</i> , 1997	new data available (MnO_2^+)
*	14		$OH + Mn^{2+} \rightarrow OH^- + Mn^{3+}$	$2.6 \cdot 10^7$		Baral <i>et al.</i> , 1986	new data available; consistent to other
				$2 \cdot 10^7$		Jacobsen <i>et al.</i> , 1997	(new) Mn reactions
	15	11	$O_2^- + Cu^+ (+ 2 H^+) \rightarrow H_2O_2 + Cu^{2+}$	$9.4 \cdot 10^9$		von Piechowski <i>et al.</i> , 1993	measurement instead of computer
				$1 \cdot 10^{10}$		Rabani <i>et al.</i> , 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 <i>et al.</i> , 1992	
	18	14	$HO_2 + Cu^{2+} \rightarrow O_2 + Cu^+ + H^+$	$1.2 \cdot 10^9$		Cabelli <i>et al.</i> , 1987	to be consistent to R19 (pH: 3-6.5;
				$1 \cdot 10^8$		Rabani <i>et al.</i> , 1973	former value: pH = 4.5)
	19	15	$O_2^- + Cu^{2+} \rightarrow O_2 + Cu^+$	$1.1 \cdot 10^{10}$		Cabelli <i>et al.</i> , 1987	"
				$8 \cdot 10^9$		Rabani <i>et al.</i> , 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 <i>et al.</i> , 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 <i>et al.</i> , 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 <i>et al.</i> , 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	$O_3 + O_2^- \xrightarrow{H^+} 2 O_2 + OH^- \rightarrow O_3^- + O_2$	$1.5 \cdot 10^9$	2200	Sehested <i>et al.</i> , 1983	split into elementary steps
						Hesper and Herrmann, 2000	
	25		$HO_3 \rightarrow OH + O_2$	330	4500	Bühler <i>et al.</i> , 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 <i>et al.</i> , 1985	
*	27	22	$HO_2 + O_2^- \xrightarrow{H^+} H_2O_2 + O_2$	$9.7 \cdot 10^7$	1060	Bielski <i>et al.</i> , 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 <i>et al.</i> , 1989	
	30	25	$H_2O_2 + OH \rightarrow HO_2 + H_2O$	$3.0 \cdot 10^7$	1680	Christensen <i>et al.</i> , 1982	

*	31	26	$\text{CH}_3\text{OOH} + \text{OH} \rightarrow \text{CH}_3\text{O}_2 + \text{H}_2\text{O}$	$3 \cdot 10^7$ $2.4 \cdot 10^7$	1680	31/32: Sum is equal as before	consideration of another reaction pathway
*	32		$\text{CH}_3\text{OOH} + \text{OH} \rightarrow \text{HO}_2 + \text{HCOOH}$	$6.0 \cdot 10^6$	1680	branching ratio 0.8 : 0.2 (correlation for H abstractions)	
	33	27	$\text{HSO}_3^- + \text{OH} \rightarrow \text{H}_2\text{O} + \text{SO}_3^-$	$2.7 \cdot 10^9$		Buxton <i>et al.</i> , 1996a	
*	34	28	$\text{SO}_3^{2-} + \text{OH} \rightarrow \text{OH}^- + \text{SO}_3^-$	$4.6 \cdot 10^9$		Buxton <i>et al.</i> , 1996a	
*	35		$\text{MnO}_2^+ + \text{MnO}_2^+ \rightarrow 2 \text{Mn}^{2+} + \text{H}_2\text{O}_2$	$6 \cdot 10^6$		Jacobsen <i>et al.</i> , 1997	new data available (MnO_2^+)
	36		$\text{Cu}^+ + \text{O}_2 \rightarrow \text{Cu}^{2+} + \text{O}_2^-$	$4.6 \cdot 10^5$		Bjergbakke <i>et al.</i> , 1976	
	37		$\text{Fe}^{2+} + \text{O}_3 \rightarrow \text{FeO}^{2+} + \text{O}_2$	$8.2 \cdot 10^5$		Logager <i>et al.</i> , 1992	new data available (FeO^{2+})
*	38		$\text{FeO}^{2+} + \text{H}_2\text{O}_2 \rightarrow \text{Fe}^{3+} + \text{HO}_2 + \text{OH}^-$	$9.5 \cdot 10^3$	2766	Jacobsen <i>et al.</i> , 1998a)	"
*	39		$\text{FeO}^{2+} + \text{H}_2\text{O} \rightarrow \text{Fe}^{3+} + \text{OH} + \text{OH}^-$	$2.34 \cdot 10^4$	4089	Jacobsen <i>et al.</i> , 1998a)	"
*	40		$\text{FeO}^{2+} + \text{HO}_2 \rightarrow \text{Fe}^{3+} + \text{O}_2 + \text{OH}^-$	$2.0 \cdot 10^6$		Jacobsen <i>et al.</i> , 1997a	"
*	41		$\text{FeO}^{2+} + \text{OH} \rightarrow \text{Fe}^{3+} + \text{H}_2\text{O}_2$	$1.0 \cdot 10^7$		Logager <i>et al.</i> , 1992	"
*	42		$\text{FeO}^{2+} + \text{HONO} \rightarrow \text{Fe}^{3+} + \text{NO}_2 + \text{OH}^-$	$1.1 \cdot 10^4$	4150	Jacobsen <i>et al.</i> , 1998b)	"
*	43		$\text{FeO}^{2+} + \text{HSO}_3^- \rightarrow \text{Fe}^{3+} + \text{SO}_3^- + \text{OH}^-$	$2.5 \cdot 10^5$		Jacobsen <i>et al.</i> , 1998b)	"
	44		$\text{FeO}^{2+} + \text{Cl}^- \xrightarrow{\text{H}^+} \text{Fe}^{3+} + \text{ClOH}^-$	100		Jacobsen <i>et al.</i> , 1998b)	"
*	45		$\text{FeO}^{2+} + \text{Mn}^{2+} \xrightarrow{2\text{H}^+} \text{Mn}^{3+} + \text{Fe}^{3+} + \text{H}_2\text{O}$	$1.0 \cdot 10^4$	2562	Jacobsen <i>et al.</i> , 1998b)	"
*	46		$\text{FeO}^{2+} + \text{HCOOH} \xrightarrow{\text{H}^+} \text{Fe}^{3+} + \text{COOH} + \text{H}_2\text{O}$	160	2680	Jacobsen <i>et al.</i> , 1998b)	"
*	47		$\text{FeO}^{2+} + \text{HCOO}^- \rightarrow \text{Fe}^{3+} + \text{COOH} + \text{OH}^-$	$3 \cdot 10^5$		Jacobsen <i>et al.</i> , 1998b)	"
*	48		$\text{FeO}^{2+} + \text{C}_2\text{H}_5\text{OH} \rightarrow \text{Fe}^{3+} + \text{CH}_3\text{CHOH} + \text{OH}^-$	$2.5 \cdot 10^3$		Jacobsen <i>et al.</i> , 1998b)	"
*	49		$\text{FeO}^{2+} + \text{CH}_2(\text{OH})_2 \rightarrow \text{Fe}^{3+} + \text{OH}^- + \text{CH}(\text{OH})_2$	400	5352	Jacobsen <i>et al.</i> , 1998b)	"
*	50		$\text{FeO}^{2+} + \text{NO}_2^- \xrightarrow{\text{H}^+} \text{Fe}^{3+} + \text{NO}_2 + \text{OH}^-$	$1 \cdot 10^5$		Jacobsen <i>et al.</i> , 1998b)	"
	51		$\text{FeO}^{2+} + \text{Fe}^{2+} \rightarrow 2 \text{Fe}^{3+} + 2 \text{OH}^-$	$7.2 \cdot 10^4$	842	Jacobsen <i>et al.</i> , 1997a)	"
*	52		$\text{FeO}^{2+} + \text{Fe}^{2+} \xrightarrow{2\text{H}_2\text{O}^+} \text{FeOH}_2\text{Fe}^{4+} + 2 \text{OH}^-$	$1.8 \cdot 10^4$	5052	Jacobsen <i>et al.</i> , 1997a)	"
*	53		$\text{FeOH}_2\text{Fe}^{4+} + \text{H}^+ \xrightarrow{\text{H}^+} 2 \text{Fe}^{3+} + \text{H}_2\text{O}$	1.95	5653	Jacobsen <i>et al.</i> , 1997a)	"
*	54		$\text{FeOH}_2\text{Fe}^{4+} \rightarrow 2 \text{Fe}^{3+} + 2 \text{OH}^-$	0.49	8780	Jacobsen <i>et al.</i> , 1997a)	"
*	55		$\text{MnO}^{2+} + \text{Mn}^{2+} \xrightarrow{2\text{H}^+} 2 \text{Mn}^{3+} + \text{H}_2\text{O}$	$1 \cdot 10^5$		Jacobsen <i>et al.</i> , 1998a)	new data available
*	56		$\text{Mn}^{2+} + \text{O}_3 \rightarrow \text{MnO}^{2+} + \text{O}_2$	$1.65 \cdot 10^3$		Jacobsen <i>et al.</i> , 1998a)	new data available
*	57		$\text{Cu}^+ + \text{O}_3 \xrightarrow{\text{H}^+} \text{Cu}^{2+} + \text{OH} + \text{O}_2$	$3 \cdot 10^7$		Hoigné and Bühler, 1996	new data available
*	58		$\text{OH} + \text{O}_3 \rightarrow \text{O}_2 + \text{HO}_2$	$1 \cdot 10^8$		Sehested <i>et al.</i> , 1984	additional sink for OH/O ₃
*	59		$\text{O}^3\text{P} + \text{O}_2 \rightarrow \text{O}_3$	$4 \cdot 10^9$		Kläning <i>et al.</i> , 1984	sink for O ³ P (NO ₃ photolysis)

