Table I : Aqueous phase equilibria

Ref.	Eq. No.	Reactions	K, M	k_{298}, (forward) $M^{-n}\ s^{-1}$ a)	E_a / R, K	k_{298} (back) $M^{-n}\ s^{-1}$ a)	E_a / R, K
1,2	E1	$H_2O \rightleftharpoons H^+ + OH^-$	$1.8\cdot10^{-16}$	$2.34 \cdot 10^{-5}$	6800	$1.3 \cdot 10^{11}$	
3,2	E2	$CO_2 \rightleftharpoons H^+ + HCO_3^-$	$4.5\cdot10^{-7}$	$2.15 \cdot 10^{3}$	-913	$5 \cdot 10^{10}$	
4,2	E3	$HCl \rightleftharpoons H^+ + Cl^-$	$1.72\cdot10^{6}$	$5\cdot10^{11}$	-6890	$2.9\cdot10^{5}$	
5,2	E4	$NH_3 \rightleftharpoons NH_4^+ + OH^-$	$1.77\cdot10^{-5}$	$6.02 \cdot 10^{5}$	560	$3.4 \cdot 10^{10}$	
6	E5	$HO_2 \rightleftharpoons H^+ + O_2^-$	$1.6\cdot10^{-5}$	$8.0 \cdot 10^{5}$		$5 \cdot 10^{10}$	
7,2	E6	$HNO_3 \rightleftharpoons H^+ + NO_3^-$	22	$1.1 \cdot 10^{12}$	-1800	$5 \cdot 10^{10}$	
8,2	E7	$HONO \rightleftharpoons H^+ + NO_2^-$	$5.3\cdot10^{-4}$	$2.65 \cdot 10^{7}$	1760	$5 \cdot 10^{10}$	
9	E8	$HNO_4 \rightleftharpoons H^+ + NO_4^-$	$1\cdot10^{-5}$	$5 \cdot 10^{5}$		$5 \cdot 10^{10}$	
9	E10	$NO_2 + HO_2 \rightleftharpoons HNO_4$	$2.2\cdot10^{9}$	$1.0 \cdot 10^{7}$		$4.6 \cdot 10^{-3}$	
10,2	E12	$SO_2 + H_2O \rightleftharpoons HSO_3^- + H^+$	$3.13\cdot10^{-4}$	$6.27 \cdot 10^{4}$	-1940	$2.0 \cdot 10^{8}$	
10,2	E13	$HSO_3^- \rightleftharpoons SO_3^{2-} + H^+$	$6.22\cdot10^{-8}$	3110	-1960	$5 \cdot 10^{10}$	
11,2	E14	$HSO_4^- \rightleftharpoons SO_4^{2-} + H^+$	$1.02\cdot10^{-2}$	$1.02 \cdot 10^{9}$	-2700	$1 \cdot 10^{11}$	
1,2	E15	$HCOOH \rightleftharpoons HCOO^- + H^+$	$1.77\cdot10^{-4}$	$8.85 \cdot 10^{6}$	-12	$5 \cdot 10^{10}$	
1,2	E16	$HAc \rightleftharpoons Ac^- + H^+$	$1.75\cdot10^{-5}$	$8.75 \cdot 10^{5}$	-46	$5 \cdot 10^{10}$	
12	E17	$Fe^{3+} + H_2O \rightleftharpoons [Fe(OH)]^{2+} + H^+$	$1.1\cdot10^{-4}$	$4.7 \cdot 10^{4}$		$4.3 \cdot 10^{8}$	
13,14	E18	$HCHO + H_2O \rightleftharpoons CH_2(OH)_2$	36	0.18	-4030	$5.1 \cdot 10^{-3}$	