Table 5: 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 <i>et al.</i> , 1997	correct formulation
		29	$N_2O_5 + H_2O \rightarrow 2H^+ + 2NO_3^-$	$5 \cdot 10^9$		estimated	wrong formulation
*	62	30	$NO_3 + OH^- \rightarrow NO_3^- + OH$	$9.4 \cdot 10^7$	2700	Exner <i>et al.</i> , 1992	
*	63	31	$NO_3 + Fe^{2+} \rightarrow NO_3^- + Fe^{3+}$	$8 \cdot 10^6$		Pikaev <i>et al.</i> , 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 <i>et al.</i> , 1994	
*	66	34	$NO_3 + CH_3OOH \rightarrow NO_3^- + H^+ + CH_3O_2$	$4.9 \cdot 10^6$	2000	$k = k_{H_2O_2}$	
	67	35	$NO_3 + HO_2 \rightarrow NO_3^- + H^+ + O_2$	$3.0 \cdot 10^9$		Sehested <i>et al.</i> , 1994	
*	68	36	$NO_3 + O_2^- \rightarrow NO_3^- + O_2$	$3.0 \cdot 10^9$		$k = k_{HO_2}$	
	69	37	$NO_3 + HSO_3^- \rightarrow NO_3^- + H^+ + SO_3^-$	$1.3 \cdot 10^9$	2000	Exner <i>et al.</i> , 1992	
*	70	38	$NO_3 + SO_3^{2-} \rightarrow NO_3^- + SO_3^-$	$3.0 \cdot 10^8$		Exner <i>et al.</i> , 1992	
*	71	39	$NO_3 + HSO_4^- \rightarrow NO_3^- + H^+ + SO_4^-$	$2.6 \cdot 10^5$		Raabe, 1996	
	72	40	$NO_3 + SO_4^{2-} \rightarrow NO_3^- + SO_4^-$	$5.6 \cdot 10^3$		Logager <i>et al.</i> , 1993	corrected value
				$1 \cdot 10^5$			
*	73	41	$NO_2 + OH \rightarrow NO_3^- + H^+$	$1.2 \cdot 10^{10}$		Wagner <i>et al.</i> , 1980	correct product; in 2.3 for simplification lumped to HNO ₃
			NO₂ + OH → HOONO				
*	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	$NO_2^- + OH \rightarrow NO_2 + OH^-$	$1.1 \cdot 10^{10}$		Barker <i>et al.</i> , 1970	measurement in more alkaline solution
				$9.1 \cdot 10^9$			
*	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	$NO_2^- + Cl_2^- \rightarrow 2Cl^- + NO_2$	$6 \cdot 10^7$		Jacobi, 1996	
*	81	49	$NO_2^- + Br_2^- \rightarrow 2Br^- + NO_2$	$1.2 \cdot 10^7$	1720	Shoute <i>et al.</i> , 1991	
						Jacobi, 1996	
*	82	50	$NO_2^- + CO_3^- \rightarrow CO_3^{2-} + NO_2$	$6.6 \cdot 10^5$	850	Huie <i>et al.</i> , 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	$\text{HNO}_2 + \text{OH} \rightarrow \text{NO}_2 + \text{H}_2\text{O}$	$1 \cdot 10^9$ $1.1 \cdot 10^{10}$	<i>Rettich, 1978</i> <i>Barker et al., 1970</i>	measurement in more alkaline solution
85		$\text{NO}_2^+ + \text{Cl}^- \rightarrow \text{ClNO}_2$	$1 \cdot 10^{10}$	Chr. George, pers. comm., 1999	considering of XNO ₂ chemistry
86		$\text{NO}_2^+ + \text{Br}^- \rightarrow \text{BrNO}_2$	$1 \cdot 10^{10}$	Chr. George, pers. comm., 1999	"
87		$\text{ClNO}_2 + \text{Br}^- \rightarrow \text{NO}_2^- + \text{BrCl}$	$5 \cdot 10^6$	Chr. George, pers. comm., 1999	"
88		$\text{BrNO}_2 + \text{Br}^- \rightarrow \text{NO}_2^- + \text{Br}_2$	$2.55 \cdot 10^4$	Chr. George, pers. comm., 1999	"
89		$\text{BrNO}_2 + \text{Cl}^- \rightarrow \text{NO}_2^- + \text{BrCl}$	10	Chr. George, pers. comm., 1999	"

Table 6: Sulfur-Chemistry

red.	No. 2.4	No. 2.3	Reaction	k_{298} , $\text{M}^{-n} \text{s}^{-1}$	E_a / R , K	Reference	comment
	90	53	$\text{HMS}^- + \text{OH} \rightarrow \text{H}_2\text{O} + \text{HO}_2 + \text{HCOOH} + \text{HSO}_3^-$ $\text{H}_2\text{O} + \text{CHOHSO}_3^-$	$3 \cdot 10^8$		Barlow et al., 1997b)	correct products; split into elementary steps
*	91	54	$\text{HMS}^- + \text{SO}_4^{2-} \rightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{HCHO} + \text{SO}_3^-$ $\text{SO}_4^{2-} + \text{OHCH}_2\text{SO}_3$	$2.8 \cdot 10^6$ $1.3 \cdot 10^6$		Barlow et al., 1997b)	"
*	92	55	$\text{HMS}^- + \text{NO}_3^- \rightarrow \text{NO}_3^- + \text{H}^+ + \text{HCHO} + \text{SO}_3^-$ $\text{NO}_3^- + \text{OHCH}_2\text{SO}_3$	$4.2 \cdot 10^6$		Herrmann et al., 1996a) Barlow et al., 1997b)	"
*	93	56	$\text{HMS}^- + \text{Cl}_2^- \rightarrow 2 \text{Cl}^- + \text{H}^+ + \text{HCHO} + \text{SO}_3^-$ $2 \text{Cl}^- + \text{OHCH}_2\text{SO}_3$	$5.0 \cdot 10^5$		Jacobi, 1996 Barlow et al., 1997b)	"
*	94	57	$\text{HMS}^- + \text{Br}_2^- \rightarrow 2 \text{Br}^- + \text{H}^+ + \text{HCHO} + \text{SO}_3^-$ $2 \text{Br}^- + \text{OHCH}_2\text{SO}_3$	$5.0 \cdot 10^4$		estimated as $k = 0.1k(\text{Cl}_2^-)$	"
*	95		$\text{OHCH}_2\text{SO}_3 \rightarrow \text{SO}_3 + \text{CH}_2\text{OH}$	$1 \cdot 10^5$		estimated	sink for OHCH ₂ SO ₃
*	96		$\text{SO}_3 + \text{H}_2\text{O} \rightarrow \text{SO}_4^{2-} + 2 \text{H}^+$	$1 \cdot 10^{10}$		estimated as diffusion controlled	sink for SO ₃
	97		$\text{CHOSO}_3^- + \text{O}_2 \rightarrow \text{O}_2\text{CHOHSO}_3^-$	$2.6 \cdot 10^9$		Barlow et al., 1997b	split into elementary steps; consideration of side reactions
	98		$\text{O}_2\text{CHOHSO}_3^- \rightarrow \text{HO}_2 + \text{CHOSO}_3^-$	$1.7 \cdot 10^4$		Barlow et al., 1997b	"
	99		$\text{O}_2\text{CHOHSO}_3^- \rightarrow \text{O}_2\text{CHO} + \text{HSO}_3^-$	$7.0 \cdot 10^3$		Barlow et al., 1997b	"
	100		$\text{CHOSO}_3^- + \text{H}_2\text{O} \rightarrow \text{HSO}_3^- + \text{HCOOH}$	$1.26 \cdot 10^{-2}$		Buxton et al., 1997	"
	101		$\text{O}_2\text{CHO} + \text{H}_2\text{O} \rightarrow \text{HCOOH} + \text{HO}_2$	44.32		Barlow et al., 1997b	"
*	102		$\text{CHOHSO}_3^{2-} + \text{O}_2 \rightarrow \text{CHOHSO}_3^- + \text{O}_2^-$	$1.6 \cdot 10^9$		Barlow et al., 1997b	"
	103	58	$\text{HSO}_3^- + \text{H}_2\text{O}_2 + \text{H}^+ \rightarrow \text{SO}_4^{2-} + \text{H}_2\text{O} + 2 \text{H}^+$	$6.9 \cdot 10^7$ $7.2 \cdot 10^7$	4000	Zellner et al., 1994 Lind et al., 1987	to be consistent to 104/105
*	104	59	$\text{HSO}_3^- + \text{CH}_3\text{OOH} + \text{H}^+ \rightarrow \text{SO}_4^{2-} + 2 \text{H}^+ + \text{CH}_3\text{OH}$	$1.8 \cdot 10^7$ $1.7 \cdot 10^7$	3800	Lind et al., 1987	corrected value
*	105	60	$\text{HSO}_3^- + \text{CH}_3\text{C}(\text{O})\text{OOH} + \text{H}^+ \rightarrow \text{SO}_4^{2-} + 2 \text{H}^+ + \text{prod.} -$ 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	$\text{SO}_2 + \text{O}_3 (+ \text{H}_2\text{O}) \rightarrow \text{HSO}_4^- + \text{O}_2 + \text{H}^+$	$2.4 \cdot 10^4$		Hoffmann, 1986	

	107	62	$\text{HSO}_3^- + \text{O}_3 \rightarrow \text{HSO}_4^- + \text{O}_2$	$3.7 \cdot 10^5$	5530	Hoffmann, 1986	
	108	63	$\text{SO}_3^{2-} + \text{O}_3 \rightarrow \text{SO}_4^{2-} + \text{O}_2$	$1.5 \cdot 10^9$	5280	Hoffmann, 1986	
*	109	64	$[\text{Fe}(\text{OH})]^{2+} + \text{HSO}_3^- \rightarrow \text{Fe}^{2+} + \text{SO}_3^- + \text{H}_2\text{O}$	39		Ziajka <i>et al.</i> , 1994	
			30				
	110	65	$\text{Fe}^{2+} + \text{SO}_5^- (+ \text{H}_2\text{O}) \rightarrow [\text{Fe}(\text{OH})]^{2+} + \text{HSO}_5^-$	$4.3 \cdot 10^7$ $2.65 \cdot 10^7$	5809	Herrmann <i>et al.</i> , 1996a Williams, 1996	T dependent value
	111	66	$\text{Fe}^{2+} + \text{HSO}_5^- \rightarrow [\text{Fe}(\text{OH})]^{2+} + \text{SO}_4^-$	$3 \cdot 10^4$		Ziajka <i>et al.</i> , 1994	
*	112		$\text{Mn}^{2+} + \text{HSO}_5^- \rightarrow \text{SO}_4^- + \text{Mn}^{3+} + \text{OH}^-$	$3 \cdot 10^4$		estimated equal as $k_{(\text{Fe}^{2+} + \text{HSO}_5^-)}$	completion of Mn chemistry
*	113	67	$\text{Mn}^{2+} + \text{SO}_5^- (+ \text{H}_2\text{O}) \rightarrow \text{Mn}^{3+} + \text{HSO}_5^- + \text{OH}^-$	$4.6 \cdot 10^6$ $1 \cdot 10^{10}$		Herrmann <i>et al.</i> , 1996a Berglund <i>et al.</i>, 1994	to be consistent to R146
	114		$\text{Fe}^{2+} + \text{SO}_4^- (+ \text{H}_2\text{O}) \rightarrow [\text{Fe}(\text{OH})]^{2+} + \text{SO}_4^{2-} + \text{H}^+$	$3.5 \cdot 10^7$ $4.6 \cdot 10^9$	-2165	Ziajka <i>et al.</i> , 1994 Buxton <i>et al.</i> , 1997	T dependent value
*	115		$\text{Fe}^{2+} + \text{S}_2\text{O}_8^{2-} (+ \text{H}_2\text{O}) \rightarrow [\text{Fe}(\text{OH})]^{2+} + \text{SO}_4^{2-} + \text{SO}_4^{2-} + \text{H}^+$	17		Ziajka <i>et al.</i> , 1994 Buxton <i>et al.</i> , 1997	measurement instead of estimate
*	116	68	$\text{SO}_5^- + \text{SO}_5^- \rightarrow \text{S}_2\text{O}_8^{2-} + \text{O}_2$	$1.8 \cdot 10^8$ $4.8 \cdot 10^7$	2600	Herrmann <i>et al.</i> , 1995 Buxton <i>et al.</i> , 1997	new evidences about product ratio
	117	69	$\text{SO}_5^- + \text{SO}_5^- \rightarrow 2 \text{SO}_4^- + \text{O}_2$	$7.2 \cdot 10^6$ $2.2 \cdot 10^8$	2600	Herrmann <i>et al.</i> , 1995 Buxton <i>et al.</i> , 1997	"
	118	70	$\text{SO}_5^- + \text{HO}_2 \rightarrow \text{HSO}_5^- + \text{O}_2$ $\rightarrow \text{SO}_5\text{O}_2\text{H}^-$	$1.7 \cdot 10^9$		Buxton <i>et al.</i> , 1996b	correct product; split into elementary steps
*	119		$\text{SO}_5^- + \text{O}_2^- (+ \text{H}^+) \rightarrow \text{HSO}_5^- + \text{OH}^- + \text{O}_2$	$1.7 \cdot 10^9$ $2.34 \cdot 10^8$		Buxton <i>et al.</i> , 1996a Buxton <i>et al.</i> , 1997	split into elementary steps; sink reaction
*	120		$\text{SO}_5\text{O}_2\text{H}^- + \text{HSO}_3^- \rightarrow 2 \text{SO}_4^{2-} + 2 \text{H}^+$	$3.0 \cdot 10^5$		Buxton <i>et al.</i> , 1997	"
*	121		$\text{SO}_5\text{O}_2^{2-} + \text{HSO}_3^- \rightarrow 2 \text{SO}_4^{2-} + \text{H}^+$	$5.2 \cdot 10^6$		Buxton <i>et al.</i> , 1997	"
	122		$\text{SO}_5\text{O}_2^{2-} (+ \text{H}^+) \rightarrow \text{HSO}_5^- + \text{O}_2$	1200		Buxton <i>et al.</i> , 1997	"
	123	71	$\text{SO}_3^- + \text{O}_2 \rightarrow \text{SO}_5^-$	$2.5 \cdot 10^9$		Buxton <i>et al.</i> , 1996a	
*	124	72	$\text{SO}_5^- + \text{HSO}_3^- \rightarrow \text{HSO}_5^- + \text{SO}_3^-$	$8.6 \cdot 10^3$		Buxton <i>et al.</i> , 1996a	
*	125	73	$\text{SO}_5^- + \text{HSO}_3^- \rightarrow \text{SO}_4^{2-} + \text{SO}_4^- + \text{H}^+$	$3.6 \cdot 10^2$		Buxton <i>et al.</i> , 1996a	
*	126	74	$\text{SO}_5^- + \text{SO}_3^{2-} (+ \text{H}^+) \rightarrow \text{HSO}_5^- + \text{SO}_3^-$	$2.13 \cdot 10^5$		Buxton <i>et al.</i> , 1996a	
*	127	75	$\text{SO}_5^- + \text{SO}_3^{2-} \rightarrow \text{SO}_4^- + \text{SO}_4^{2-}$	$5.5 \cdot 10^5$		Buxton <i>et al.</i> , 1996a	
*	128	76	$\text{OH} + \text{HSO}_4^- \rightarrow \text{H}_2\text{O} + \text{SO}_4^-$	$3.5 \cdot 10^5$		Tang <i>et al.</i> , 1988	
*	129		$\text{SO}_4^- + \text{SO}_4^- \rightarrow \text{S}_2\text{O}_8^{2-}$	$1.6 \cdot 10^8$ $6.1 \cdot 10^8$	840	Herrmann <i>et al.</i> , 1995a) Ervens, 1997	T dependent value
*	130		$\text{SO}_4^- + \text{HSO}_3^- \rightarrow \text{SO}_4^{2-} + \text{SO}_3^- + \text{H}^+$	$3.2 \cdot 10^8$ $5.8 \cdot 10^8$		Reese, 1997 mean value of Reese, 1997; Wine <i>et al.</i> , 1989; Buxton <i>et al.</i> , 1996a	mean value of all available data
*	131		$\text{SO}_4^- + \text{SO}_3^{2-} \rightarrow \text{SO}_4^{2-} + \text{SO}_3^-$	$3.2 \cdot 10^8$	1200	Reese, 1997	

*									
*	132	77	$SO_4^- + Fe^{2+} \rightarrow [Fe(SO_4)]^+$ $SO_4^- + Mn^{2+} \rightarrow SO_4^{2-} + Mn^{3+}$	$3.4 \cdot 10^8$ $3 \cdot 10^8$ $2 \cdot 10^7$ $1.4 \cdot 10^7$	4089	mean value of Reese, 1997; Wine <i>et al.</i> , 1989., Buxton <i>et al.</i> , 1996a McElroy and Waygood, 1990 Neta and Huie, 1987 Buxton <i>et al.</i> , 1996b	mean value of all available data no evidence that rxn. takes place T dependent value		
*	133		$SO_4^- + Cu^+ \rightarrow SO_4^{2-} + Cu^{2+}$	$3 \cdot 10^8$		estimated equal as $k_{(Fe^{2+} + SO_4^- \rightarrow FeSO_4^+)}$; McElroy and Waygood, 1990)	formulated analagous to Fe/ Mn chemistry		
*	134	78	$SO_4^- + H_2O_2 \rightarrow SO_4^{2-} + H^+ + HO_2$	$2.8 \cdot 10^7$ $1.7 \cdot 10^7$		Reese, 1997 mean value of Reese, 1997; Wine <i>et al.</i> , 1989; Maruthamutu and Neta, 1978	mean value of all available data		
*	135	79	$SO_4^- + CH_3OOH \rightarrow SO_4^{2-} + H^+ + CH_3O_2$	$2.8 \cdot 10^7$ $1.7 \cdot 10^7$		$k = k_{H_2O_2}$	equal as $k_{H_2O_2}$		
*	136	80	$SO_4^- + HO_2 \rightarrow SO_4^{2-} + H^+ + O_2$	$3.5 \cdot 10^9$		Jiang <i>et al.</i> , 1992			
*	137	81	$SO_4^- + O_2^- \rightarrow SO_4^{2-} + O_2$	$3.5 \cdot 10^9$		$k_{HO_2} = k_{O_2^-}$.			
*	138	82	$SO_4^- + NO_3^- \rightarrow SO_4^{2-} + NO_3$	$5.0 \cdot 10^4$		Exner <i>et al.</i> , 1992			
*	139	83	$SO_4^- + OH^- \rightarrow SO_4^{2-} + OH$	$1.4 \cdot 10^7$		Herrmann <i>et al.</i> , 1995b			
	140	84	$SO_4^- + H_2O \rightarrow SO_4^{2-} + H^+ + OH$	11	1110	Herrmann <i>et al.</i> , 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 <i>et al.</i> , 1996			
*	145		$OH + SO_4^- \rightarrow HSO_5^-$	$1.0 \cdot 10^{10}$		Wilhelm <i>et al.</i> , 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 <i>et al.</i> , 1994			
*	147		$SO_5^- + HC_2O_4^- \rightarrow HSO_5^- + C_2O_4^-$	$5 \cdot 10^3$		Herrmann <i>et al.</i> , 2000			
*	148		$SO_5^- + C_2O_4^{2-} \rightarrow HSO_5^- + C_2O_4^-$	$1 \cdot 10^4$		Herrmann <i>et al.</i> , 2000	consideration of C_2 -difunctional compounds		
*	149		$SO_5^- + CH(OH)_2CH(OH)_2 \rightarrow HSO_5^- +$ $C(OH)_2CH(OH)_2$	$5 \cdot 10^5$		Herrmann <i>et al.</i> , 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 <i>Exner et al., 1993</i>	"
*	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 <i>et al.</i> , 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 <i>et al.</i> , 1996	"
	156		$CH_2OH + O_2 \rightarrow O_2CH_2OH$	$2 \cdot 10^9$		von Sonntag, 1987	explicit 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 <i>et al.</i> , 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 <i>et al.</i> , 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 <i>et al.</i> , 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	explicit 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	$\text{CH}_2(\text{OH})_2 + \text{OH} (+\text{O}_2) \rightarrow \text{H}_2\text{O} + \text{HO}_2 + \text{HCOOH}$ $\rightarrow \text{H}_2\text{O} + \text{CH}(\text{OH})_2$	$1.0 \cdot 10^9$	1020	Hart <i>et al.</i> , 1964; Chin and Wine, 1994	split into elementary steps
*	169	102	$\text{CH}_2(\text{OH})_2 + \text{SO}_4^- (+\text{O}_2) \rightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{HO}_2 +$ HCOOH $\rightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{CH}(\text{OH})_2$	$1.4 \cdot 10^7$	1300	Buxton <i>et al.</i> , 1990	"
*	170	103	$\text{CH}_2(\text{OH})_2 + \text{NO}_3 (+\text{O}_2) \rightarrow \text{NO}_3^- + \text{HO}_2 + \text{HCOOH}$ $\rightarrow \text{NO}_3^- + \text{H}^+ + \text{CH}(\text{OH})_2$	$1.0 \cdot 10^6$	4500	Exner <i>et al.</i> , 1993	"
*	171	104	$\text{CH}_2(\text{OH})_2 + \text{Cl}_2^- (+\text{O}_2) \rightarrow 2 \text{Cl}^- + \text{HO}_2 + \text{HCOOH}$ $\rightarrow 2 \text{Cl}^- + \text{H}^+ + \text{CH}(\text{OH})_2$	$3.1 \cdot 10^4$ $3.6 \cdot 10^4$	4400 4330	Zellner <i>et al.</i> , 1996 Jacobi <i>et al.</i> , 1999	" more actual data
*	172	105	$\text{CH}_2(\text{OH})_2 + \text{Br}_2^- (+\text{O}_2) \rightarrow 2 \text{Br}^- + \text{HO}_2 + \text{HCOOH}$ $\rightarrow 2 \text{Br}^- + \text{H}^+ + \text{CH}(\text{OH})_2$	$3 \cdot 10^3$		estimated	split into elementary steps
*	173	106	$\text{CH}_2(\text{OH})_2 + \text{CO}_3^- (+\text{O}_2) \rightarrow \text{CO}_3^{2-} + \text{HO}_2 + \text{HCOOH}$ $\rightarrow \text{CO}_3^{2-} + \text{H}^+ + \text{CH}(\text{OH})_2$	$1.3 \cdot 10^4$		Zellner <i>et al.</i> , 1996	"
	174		$\text{CH}(\text{OH})_2 + \text{O}_2 \rightarrow \text{HO}_2 + \text{HCOOH}$	$2 \cdot 10^9$		estimated	explicit consideration of alkyl /peroxyl radicals
	175	107	$\text{CH}_3\text{CH}(\text{OH})_2 + \text{OH} (+\text{O}_2) \rightarrow \text{H}_2\text{O} + \text{HO}_2 + \text{HAc}$ $\rightarrow \text{H}_2\text{O} + \text{CH}_3\text{C}(\text{OH})_2$	$1.2 \cdot 10^9$		Schuchmann and von Sonntag, 1988	split into elementary steps
	176	108	$\text{CH}_3\text{CHO} + \text{OH} (+\text{H}_2\text{O} + \text{O}_2) \rightarrow \text{H}_2\text{O} + \text{HO}_2 + \text{HAc}$ $\rightarrow \text{H}_2\text{O} + \text{CH}_3\text{C}(\text{OH})_2$	$3.6 \cdot 10^9$		Schuchmann and von Sonntag, 1988	"
*	177	109	$\text{CH}_3\text{CHO} + \text{SO}_4^- (+\text{H}_2\text{O} + \text{O}_2) \rightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{HO}_2 +$ HAc $\rightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{CH}_3\text{CO}$	$2 \cdot 10^7$		estimated	"
*	178	110	$\text{CH}_3\text{CH}(\text{OH})_2 + \text{SO}_4^- (+\text{O}_2) \rightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{HO}_2 +$ HAc $\rightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{CH}_3\text{C}(\text{OH})_2$	$2 \cdot 10^7$		estimated	"
*	179	111	$\text{CH}_3\text{CH}(\text{OH})_2 + \text{NO}_3 (+\text{O}_2) \rightarrow \text{NO}_3^- + \text{H}^+ + \text{HO}_2 + \text{HAc}$ $\rightarrow \text{NO}_3^- + \text{H}^+ + \text{CH}_3\text{C}(\text{OH})_2$	$1.9 \cdot 10^6$		Zellner <i>et al.</i> , 1996	"
*	180	112	$\text{CH}_3\text{CHO} + \text{Cl}_2^- (+\text{O}_2) \rightarrow 2 \text{Cl}^- + \text{H}^+ + \text{HO}_2 + \text{HAc}$ $\rightarrow 2 \text{Cl}^- + \text{H}^+ + \text{CH}_3\text{CO}$	$4 \cdot 10^4$		Jacobi, 1996	"
*	181	113	$\text{CH}_3\text{CHO} + \text{Br}_2^- (+\text{O}_2) \rightarrow 2 \text{Br}^- + \text{H}^+ + \text{HO}_2 + \text{HAc}$ $\rightarrow 2 \text{Br}^- + \text{H}^+ + \text{CH}_3\text{CO}$	$4 \cdot 10^4$ $4 \cdot 10^3$		estimated estimated: $k_{\text{Br}_2^-} = 0.1 \cdot k_{\text{Cl}_2^-}$	" better estimate
*	182	114	$\text{CH}_3\text{CHO} + \text{CO}_3^- (+\text{O}_2) \rightarrow \text{CO}_3^{2-} + \text{H}^+ + \text{HO}_2 + \text{HAc}$ $\rightarrow \text{CO}_3^{2-} + \text{H}^+ + \text{CH}_3\text{CO}$	$1 \cdot 10^4$		estimated	split into elementary steps
	183	115	$\text{HCOOH} + \text{OH} (+\text{O}_2) \rightarrow \text{H}_2\text{O} + \text{HO}_2 + \text{CO}_2$ $\rightarrow \text{H}_2\text{O} + \text{CO}_2\text{H}$	$1.3 \cdot 10^8$	1000	Buxton <i>et al.</i> , 1988a; Chin and Wine, 1994	"
	184	116	$\text{HCOO}^- + \text{OH} (+\text{O}_2) \rightarrow \text{OH}^- + \text{HO}_2 + \text{CO}_2$ $\rightarrow \text{OH}^- + \text{CO}_2\text{H}$	10^9 $3.2 \cdot 10^9$	1000	Buxton <i>et al.</i> , 1988a; Elliot and Simsons, 1984	"