14,15	E19	$CH_3CHO + H_2O \rightleftharpoons CH_3CH(OH)_2$	$2.46\cdot10^{-2}$	$1.4 \cdot 10^{-4}$	-2500	$5.69 \cdot 10^{-3}$	
13	E20	$CH_2(OH)_2 + HSO_3^- \rightleftharpoons HMS^- + H_2O$	$2\cdot10^{8}$	0.436	2990	$2.2 \cdot 10^{-9}$	
13	E21	$CH_2(OH)_2 + SO_3^{2-} \rightleftharpoons HMS^- + OH^-$	33	$1.35 \cdot 10^{5}$		$4.15 \cdot 10^{3}$	
17	E22	$Cl + Cl^- \rightleftharpoons Cl_2^-$	$1.4\cdot10^{5}$	$8.5\cdot10^{9}$		$6\cdot10^{4}$	
18	E23	$Br + Br^- \rightleftharpoons Br_2^-$	$6.3\cdot10^{5}$	$1.2 \cdot 10^{10}$		$1.9 \cdot 10^{4}$	
19	E24	$Cl^- + OH \rightleftharpoons ClOH^-$	0.7	$4.3\cdot10^{9}$		$6.1\cdot10^{9}$	
19	E25	$ClOH^- + H^+ \rightleftharpoons Cl + H_2O$	$5.1\cdot10^{6}$	$2.1\cdot10^{10}$		4100	
20	E26	$Br^- + OH \rightleftharpoons BrOH^-$	333	$1.1\cdot10^{10}$		$3.3\cdot10^{7}$	
20,21	E27	$BrOH^- + H^+ \rightleftharpoons Br + H_2O$	$1.8\cdot10^{12}$	$4.4\cdot10^{10}$		$2.45\cdot10^{-2}$	
22	E28	$HO_3 \rightleftharpoons H^+ + O_3^-$	$6.3 \cdot10^{-9}$	330		$5.2\cdot10^{10}$	
23	E29	$CHOHSO_3^- \rightleftharpoons CHOSO_3^{2-} + H^+$	$1.34 \cdot10^{-6}$	$5.9\cdot10^{4}$		$4.4\cdot10^{10}$	
(E)	E30	$SO_5O_2H^- \rightleftharpoons SO_5O_2^{2-} + H^+$	$1.5 \cdot10^{-5}$	$7.5\cdot10^{5}$		$5\cdot10^{10}$	
(E)*	E31	$H_2C_2O_4 \rightleftharpoons H^+ + HC_2O_4^-$	$6.4 \cdot10^{-2}$	$3.2\cdot10^{9}$		$5\cdot10^{10}$	
(E)*	E32	$HC_2O_4^- \rightleftharpoons H^+ + C_2O_4^{2-}$	$5.2 \cdot10^{-5}$	$2.6\cdot10^{6}$		$5\cdot10^{10}$	
24	E33	$CH(OH)_2COOH \rightleftharpoons H^+ + CH(OH)_2COO^-$	$3.16\cdot10^{-4}$	$6.32\cdot10^{6}$		$2\cdot10^{10}$	
25	E34	$CHOCHO + H_2O \rightleftharpoons (CH(OH)_2)_2$	$3.9 \cdot10^{3}$	21.5		$5.5\cdot10^{-3}$	
26	E35	$[Fe(C_2O_4)]^+ \rightleftharpoons Fe^{3+} + C_2O_4^{2-}$	$2.5 \cdot10^{9}$	$7.5\cdot10^{6}$		$3\cdot10^{-3}$	
(E)*	E36	$[Fe(C_2O_4)_2]^- \rightleftharpoons$	$6.3 \cdot10^{6}$	$1.89\cdot10^{4}$		$3\cdot10^{-3}$	