*	185	117	$\text{HCOOH} + \text{SO}_4^- (+ \text{O}_2) \rightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{HO}_2 + \text{CO}_2$ $\rightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{CO}_2\text{H}$	$2.5 \cdot 10^6$		Reese, 1997	"
*	186	118	$\text{HCOO}^- + \text{SO}_4^- (+ \text{O}_2) \rightarrow \text{SO}_4^{2-} + \text{HO}_2 + \text{CO}_2$ $\rightarrow \text{SO}_4^{2-} + \text{CO}_2\text{H}$	$2.1 \cdot 10^7$		Reese, 1997	"
*	187	119	$\text{HCOOH} + \text{NO}_3 (+ \text{O}_2) \rightarrow \text{NO}_3^- + \text{H}^+ + \text{HO}_2 + \text{CO}_2$ $\rightarrow \text{NO}_3^- + \text{H}^+ + \text{CO}_2\text{H}$	$3.8 \cdot 10^5$	3400	Exner <i>et al.</i> , 1994	"
*	188	120	$\text{HCOO}^- + \text{NO}_3 (+ \text{O}_2) \rightarrow \text{NO}_3^- + \text{HO}_2 + \text{CO}_2$ $\rightarrow \text{NO}_3^- + \text{CO}_2\text{H}$	$5.1 \cdot 10^7$	2200	Exner <i>et al.</i> , 1994	"
*	189	121	$\text{HCOOH} + \text{Cl}_2^- (+ \text{O}_2) \rightarrow 2 \text{Cl}^- + \text{H}^+ + \text{HO}_2 + \text{CO}_2$ $\rightarrow 2 \text{Cl}^- + \text{H}^+ + \text{CO}_2\text{H}$	5500 $8 \cdot 10^4$	4500 4450	Jacobi <i>et al.</i> , 1999 Jacobi <i>et al.</i> , 1999	" more actual value
*	190	122	$\text{HCOO}^- + \text{Cl}_2^- (+ \text{O}_2) \rightarrow 2 \text{Cl}^- + \text{HO}_2 + \text{CO}_2$ $\rightarrow 2 \text{Cl}^- + \text{CO}_2\text{H}$	$1.3 \cdot 10^6$		Jacobi <i>et al.</i> , 1996 Jacobi <i>et al.</i> , 1999	split into elementary steps
*	191	123	$\text{HCOOH} + \text{Br}_2^- (+ \text{O}_2) \rightarrow 2 \text{Br}^- + \text{H}^+ + \text{HO}_2 + \text{CO}_2$ $\rightarrow 2 \text{Br}^- + \text{H}^+ + \text{CO}_2\text{H}$	$4 \cdot 10^3$		Reese <i>et al.</i> , 1999	"
*	192	124	$\text{HCOO}^- + \text{Br}_2^- (+ \text{O}_2) \rightarrow 2 \text{Br}^- + \text{HO}_2 + \text{CO}_2$ $\rightarrow 2 \text{Br}^- + \text{CO}_2\text{H}$	$4.9 \cdot 10^3$		Jacobi, 1996	"
*	193	125	$\text{HCOO}^- + \text{CO}_3^- (+ \text{O}_2) \rightarrow \text{CO}_3^{2-} + \text{H}^+ + \text{HO}_2 + \text{CO}_2$ $\rightarrow \text{CO}_3^{2-} + \text{H}^+ + \text{CO}_2\text{H}$	$1.4 \cdot 10^5$	3300	Zellner <i>et al.</i> , 1996	"
	194	126	$\text{CO}_2\text{H} + \text{O}_2 \rightarrow \text{CO}_2 + \text{HO}_2$	$2 \cdot 10^9$		estimated	explicite consideration of alkyl /peroxy radicals
	195	127	$\text{HAc} + \text{OH} (+ \text{O}_2) \rightarrow \text{H}_2\text{O} + \text{HO}_2 + \text{ACO}_3$ $\rightarrow \text{H}_2\text{O} + \text{CH}_2\text{COOH}$	$1.5 \cdot 10^7$	1330	Thomas, 1965; Chin and Wine, 1994	split into elementary steps
	196	128	$\text{Ac}^- + \text{OH} (+ \text{O}_2) \rightarrow \text{OH}^- + \text{HO}_2 + \text{ACO}_3$ $\rightarrow \text{H}_2\text{O} + \text{CH}_2\text{COO}^-$	$1 \cdot 10^8$	1800	Fisher and Hamill, 1973; Chin and Wine, 1994	"
*	197	129	$\text{HAc} + \text{SO}_4^- (+ \text{O}_2) \rightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{HO}_2 + \text{ACO}_3$ $\rightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{CH}_2\text{COOH}$	$2.0 \cdot 10^5$		Reese, 1997	"
*	198	130	$\text{Ac}^- + \text{SO}_4^- (+ \text{O}_2) \rightarrow \text{SO}_4^{2-} + \text{CH}_3\text{O}_2 + \text{CO}_2$ $\rightarrow \text{SO}_4^{2-} + \text{CH}_3 + \text{CO}_2$	$2.8 \cdot 10^7$	1210	Reese, 1997; Huie and Clifton, 1990	"
*	199	131	$\text{HAc} + \text{NO}_3 (+ \text{O}_2) \rightarrow \text{NO}_3^- + \text{H}^+ + \text{HO}_2 + \text{ACO}_3$ $\rightarrow \text{NO}_3^- + \text{H}^+ + \text{CH}_2\text{COOH}$	$1.4 \cdot 10^4$	3800	Exner <i>et al.</i> , 1994	"
*	200	132	$\text{Ac}^- + \text{NO}_3 (+ \text{O}_2) \rightarrow \text{NO}_3^- + \text{CH}_3\text{O}_2 + \text{CO}_2$ $\rightarrow \text{NO}_3^- + \text{CH}_3 + \text{CO}_2$	$2.9 \cdot 10^6$	3800	Exner <i>et al.</i> , 1994	"
*	201	133	$\text{HAc} + \text{Cl}_2^- (+ \text{O}_2) \rightarrow 2 \text{Cl}^- + \text{H}^+ + \text{HO}_2 + \text{ACO}_3$ $\rightarrow 2 \text{Cl}^- + \text{H}^+ + \text{CH}_2\text{COOH}$	1950 1500	4800 4930	Jacobi <i>et al.</i> , 1998 Jacobi <i>et al.</i> , 1999	" more actual value
*	202	134	$\text{Ac}^- + \text{Cl}_2^- (+ \text{O}_2) \rightarrow 2 \text{Cl}^- + \text{CH}_3\text{O}_2 + \text{CO}_2$ $\rightarrow 2 \text{Cl}^- + \text{CH}_3 + \text{CO}_2$	$2.6 \cdot 10^5$	4800	Jacobi <i>et al.</i> , 1996	split into elementary steps

*	203	135	$\text{HAc} + \text{Br}_2^- (+ \text{O}_2) \rightarrow 2 \text{Br}^- + \text{H}^+ + \text{HO}_2 + \text{ACO}_3$ $\rightarrow 2 \text{Br}^- + \text{H}^+ + \text{CH}_2\text{COOH}$	10		Reese <i>et al.</i> , 1999	"
*	204	136	$\text{Ac}^- + \text{Br}_2^- (+ \text{O}_2) \rightarrow 2 \text{Br}^- + \text{CH}_3\text{O}_2 + \text{CO}_2$ $\rightarrow 2 \text{Br}^- + \text{CH}_3 + \text{CO}_2$	100		Jacobi, 1996	"
*	205	137	$\text{Ac}^- + \text{CO}_3^- (+ \text{O}_2) \rightarrow \text{CO}_3^{2-} + \text{CH}_3\text{O}_2 + \text{CO}_2$ $\rightarrow \text{CO}_3^{2-} + \text{CH}_3 + \text{CO}_2$	580		Zellner <i>et al.</i> , 1996	"
	206		$\text{CH}_2\text{COOH} + \text{O}_2 \rightarrow \text{ACO}_3$	$1.7 \cdot 10^9$		Schuchmann <i>et al.</i> , 1985	explicit consideration of alkyl /peroxy radicals
	207		$\text{CH}_3 + \text{O}_2 \rightarrow \text{CH}_3\text{O}_2$	$4.1 \cdot 10^9$		Marchaj <i>et al.</i> , 1991	"
	208	138	$\text{CH}_3\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow \text{HCHO} + \text{CH}_3\text{OH} + \text{O}_2$	$1.7 \cdot 10^8$	2200	Herrmann <i>et al.</i> , 1999b)	consideration of additional reaction pathways (correlation)
	209		$\text{CH}_3\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{O} + \text{CH}_3\text{O} + \text{O}_2$	$3.6 \cdot 10^7$	2200	Herrmann <i>et al.</i> , 1999b)	
	210		$\text{ACO}_3 + \text{ACO}_3 \rightarrow 2 \text{CH}_3\text{O}_2 + 2 \text{CO}_2 + \text{O}_2$	$1.5 \cdot 10^8$		estimated equal as $k_{(2 \text{ETHPX})}$	
	211	139	$\text{CH}_3\text{O}_2 + \text{HSO}_3^- \rightarrow \text{CH}_3\text{OOH} + \text{SO}_3^-$	$5 \cdot 10^5$		Herrmann <i>et al.</i> , 1999b)	correct products;
*	212	140	$\text{ETHP} + \text{ETHP} \rightarrow \text{products}$ $\rightarrow \text{EtOH} + \text{CH}_3\text{CHO} + \text{O}_2$	$1.6 \cdot 10^8$	-750	Herrmann <i>et al.</i> , 1999	correct products; consideration of different reaction pathways (correlation)
	213		$\text{ETHP} + \text{ETHP} \rightarrow \text{CH}_3\text{CH}_2\text{O} + \text{CH}_3\text{CH}_2\text{O} + \text{O}_2$	$1 \cdot 10^8$	-750	Herrmann <i>et al.</i> , 1999	correct products; consideration of different reaction pathways (correlation)
*	214		$\text{CH}_3\text{CH}_2\text{O} + \text{O}_2 \rightarrow \text{HO}_2 + \text{CH}_3\text{CHO}$	$6 \cdot 10^6$		estimated	sink reaction
	215		$\text{CH}_3\text{CH}_2\text{O} \rightarrow \text{CH}_3\text{CHOH}$	$1 \cdot 10^6$		estimated	sink reaction
*	216		$\text{Fe}^{2+} + \text{CH}_3\text{O}_2 \rightarrow \text{FeCH}_3\text{O}_2^{2+}$	$8.6 \cdot 10^5$		Khaikin <i>et al.</i> , 1996	$\text{FeCH}_3\text{O}_2^+$: new considered
*	217		$\text{FeCH}_3\text{O}_2^{2+} + \text{H}^+ \rightarrow \text{Fe}^{3+} + \text{O}_2$	$3.0 \cdot 10^4$		Khaikin <i>et al.</i> , 1996	$\text{FeCH}_3\text{O}_2^+$: new considered
*	218		$\text{FeCH}_3\text{O}_2^{2+} \rightarrow \text{Fe}^{3+} + \text{CH}_3\text{OOH} + \text{OH}^-$	100		Khaikin <i>et al.</i> , 1996	$\text{FeCH}_3\text{O}_2^+$: new considered
	219		$\text{OH} + \text{HC}_2\text{O}_4^- \rightarrow \text{H}_2\text{O} + \text{C}_2\text{O}_4^-$	$3.2 \cdot 10^7$		Getoff <i>et al.</i> , 1971	consideration of C_2 -difunctional compounds
*	220		$\text{NO}_3 + \text{HC}_2\text{O}_4^- \rightarrow \text{NO}_3^- + \text{H}^+ + \text{C}_2\text{O}_4^-$	$6.8 \cdot 10^7$		Raabe, 1996	"
*	221		$\text{Cl}_2^- + \text{HC}_2\text{O}_4^- \rightarrow 2 \text{Cl}^- + \text{H}^+ + \text{C}_2\text{O}_4^-$	$1.3 \cdot 10^6$		estimated (ETR)	"
*	222		$\text{Br}_2^- + \text{HC}_2\text{O}_4^- \rightarrow 2 \text{Br}^- + \text{H}^+ + \text{C}_2\text{O}_4^-$	$3.7 \cdot 10^3$		estimated (ETR)	"
*	223		$\text{SO}_4^- + \text{HC}_2\text{O}_4^- \rightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{C}_2\text{O}_4^-$	$3.35 \cdot 10^5$		Buxton <i>et al.</i> , 1999	"
	224		$\text{OH} + \text{C}_2\text{O}_4^{2-} \rightarrow \text{OH}^- + \text{C}_2\text{O}_4^-$	$5.3 \cdot 10^6$		Getoff <i>et al.</i> , 1971	"
*	225		$\text{NO}_3 + \text{C}_2\text{O}_4^{2-} \rightarrow \text{NO}_3^- + \text{C}_2\text{O}_4^-$	$2.2 \cdot 10^8$		Raabe, 1996	"
*	226		$\text{Cl}_2^- + \text{C}_2\text{O}_4^{2-} \rightarrow 2 \text{Cl}^- + \text{H}^+ + \text{C}_2\text{O}_4^-$	$4.0 \cdot 10^6$		estimated (ETR)	"
*	227		$\text{Br}_2^- + \text{C}_2\text{O}_4^{2-} \rightarrow 2 \text{Br}^- + \text{C}_2\text{O}_4^-$	$1.1 \cdot 10^4$		estimated (ETR)	"
*	228		$\text{SO}_4^- + \text{C}_2\text{O}_4^{2-} \rightarrow \text{SO}_4^{2-} + \text{C}_2\text{O}_4^-$	$1.05 \cdot 10^6$		Buxton <i>et al.</i> , 1999a	"
	229		$\text{C}_2\text{O}_4^- + \text{O}_2 \rightarrow \text{CO}_2 + \text{CO}_2 + \text{O}_2^-$	$2.0 \cdot 10^9$		estimated	"
	230		$\text{OH} + \text{CH}(\text{OH})_2\text{CH}(\text{OH})_2 \rightarrow \text{H}_2\text{O} + \text{C}(\text{OH})_2\text{CH}(\text{OH})_2$	$1.1 \cdot 10^9$	1516	Buxton <i>et al.</i> , 1997	"