		$[Fe(C_2O_4)]^+ + C_2O_4^{2-}$				
27	E37	$SO_4^- + Cl^- \rightleftharpoons SO_4^{2-} + Cl$	1.2	$2.52\cdot10^8$		$2.1\cdot10^8$
28	E38	$NO_3 + Cl^- \rightleftharpoons NO_3^- + Cl$	3.4	$3.4\cdot10^8$	4300	$1\cdot10^8$
29	E39	$CH_3CO + H_2O \rightleftharpoons CH_3C(OH)_2$	367	$1.1\cdot10^7$	1000	$3\cdot10^4$
30	E40	$ACO_3 \rightleftharpoons O_2CH_2COO^- + H^+$	$1.75\cdot10^{-5}$	$8.75\cdot10^5$	-46	$5\cdot10^{10}$

* k_f and k_b estimated from pKa value.

<u>Table II:</u> HO$_x$- and TMI-Chemistry

Ref		Reaction	k_{298}, $M^{-n}\,s^{-1}$ a)	E_a / R, K
31	R1	$H_2O_2 + Fe^{2+} \rightarrow OH + OH^- + Fe^{3+}$	50	
32	R2	$H_2O_2 + Cu^+ \rightarrow OH + OH^- + Cu^{2+}$	$7.0 \cdot 10^3$	
33	R3	$O_2^- + Fe^{3+} \rightarrow O_2 + Fe^{2+}$	$1.5 \cdot 10^8$	
34	R4	$HO_2 + [Fe(OH)]^{2+} \rightarrow Fe^{2+} + O_2 + H_2O$	$1.3 \cdot 10^5$	
35	R5	$O_2^- + [Fe(OH)]^{2+} \rightarrow O_2 + Fe^{2+} + OH^-$	$1.5 \cdot 10^8$	
33	R6	$O_2^- + Fe^{2+}\ (+ 2H^+) \rightarrow H_2O_2 + Fe^{3+}$	$1.0 \cdot 10^7$	
35	R7	$HO_2 + Fe^{2+}\ (+ H^+) \rightarrow H_2O_2 + Fe^{3+}$	$1.2 \cdot 10^6$	5050
36	R8	$OH + Fe^{2+} \rightarrow [Fe(OH)]^{2+}$	$4.3 \cdot 10^8$	1100
37	R9	$O_2^- + Cu^+\ (+ 2H^+) \rightarrow H_2O_2 + Cu^{2+}$	$1\cdot10^{10}$	
37	R10	$HO_2 + Cu^+\ (+ H^+) \rightarrow H_2O_2 + Cu^{2+}$	$2.3 \cdot 10^9$	
37	R11	$HO_2 + Cu^{2+} \rightarrow O_2 + Cu^+ + H^+$	$1 \cdot 10^8$	
37	R12	$O_2^- + Cu^{2+} \rightarrow O_2 + Cu^+$	$8 \cdot 10^9$	
38	R13	$Fe^{3+} + Cu^+ \rightarrow Fe^{2+} + Cu^{2+}$	$1.3 \cdot 10^7$	
38	R14	$[Fe(OH)]^{2+} + Cu^+ \rightarrow Fe^{2+} + Cu^{2+} + OH^-$	$1.3 \cdot 10^7$	
39,40	R15	$O_3 + O_2^- \rightarrow O_3^- + O_2$	$1.5 \cdot 10^9$	2165
22	R16	$HO_3 \rightarrow OH + O_2$	330	
41	R17	$H_2O_2 + OH \rightarrow HO_2 + H_2O$	$3.0 \cdot 10^7$	1680
42	R18	$HSO_3^- + OH \rightarrow H_2O + SO_3^-$	$2.7 \cdot 10^9$	
43	R19	$Cu^+ + O_2 \rightarrow Cu^{2+} + O_2^-$	$4.6 \cdot 10^5$	
44	R20	$Fe^{2+} + O_3 \rightarrow FeO^{2+} + O_2$	$8.2 \cdot 10^5$	4690
45	R21	$FeO^{2+} + Cl^-\ (+ H^+) \rightarrow Fe^{3+} + ClOH^-$	100	
45	R22	$FeO^{2+} + Fe^{2+} \rightarrow 2\,Fe^{3+} + 2\,OH^-$	$7.2\cdot10^4$	842

<u>Table III:</u> N-Chemistry

Ref		Reaction	k_{298}, $M^{-n}\,s^{-1}$ a)	E_a / R, K
(E)	R23	$N_2O_5 \rightarrow NO_2^+ + NO_3^-$	$1\cdot10^7$	
46	R24	$NO^{2+} + H_2O \rightarrow NO_3^- + 2H^+$	$8.9\cdot10^7$	

47	R25	$NO_3 + HSO_3^- \rightarrow NO_3^- + H^+ + SO_3^-$	$1.3 \cdot 10^9$	2000
48	R26	$NO_3 + SO_4^{2-} \rightarrow NO_3^- + SO_4^-$	$1 \cdot 10^5$	
16	R27	$NO_4^- \rightarrow NO_2^- + O_2$	0.8	
49	R28	$HNO_4 + HSO_3^- \rightarrow HSO_4^- + NO_3 + H^+$	$3.3 \cdot 10^5$	
50	R29	$NO_2^+ + Cl^- \rightarrow ClNO_2$	$1 \cdot 10^{10}$	
50	R30	$NO_2^+ + Br^- \rightarrow BrNO_2$	$1 \cdot 10^{10}$	
50	R31	$ClNO_2 + Br^- \rightarrow NO_2^- + BrCl$	$5 \cdot 10^6$	
50	R32	$BrNO_2 + Br^- \rightarrow NO_2^- + Br_2$	$2.55 \cdot 10^4$	
50	R33	$BrNO_2 + Cl^- \rightarrow NO_2^- + BrCl$	10	