*	231	$\text{NO}_3 + \text{CH}(\text{OH})_2\text{CH}(\text{OH})_2 \rightarrow \text{H}^+ + \text{NO}_3^- + \text{C}(\text{OH})_2\text{CH}(\text{OH})_2$	$1.1 \cdot 10^6$	3368	Herrmann <i>et al.</i> , 1995c	"
*	232	$\text{Cl}_2^- + \text{CH}(\text{OH})_2\text{CH}(\text{OH})_2 \rightarrow \text{H}^+ + 2 \text{Cl}^- + \text{C}(\text{OH})_2\text{CH}(\text{OH})_2$	$4.0 \cdot 10^4$		Herrmann <i>et al.</i> , 1995c	"
*	233	$\text{Br}_2^- + \text{CH}(\text{OH})_2\text{CH}(\text{OH})_2 \rightarrow \text{H}^+ + 2 \text{Br}^- + \text{C}(\text{OH})_2\text{CH}(\text{OH})_2$	500		estimated (H abstr.)	"
*	234	$\text{SO}_4^- + \text{CH}(\text{OH})_2\text{CH}(\text{OH})_2 \rightarrow \text{H}^+ + \text{SO}_4^{2-} + \text{C}(\text{OH})_2\text{CH}(\text{OH})_2$	$2.35 \cdot 10^7$	1395	Mirabel <i>et al.</i> , 1996	"
	235	$\text{C}(\text{OH})_2\text{CH}(\text{OH})_2 + \text{O}_2 \rightarrow \text{O}_2\text{C}(\text{OH})_2\text{CH}(\text{OH})_2$	$1.38 \cdot 10^9$		Mirabel <i>et al.</i> , 1996	"
	236	$\text{O}_2\text{C}(\text{OH})_2\text{CH}(\text{OH})_2 \rightarrow \text{HO}_2 + \text{CH}(\text{OH})_2\text{COOH}$	$2 \cdot 10^9$		estimated	"
	237	$\text{OH} + \text{CH}(\text{OH})_2\text{COOH} \rightarrow \text{H}_2\text{O} + \text{C}(\text{OH})_2\text{COOH}$	$1.1 \cdot 10^9$	1516	estimate equal as k ((CH(OH) ₂) ₂)	"
*	238	$\text{NO}_3 + \text{CH}(\text{OH})_2\text{COOH} \rightarrow \text{H}^+ + \text{NO}_3^- + \text{C}(\text{OH})_2\text{COOH}$	$1.1 \cdot 10^6$	3368	estimate equal as k ((CH(OH) ₂) ₂)	"
*	239	$\text{Cl}_2^- + \text{CH}(\text{OH})_2\text{COOH} \rightarrow \text{H}^+ + 2 \text{Cl}^- + \text{C}(\text{OH})_2\text{COOH}$	$4.0 \cdot 10^4$		estimate equal as k ((CH(OH) ₂) ₂)	"
*	240	$\text{Br}_2^- + \text{CH}(\text{OH})_2\text{COOH} \rightarrow \text{H}^+ + 2 \text{Br}^- + \text{C}(\text{OH})_2\text{COOH}$	500		estimate equal as k ((CH(OH) ₂) ₂)	"
*	241	$\text{SO}_4^- + \text{CH}(\text{OH})_2\text{COOH} \rightarrow \text{H}^+ + \text{SO}_4^{2-} + \text{C}(\text{OH})_2\text{COOH}$	$2.35 \cdot 10^7$	1395	estimate equal as k ((CH(OH) ₂) ₂)	"
	242	$\text{C}(\text{OH})_2\text{COOH} + \text{O}_2 \rightarrow \text{O}_2\text{C}(\text{OH})_2\text{COOH}$	$2 \cdot 10^9$		estimated	additional reactions of peroxy radicals
	243	$\text{O}_2\text{C}(\text{OH})_2\text{COOH} \rightarrow \text{HO}_2 + \text{H}_2\text{C}_2\text{O}_4$	$2 \cdot 10^9$		estimated	"
*	244	$\text{CH}_3\text{CO} + \text{O}_2 \rightarrow \text{ACO}_3$	$2 \cdot 10^9$		estimated	"
*	245	$\text{ACO}_3 + \text{O}_2^- \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO}^-$	$1 \cdot 10^9$		Schuchmann and v. Sonntag, 1988	"
	246	$\text{CH}_3\text{C}(\text{OH})_2 + \text{O}_2 \rightarrow \text{CH}_3\text{C}(\text{OH})_2\text{O}_2$	$2 \cdot 10^9$		estimated	"
	247	$\text{CH}_3\text{C}(\text{OH})_2\text{O}_2 \rightarrow 2 \text{H}^+ + \text{Ac}^- + \text{O}_2^-$	$1 \cdot 10^5$		estimated	"
*	248	$\text{CH}_3\text{O} + \text{O}_2 \rightarrow \text{HCHO} + \text{HO}_2$	$1.2 \cdot 10^6$		estimated as in the gas phase	"
	249	$\text{CH}_3\text{O} \rightarrow \text{CH}_2\text{OH}$	$1 \cdot 10^6$		estimated	"
	250	$2 \text{O}_2\text{CH}_2\text{COO}^- (+ \text{H}_2\text{O}) \rightarrow 2 \text{CH}(\text{OH})_2\text{COO}^- + \text{H}_2\text{O}_2$	$2 \cdot 10^7$		Schuchmann <i>et al.</i> , 1985	"
*	251	$2 \text{O}_2\text{CH}_2\text{COO}^- \rightarrow 2 \text{HCHO} + \text{H}_2\text{O}_2 + 2 \text{OH}^- + 2 \text{CO}_2$	$1.88 \cdot 10^7$		Schuchmann <i>et al.</i> , 1985	"
*	252	$2 \text{O}_2\text{CH}_2\text{COO}^- (+ \text{H}_2\text{O}) \rightarrow \text{CH}(\text{OH})_2\text{COO}^- + \text{CH}_3\text{COO}^- + \text{O}_2$	$1.88 \cdot 10^7$		Schuchmann <i>et al.</i> , 1985	"
*	253	$2 \text{O}_2\text{CH}_2\text{COO}^- (+ \text{H}_2\text{O}) \rightarrow 2 \text{O}_2^- + \text{CH}(\text{OH})_2\text{COO}^- + 2 \text{H}_2\text{O}$	$7.5 \cdot 10^6$		Schuchmann <i>et al.</i> , 1985	"
	254	$\text{CO}_2^- + \text{O}_2 \rightarrow \text{CO}_2 + \text{O}_2^-$	$4 \cdot 10^9$		estimated	"
	255	$\text{CH}_2\text{COO}^- + \text{O}_2 \rightarrow \text{O}_2\text{CH}_2\text{COO}^-$	$2 \cdot 10^9$			"

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	<i>Huie and Clifton, 1990;</i> <i>Herrmann et al., 1997</i>	back reaction included => E51
	257	142	$NO_3 + Cl^- \rightarrow NO_3^- + Cl^-$	$1.0 \cdot 10^7$	4300	<i>Exner et al., 1992</i>	back reaction included => E52
*	258	143	$Cl_2^- + Cl_2^- \rightarrow Cl_2 + 2 Cl^-$	$8.7 \cdot 10^8$		<i>Zellner et al., 1996</i>	
	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	$Cl_2^- + Cu^+ \rightarrow 2 Cl^- + Cu^{2+}$	$1 \cdot 10^7$		$k_{Cu^+} = k_{Fe^{2+}}$	better estimate (more consistent to other
	266	147	$Cl_2^- + H_2O_2 \rightarrow 2 Cl^- + H^+ + HO_2$	$1 \cdot 10^8$		$k_{Cu^+} \cong 10 \cdot k_{Fe^{2+}}$	Cl_2^-/Br_2^- ratios)
*				$7 \cdot 10^5$	3340	<i>Elliot, 1989</i>	more actual value
*	267	148	$Cl_2^- + CH_3OOH \rightarrow 2 Cl^- + H^+ + CH_3O_2$	$5 \cdot 10^4$		Jacobi et al., 1999	
				$7 \cdot 10^5$	3340	$k_{CH_3OOH} = k_{H_2O_2}$	
*	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	7900	Wang and Margerum, 1994	correct rounded
	273		$Cl_2^- + H_2O \rightarrow H^+ + 2 Cl^- + OH$	0.4		Jacobi, 1996	new data available
				6			

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 <i>et al.</i> , 1997	better reference
	275	156	$NO_3 + Br^- \rightarrow NO_3^- + Br$	$3.8 \cdot 10^9$		Zellner <i>et al.</i> , 1996	
	276	157	$Br_2^- + Br_2^- \rightarrow Br_2 + 2 Br^-$	$1.7 \cdot 10^9$		Reese, 1998 Reese <i>et al.</i> , 1999	
	277	158	$Br_2^- + Fe^{2+} \rightarrow 2 Br^- + Fe^{3+}$	$3.6 \cdot 10^6$	3330	Thornton and Laurence, 1973	additional ramification
*	278		$Br_2^- + Mn^{2+} \rightarrow MnBr_2^+$	$6.3 \cdot 10^6$	4330	Laurence and Thornton, 1973	
*	279	159	$Br_2^- + Mn^{2+} \rightarrow 2 Br^- + Mn^{3+}$	$6.3 \cdot 10^6$	4330	Laurence and Thornton, 1973	additional ramification following sink
*	280		$MnBr_2^+ \rightarrow Br_2^- + Mn^{2+}$	$3 \cdot 10^5$		Laurence and Thornton, 1973	
*	281		$MnBr_2^+ \rightarrow 2 Br^- + Mn^{3+}$	$2.2 \cdot 10^5$		Laurence and Thornton, 1973	
	282	160	$Br_2^- + Cu^+ \rightarrow 2 Br^- + Cu^{2+}$	$3.6 \cdot 10^6$		$k_{Cu^+} = k_{Fe^{2+}}$ Reese, 1997	
	283	161	$Br_2^- + H_2O_2 \rightarrow 2 Br^- + H^+ + HO_2$	$1.0 \cdot 10^5$		Reese, 1997	
*	284	162	$Br_2^- + MHP \rightarrow 2 Br^- + H^+ + CH_3O_2$	$1.0 \cdot 10^5$		$k_{R174} = k_{R172}$ Jacobi, 1996	
*	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 <i>et al.</i> , 1991; Jacobi, 1996	
*	289	167	$Br_2^- + SO_3^{2-} \rightarrow 2 Br^- + SO_3^-$	$3.3 \cdot 10^7$	650	Shoute <i>et al.</i> , 1991; Jacobi, 1996	
	290	168	$Br_2 + H_2O \rightarrow Br^- + H^+ + HOBr$	1.7	7500	Beckwith <i>et al.</i> , 1996	
	291		$BrOH^- \rightarrow Br + OH^-$	$4.2 \cdot 10^6$		Zehavi and Rabani, 1972	completion of $BrOH^-$ chemistry

Table 10: 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 <i>et al.</i> , 1988a,b	
*	294	171	$CO_3^{2-} + SO_4^- \rightarrow SO_4^{2-} + CO_3^-$	$4.1 \cdot 10^7$		<i>estimated</i> Padmaja <i>et al.</i> , 1993	measurement instead of estimate
*	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	$CO_3^{2-} + NO_3^- \rightarrow NO_3^- + CO_3^-$	$4.1 \cdot 10^7$		<i>estimated</i>	
*	297		$HCO_3^- + NO_3^- \rightarrow NO_3^- + CO_3^- + H^+$	$4.1 \cdot 10^7$		<i>estimated</i> $k_{HCO_3^-} = k_{CO_3^{2-}}$	reactions of HCO_3^- added for completion
*	298	174	$CO_3^{2-} + Cl_2^- \rightarrow 2 Cl^- + CO_3^-$	$2.7 \cdot 10^6$		<i>estimated</i>	
*	299		$HCO_3^- + Cl_2^- \rightarrow 2 Cl^- + CO_3^- + H^+$	$2.7 \cdot 10^6$		<i>estimated</i>	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 <i>et al.</i> , 1991b	
*	301		$HCO_3^- + Br_2^- \rightarrow 2 Cl^- + CO_3^-$	$1.1 \cdot 10^5$		<i>estimated</i>	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	$CO_3^- + Fe^{2+} \rightarrow CO_3^{2-} + Fe^{3+}$	$2 \cdot 10^7$		<i>estimated</i>	
*	304	178	$CO_3^- + Mn^{2+} \rightarrow CO_3^{2-} + Mn^{3+}$	$1.5 \cdot 10^7$		Cope <i>et al.</i> , 1978	
*	305	179	$CO_3^- + Cu^+ \rightarrow CO_3^{2-} + Cu^{2+}$	$2 \cdot 10^7$		<i>estimated</i>	
*	306	180	$CO_3^- + H_2O_2 \rightarrow HCO_3^- + HO_2$	$4.3 \cdot 10^5$		Draganic <i>et al.</i> , 1991	
*	307	181	$CO_3^- + CH_3OOH \rightarrow HCO_3^- + CH_3O_2$	$4.3 \cdot 10^5$		$k_{H_2O_2} = k_{CH_3OOH}$	
*	308	182	$CO_3^- + HO_2 \rightarrow HCO_3^- + O_2$	$6.5 \cdot 10^8$		$k_{HO_2} = k_{O_2}$	
*	309	183	$CO_3^- + O_2^- \rightarrow CO_3^{2-} + O_2$	$6.5 \cdot 10^8$		Eriksen <i>et al.</i> , 1985	
*	310	184	$CO_3^- + HSO_3^- \rightarrow HCO_3^- + SO_3^-$	$1 \cdot 10^7$		<i>estimated</i>	
*	311	185	$CO_3^- + SO_3^{2-} \rightarrow CO_3^{2-} + SO_3^-$	$5.0 \cdot 10^6$	470	Exner <i>et al.</i> , 1990; Huie <i>et al.</i> , 1991a	
*	312		$CO_3^- + NO_2 \rightarrow CO_2 + NO_3^-$	$1 \cdot 10^9$		Lilie <i>et al.</i> , 1978	sinks added for CO_3^-
*	313		$CO_3^- + O_3 \rightarrow CO_2 + O_2 + O_2^-$	$1 \cdot 10^5$		Sehested <i>et al.</i> , 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	$\text{H}_2\text{O}_2 + \text{h}\nu \rightarrow 2 \text{OH}$	$7.19 \cdot 10^{-6}$	$0.98 \pm 0.03^{\text{a}}$ $0.96 \pm 0.03^{\text{b}}$	Zellner <i>et al.</i> , 1990 Zellner <i>et al.</i> , 1990	
*	315	187	$[\text{Fe}(\text{OH})]^{2+} + \text{h}\nu \rightarrow \text{Fe}^{2+} + \text{OH}$	$4.51 \cdot 10^{-3}$	$0.312 \pm 0.03 \dots 0.074 \pm 0.015^{\text{c}}$	Benkelberg and Warneck, 1995	
*	316	188	$[\text{Fe}(\text{OH})_2]^+ + \text{h}\nu \rightarrow \text{Fe}^{2+} + \text{OH} + \text{OH}^-$	$5.77 \cdot 10^{-3}$	$0.255 \dots 0.07^{\text{d}}$	Benkelberg <i>et al.</i> , 1991	
*	317	189	$[\text{Fe}(\text{SO}_4)]^+ + \text{h}\nu \rightarrow \text{Fe}^{2+} + \text{SO}_4^-$	$6.43 \cdot 10^{-3}$	$(7.9 \pm 0.34 \dots 1.56 \pm 0.02) \cdot 10^{-3}^{\text{c}}$	Benkelberg and Warneck, 1995	
*	318	190	$\text{NO}_2^- + \text{h}\nu (+ \text{H}^+) \rightarrow \text{NO} + \text{OH}$	$2.57 \cdot 10^{-5}$	$0.07 \pm 0.01^{\text{a}}$ $0.046 \pm 0.009^{\text{b}}$	Zellner <i>et al.</i> , 1990 Zellner <i>et al.</i> , 1990	
	319	191	$\text{NO}_3^- + \text{h}\nu (+ \text{H}^+) \rightarrow \text{NO}_2 + \text{OH}$	$4.28 \cdot 10^{-7}$	0.017 ± 0.003	Zellner <i>et al.</i> , 1990	
*	320		$[\text{Fe}(\text{C}_2\text{O}_4)_2]^- + \text{h}\nu \rightarrow \text{Fe}^{2+} + \text{C}_2\text{O}_4^{2-} + \text{C}_2\text{O}_4^-$	$2.47 \cdot 10^{-2}$	1.0 ± 0.25 (436 nm)	Zuo and Hoigné, 1992	oxalate chemistry
*	321		$[\text{Fe}(\text{C}_2\text{O}_4)_3]^{3-} + \text{h}\nu \rightarrow \text{Fe}^{2+} + 2 \text{C}_2\text{O}_4^{2-} + \text{C}_2\text{O}_4^-$	$1.55 \cdot 10^{-2}$	0.6 ± 0.46 (436 nm)	Zuo and Hoigné, 1992	"
*	322		$\text{CH}_3\text{O}_2\text{H} + \text{h}\nu \rightarrow \text{CH}_3\text{O} + \text{OH}$	$7.19 \cdot 10^{-6}$		$j_{\text{P1}} = j_{\text{P9}}$	analogous to H_2O_2 (also other reactions treated as being equal)
*	323		$\text{NO}_3 + \text{h}\nu \rightarrow \text{NO} + \text{O}_2$	$2.32 \cdot 10^{-2}$		estimated as in the gas phase	additional sinks for NO_3
*	324		$\text{NO}_3 + \text{h}\nu \rightarrow \text{NO}_2 + \text{O}^{\text{3P}}$	$2.01 \cdot 10^{-1}$		estimated as in the gas phase	additional sinks for NO_3

^a $\lambda = 308$ nm, T = 298 K; ^b $\lambda = 351$ nm, T = 298 K; ^c $\lambda = 280 \dots 370$ nm; ^d $\lambda = 290 \dots 365$ 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	$\text{H}_2\text{O} \rightleftharpoons \text{H}^+ + \text{OH}^-$	$1.8 \cdot 10^{-16}$	$2.34 \cdot 10^{-5}$	6800	a	$1.3 \cdot 10^{11}$		c	
	2	2	$\text{CO}_2 + \text{H}_2\text{O} \rightleftharpoons \text{H}_2\text{CO}_3$	$7.7 \cdot 10^{-7}$	$4.3 \cdot 10^{-2}$	9250	b	$5.6 \cdot 10^4$	8500	x	
	3	3	$\text{H}_2\text{CO}_3 \rightleftharpoons \text{H}^+ + \text{HCO}_3^-$	$2 \cdot 10^{-4}$	$1 \cdot 10^7$		c	$5 \cdot 10^{10}$		c	
*	4	4	$\text{HCO}_3^- \rightleftharpoons \text{H}^+ + \text{CO}_3^{2-}$	$4.69 \cdot 10^{-11}$	2.35	1820	a	$5 \cdot 10^{10}$		c	
	5	5	$\text{HCl} \rightleftharpoons \text{H}^+ + \text{Cl}^-$	$1.72 \cdot 10^6$	$8.6 \cdot 10^{16}$ $5 \cdot 10^{11}$	-6890	d	$5 \cdot 10^{10}$ $2.9 \cdot 10^5$		c	$8.6 \cdot 10^{16} \gg$ diffusion controlled (vibrational freq.); based on $K \cdot k_{\text{back}}$ new: $k_{\text{f}} =$ speed of hydrogen bond breaking in water H ₂ O included in K
	6	6	$\text{NH}_3 + \text{H}_2\text{O} \rightleftharpoons \text{NH}_4^+ + \text{OH}^-$	$1.77 \cdot 10^{-5}$ $3.17 \cdot 10^{-7}$	$6.02 \cdot 10^5$	560	a	$3.4 \cdot 10^{10}$		c	
	7	7	$\text{HO}_2 \rightleftharpoons \text{H}^+ + \text{O}_2^-$	$1.6 \cdot 10^{-5}$	$8.0 \cdot 10^5$	0	e, f	$5 \cdot 10^{10}$	0	y	
	8	8	$\text{HNO}_3 \rightleftharpoons \text{H}^+ + \text{NO}_3^-$	22	$1.1 \cdot 10^{12}$	-1800	g, h	$5 \cdot 10^{10}$		c	
	9	9	$\text{HNO}_2 \rightleftharpoons \text{H}^+ + \text{NO}_2^-$	$5.3 \cdot 10^{-4}$	$2.65 \cdot 10^7$	1760	i	$5 \cdot 10^{10}$		c	
	10	10	$\text{HO}_2\text{NO}_2 \rightleftharpoons \text{H}^+ + \text{O}_2\text{NO}_2^-$	$1 \cdot 10^{-5}$	$5 \cdot 10^5$		j	$5 \cdot 10^{10}$		y	