<u>Table IV:</u> S-Chemistry

Ref		Reaction	k_{298}, M^{-n} s^{-1} a)	E_a / R, K
23	R34	$HMS^- + OH \rightarrow H_2O + CHOHSO_3^-$	$3 \cdot 10^8$	
23	R35	$CHOHSO_3^- + O_2 \rightarrow O_2CHOHSO_3^-$	$2.6 \cdot 10^9$	
23	R36	$O_2CHOHSO_3^- \rightarrow HO_2 + CHOSO_3^-$	$1.7 \cdot 10^4$	
23	R37	$O_2CHOHSO_3^- \rightarrow O_2CHO + HSO_3^-$	$7.0 \cdot 10^3$	
23	R38	$CHOSO_3^- + H_2O \rightarrow HSO_3^- + HCOOH$	$1.26 \cdot 10^{-2}$	
23	R39	$O_2CHO + H_2O \rightarrow HCOOH + HO_2$	44.32	
51	R40	$HSO_3^- + H_2O_2 + H^+ \rightarrow SO_4^{2-} + H_2O + 2\ H^+$	$7.2 \cdot 10^7$	4000
52	R41	$HSO_3^- + O_3 \rightarrow HSO_4^- + O_2$	$3.7 \cdot 10^5$	5530
53	R42	$SO_3^{2-} + O_3 \rightarrow SO_4^{2-} + O_2$	$1.5 \cdot 10^9$	5280
54,55	R43	$Fe^{2+} + SO_5^- (+ H_2O) \rightarrow [Fe(OH)]^{2+} + HSO_5^-$	$2.65 \cdot 10^7$	5809
34	R44	$Fe^{2+} + HSO_5^- \rightarrow [Fe(OH)]^{2+} + SO_4^-$	$3 \cdot 10^4$	
55	R45	$Fe^{2+} + SO_4^- \rightarrow Fe^{3+} + SO_4^{2-} + H^+$	$4.6 \cdot 10^9$	-2165
42	R46	$SO_5^- + SO_5^- \rightarrow 2\ SO_4^- + O_2$	$2.2 \cdot 10^8$	2600
43	R47	$SO_5^- + HO_2 \rightarrow SO_5O_2H^-$	$1.7 \cdot 10^9$	
56	R48	$SO_5O_2^{2-}\ (+ H^+) \rightarrow HSO_5^- + O_2$	1200	
57	R49	$SO_4^- + H_2O \rightarrow SO_4^{2-} + H^+ + OH$	11	1110
58	R50	$HSO_5^- + HSO_3^- + H^+ \rightarrow 2\ SO_4^{2-} + 3\ H^+$	$7.14 \cdot 10^6$	

<u>Table V:</u> Organic Chemistry

Ref		Reaction	k_{298}, M^{-n} s^{-1} a)	E_a / R, K
59	R51	$CH_3OH + OH (+ O_2) \rightarrow H_2O + O_2CH_2OH$	$1.0 \cdot 10^9$	580
60	R52	$O_2CH_2OH + O_2CH_2OH \rightarrow CH_3OH + O_2 + HCHO$	$1.05 \cdot 10^9$	
61	R53	$ETOH + OH (+ O_2) \rightarrow H_2O + O_2CH_3CHOH$	$1.9 \cdot 10^9$	
60	R54	$O_2CH_3CHOH \rightarrow CH_3CHO + HO_2$	52	7217