	11	11	$\text{NO}_2 + \text{HO}_2 \rightleftharpoons \text{HO}_2\text{NO}_2$	$2.2 \cdot 10^9$	$1.0 \cdot 10^7$		k	$4.6 \cdot 10^{-3}$	j	
	12	12	$\text{SO}_2 + \text{H}_2\text{O} \rightleftharpoons \text{HSO}_3^- + \text{H}^+$	$3.13 \cdot 10^{-4}$	$6.27 \cdot 10^4$	-1940	l	$2.0 \cdot 10^8$	c	
	13	13	$\text{HSO}_3^- \rightleftharpoons \text{SO}_3^{2-} + \text{H}^+$	$6.22 \cdot 10^{-8}$	3110	-1960	l	$5 \cdot 10^{10}$	c	
	14		$\text{H}_2\text{SO}_4 \rightleftharpoons \text{HSO}_4^- + \text{H}^+$	1000	$5 \cdot 10^{13}$			$5 \cdot 10^{10}$	c	added for completion
	15	14	$\text{HSO}_4^- \rightleftharpoons \text{SO}_4^{2-} + \text{H}^+$	$1.02 \cdot 10^{-2}$	$1.02 \cdot 10^9$	-2700	g	$1 \cdot 10^{11}$	c	
	16	15	$\text{HCOOH} \rightleftharpoons \text{HCOO}^- + \text{H}^+$	$1.77 \cdot 10^{-4}$	$8.85 \cdot 10^6$	-12	a	$5 \cdot 10^{10}$	c	
	17	16	$\text{HAc} \rightleftharpoons \text{Ac}^- + \text{H}^+$	$1.75 \cdot 10^{-5}$	$8.75 \cdot 10^5$	-46	a	$5 \cdot 10^{10}$	c	
	18	17	$\text{Fe}^{3+} + \text{H}_2\text{O} \rightleftharpoons [\text{Fe}(\text{OH})]^{2+} + \text{H}^+$	$1.1 \cdot 10^{-4}$	$4.7 \cdot 10^4$		m	$4.3 \cdot 10^8$	m	
*	19	18	$[\text{Fe}(\text{OH})]^{2+} + \text{H}_2\text{O} \rightleftharpoons$ $[\text{Fe}(\text{OH})_2]^+ + \text{H}^+$	$1.4 \cdot 10^{-7}$	$1.1 \cdot 10^3$		n	$8.0 \cdot 10^9$	n	
*	20	19	$\text{Fe}^{3+} + \text{SO}_4^{2-} \rightleftharpoons [\text{Fe}(\text{SO}_4)]^+$	$1.8 \cdot 10^{-2}$	$3.2 \cdot 10^3$		m	$1.8 \cdot 10^5$	m	
	21	20	$\text{HCHO} + \text{H}_2\text{O} \rightleftharpoons \text{CH}_2(\text{OH})_2$	36	0.18	-4030	q	$5.1 \cdot 10^{-3}$	p	
	22	21	$\text{CH}_3\text{CHO} + \text{H}_2\text{O} \rightleftharpoons \text{CH}_3\text{CH}(\text{OH})_2$	$2.46 \cdot 10^{-2}$	$1.4 \cdot 10^{-4}$	-2500	p	$5.69 \cdot 10^{-3}$	o	
	23	22	$\text{CH}_2(\text{OH})_2 + \text{HSO}_3^- \rightleftharpoons \text{HMS}^- + \text{H}_2\text{O}$	$2 \cdot 10^8$	0.436	2990	q	$2.2 \cdot 10^{-9}$	q	2990
	24	23	$\text{CH}_2(\text{OH})_2 + \text{SO}_3^{2-} \rightleftharpoons \text{HMS}^- + \text{OH}^-$	33	$1.35 \cdot 10^5$	2450	q	$4.15 \cdot 10^3$	q	5530
	25	24	$\text{Cl} + \text{Cl}^- \rightleftharpoons \text{Cl}_2^-$	$1.9 \cdot 10^5$	$2.7 \cdot 10^{10}$		r	$1.4 \cdot 10^5$	r	new data available
				$1.4 \cdot 10^5$	$8.5 \cdot 10^9$			$6 \cdot 10^4$		
	26	25	$\text{Br} + \text{Br}^- \rightleftharpoons \text{Br}_2^-$	$6 \cdot 10^5$	$1.2 \cdot 10^{10}$		s	$1.9 \cdot 10^4$	s	
	27	26	$\text{Cl}^- + \text{OH}^- \rightleftharpoons \text{ClOH}^-$	0.7	$4.3 \cdot 10^9$		t	$6.1 \cdot 10^9$	t	
	28	27	$\text{ClOH}^- + \text{H}^+ \rightleftharpoons \text{Cl} + \text{H}_2\text{O}$	$1.6 \cdot 10^7$	$2.1 \cdot 10^{10}$		t	$1.3 \cdot 10^3$	z	new data available
				$5.1 \cdot 10^6$				4100		
*	29	28	$\text{ClOH}^- + \text{Cl}^- \rightleftharpoons \text{Cl}_2^- + \text{OH}^-$	$2.2 \cdot 10^{-4}$	$1.0 \cdot 10^4$		u	$4.5 \cdot 10^7$	u	
	30	29	$\text{Br}^- + \text{OH}^- \rightleftharpoons \text{BrOH}^-$	333	$1.1 \cdot 10^{10}$		v	$3.3 \cdot 10^7$	v	
	31	30	$\text{BrOH}^- + \text{H}^+ \rightleftharpoons \text{Br} + \text{H}_2\text{O}$	$1.8 \cdot 10^{12}$	$4.4 \cdot 10^{10}$		v	$2.45 \cdot 10^{-2}$	w	
*	32	31	$\text{BrOH}^- + \text{Br}^- \rightleftharpoons \text{Br}_2^- + \text{OH}^-$	70	$1.9 \cdot 10^8$		v	$2.7 \cdot 10^6$	x	
*	33		$\text{Mn}^{3+} + \text{H}_2\text{O} \rightleftharpoons \text{Mn}(\text{OH})^{2+} + \text{H}^+$	0.93	$1.86 \cdot 10^{10}$		y	$2 \cdot 10^{10}$	y	detailed formulation of Mn chemistry (new data available)
*	34		$\text{O}_2^- + \text{Mn}^{2+} \rightleftharpoons \text{MnO}_2^+$	$2.3 \cdot 10^4$	$1.5 \cdot 10^8$		z	$6.5 \cdot 10^3$	z	"
*	35		$\text{HO}_2 + \text{Mn}^{2+} \rightleftharpoons \text{MnO}_2^+ + \text{H}^+$	0.17	$1.1 \cdot 10^6$		z	$6.5 \cdot 10^6$	z	"
*	36		$\text{Mn}^{3+} + \text{Mn}^{3+} \rightleftharpoons \text{Mn}^{2+} + \text{Mn}^{4+}$	$1 \cdot 10^{-3}$	$1 \cdot 10^7$		A	$1 \cdot 10^{10}$	A	"
*	37		$\text{Mn}(\text{OH})^{2+} + \text{H}_2\text{O} \rightleftharpoons \text{Mn}(\text{OH})_2^+ + \text{H}^+$	$1 \cdot 10^{-5}$	$2 \cdot 10^5$		B	$2 \cdot 10^{10}$	B	"
*	38		$\text{Mn}^{2+} + \text{HSO}_3^- \rightleftharpoons \text{MnHSO}_3^+$	$3 \cdot 10^4$	$3.1 \cdot 10^7$		C	$1.033 \cdot 10^3$	C	"
*	39		$\text{Cu}^{2+} + \text{OH}^- \rightleftharpoons \text{CuOH}^{2+}$	$1.17 \cdot 10^4$	$3.5 \cdot 10^8$		D	$3 \cdot 10^4$	E	
	40		$\text{HO}_3 \rightleftharpoons \text{H}^+ + \text{O}_3^-$	$5 \cdot 10^{-9}$	330		F	$5.2 \cdot 10^{10}$	F	sink for O_3^- (see R31/32)
*	41		$\text{HOONO} \rightleftharpoons \text{H}^+ + \text{OONO}^-$	$1 \cdot 10^{-6}$	$5 \cdot 10^4$		G	$5 \cdot 10^{10}$	(E)	HOONO new added (see reaction 81)
	42		$\text{CHOHSO}_3^- \rightleftharpoons \text{CHOSO}_3^{2-} + \text{H}^+$	$1.34 \cdot 10^{-6}$	$5.9 \cdot 10^4$		H	$4.4 \cdot 10^{10}$	H	link between acid/anion
	43		$\text{SO}_5\text{O}_2\text{H} \rightleftharpoons \text{SO}_5\text{O}_2^- + \text{H}^+$	$1.6 \cdot 10^{-5}$	$7.5 \cdot 10^5$			$5 \cdot 10^{10}$	(E)	"

*	44	$\text{H}_2\text{C}_2\text{O}_4 \rightleftharpoons \text{H}^+ + \text{HC}_2\text{O}_4^-$	$6.4 \cdot 10^{-2}$	$3.2 \cdot 10^9$		$5 \cdot 10^{10}$	(E)	consideration of C ₂ -difunctional compounds
	45	$\text{HC}_2\text{O}_4^- \rightleftharpoons \text{H}^+ + \text{C}_2\text{O}_4^{2-}$	$5.25 \cdot 10^{-5}$	$2.6 \cdot 10^6$		$5 \cdot 10^{10}$	(E)	"
	46	$\text{CH}(\text{OH})_2\text{COOH} \rightleftharpoons \text{H}^+ + \text{CH}(\text{OH})_2\text{COO}^-$	$3.16 \cdot 10^{-4}$	$6.32 \cdot 10^6$	J	$2 \cdot 10^{10}$	J	"
	47	$\text{CHOCHO} + \text{H}_2\text{O} \rightleftharpoons (\text{CH}(\text{OH})_2)_2$	$3.9 \cdot 10^3$	21.5	K	$5.5 \cdot 10^{-3}$	K	"
	48	$[\text{Fe}(\text{C}_2\text{O}_4)]^+ \rightleftharpoons [\text{Fe}]^{3+} + \text{C}_2\text{O}_4^{2-}$	$2.9 \cdot 10^9$	$3 \cdot 10^{-3}$	L	$7.5 \cdot 10^6$		"
	49	$[\text{Fe}(\text{C}_2\text{O}_4)_2]^- \rightleftharpoons [\text{Fe}(\text{C}_2\text{O}_4)]^+ + \text{C}_2\text{O}_4^{2-}$	$6.3 \cdot 10^6$	$3 \cdot 10^{-3}$	(E)	$1.89 \cdot 10^4$		"
*	50	$[\text{Fe}(\text{C}_2\text{O}_4)_3]^{3-} \rightleftharpoons [\text{Fe}(\text{C}_2\text{O}_4)_2]^- + \text{C}_2\text{O}_4^{2-}$	$3.8 \cdot 10^4$	$3 \cdot 10^{-3}$	(E)	38		"
	51	$\text{SO}_4^- + \text{Cl}^- \rightleftharpoons \text{SO}_4^{2-} + \text{Cl}$	1.2	$2.52 \cdot 10^8$	M	$2.1 \cdot 10^8$	M	dat for back reaction available
	52	$\text{NO}_3 + \text{Cl}^- \rightleftharpoons \text{NO}_3^- + \text{Cl}$	3.4	$3.4 \cdot 10^8$	N	$1 \cdot 10^8$	N	"
*	53	$\text{Cl}^- + \text{Fe}^{3+} \rightleftharpoons \text{FeCl}^{2+}$	1.39	$3 \cdot 10^3$	O	2160		
*	54	$\text{CH}_3\text{C}(\text{O})\text{OOH} \rightleftharpoons \text{CH}_3\text{C}(\text{O})\text{OO}^- + \text{H}^+$	$6.3 \cdot 10^{-9}$	315	P	$5 \cdot 10^{10}$	(E)	sink for the anion (see R255)
	55	$\text{CH}_3\text{CO} + \text{H}_2\text{O} \rightleftharpoons \text{CH}_3\text{C}(\text{OH})_2$	367	$1.1 \cdot 10^7$	Q	$3 \cdot 10^4$		hydration of acetyl radical analogous to acetaldehyde
*	56	$2 \text{Br}^- + \text{CO}_3^- \rightleftharpoons \text{Br}_2^- + \text{CO}_3^{2-}$	0.34	$3.4 \cdot 10^4$	R	$1.1 \cdot 10^5$	R	
	57	$\text{ACO}_3 \rightleftharpoons \text{O}_2\text{CH}_2\text{COO}^- + \text{H}^+$	$1.75 \cdot 10^{-5}$	$8.75 \cdot 10^5$	-46	$5 \cdot 10^{10}$	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 Klänning and Wolff, 1985; ^x Fournier 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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