62	R55	$CH_2(OH)_2 + OH \rightarrow H_2O + HO_2 + HCOOH$	$1.0 \cdot 10^9$	1020
63	R56	$CH_3CH(OH)_2 + OH \rightarrow H_2O + CH_3C(OH)_2$	$1.2 \cdot 10^9$	
63	R57	$CH_3CHO + OH \rightarrow H_2O + CH_3CO$	$3.6 \cdot 10^9$	
61	R58	$HCOOH + OH\ (+ O_2) \rightarrow H_2O + CO_2 + O_2^- + H^+$	$1.3 \cdot 10^8$	1000
64	R59	$HCOO^- + OH\ (+ O_2) \rightarrow OH^- + CO_2 + O_2^- + H^+$	$3.2 \cdot 10^9$	1000
65	R60	$CH_3COOH + OH\ (+ O_2) \rightarrow H_2O + ACO_3$	$1.5 \cdot 10^7$	1330
66	R61	$CH_3COO^- + OH\ (+ O_2) \rightarrow H_2O + O_2CH_2COO^-$	$1.0 \cdot 10^8$	1800
67	R62	$CH_3O_2 + CH_3O_2 \rightarrow CH_3OH + HCHO + O_2$	$7.4 \cdot 10^7$	2200
68	R63	$CH_3O_2 + CH_3O_2\ (+ 2O_2) \rightarrow O_2CH_2OH + O_2CH_2OH + O_2$	$3.6 \cdot 10^7$	2200
(E)	R64	$ACO_3 + ACO_3 \rightarrow 2\ CH_3O_2 + 2\ CO_2 + O_2$	$1.5 \cdot 10^8$	
67	R65	$CH_3O_2 + HSO_3^- \rightarrow CH_3OOH + SO_5^-$	$5 \cdot 10^5$	
68	R66	$ETHP + ETHP\ (+ 2O_2) \rightarrow 2\ O_2CH_3CHOH + O_2$	$1 \cdot 10^8$	
68	R67	$OH + HC_2O_4^-\ (+ O_2) \rightarrow H_2O + 2CO_2 + O_2^-$	$3.2 \cdot 10^7$	
68	R68	$OH + C_2O_4^{2-}\ (+ O_2) \rightarrow OH^- + 2CO_2 + O_2^-$	$5.3 \cdot 10^6$	
24	R69	$OH + CH(OH)_2CH(OH)_2\ (+ O_2) \rightarrow H_2O + O_2C(OH)_2CH(OH)_2$	$1.1 \cdot 10^9$	1516
(E)	R70	$O_2C(OH)_2CH(OH)_2 \rightarrow HO_2 + CH(OH)_2COOH$	$2 \cdot 10^9$	
(E)	R71	$OH + CH(OH)_2COOH\ (+ O_2) \rightarrow H_2O + O_2C(OH)_2COOH$	$1.1 \cdot 10^9$	1516
(E)	R72	$O_2C(OH)_2COOH \rightarrow HO_2 + H^+ + HC_2O_4^-$	$2 \cdot 10^9$	
(E)	R73	$CH_3C(OH)_2 + O_2 \rightarrow CH_3C(OH)_2O_2$	$2 \cdot 10^9$	
(E)	R74	$CH_3C(OH)_2O_2 \rightarrow 2\ H^+ + Ac^- + O_2^-$	$1 \cdot 10^5$	
69	R75	$2\ O_2CH_2COO^-\ (+ H_2O) \rightarrow 2\ CH(OH)_2COO^- + H_2O_2$	$2 \cdot 10^7$	

<u>Table VI:</u> Chlorine chemistry

Ref		Reaction	k_{298}, $M^{-n}\ s^{-1}$ a)	E_a / R, K
70	R76	$Cl_2^- + Fe^{2+} \rightarrow 2\ Cl^- + Fe^{3+}$	$1.0 \cdot 10^7$	3030
71	R77	$Cl_2^- + HO_2 \rightarrow 2\ Cl^- + H^+ + O_2$	$1.3 \cdot 10^{10}$	
72	R78	$Cl_2^- + HSO_3^- \rightarrow 2\ Cl^- + H^+ + SO_3^-$	$1.7 \cdot 10^8$	400
73	R79	$Cl_2 + H_2O \rightarrow H^+ + Cl^- + ClOH$	0.4	7900
17	R80	$Cl_2^- + H_2O \rightarrow H^+ + Cl^- + Cl^- + OH$	23.4	

<u>Table VII:</u> Bromine chemistry

Ref		Reaction	k_{298}, $M^{-n}\ s^{-1}$ a)	E_a / R, K
74	R81	$SO_4^- + Br^- \rightarrow SO_4^{2-} + Br$	$2.1 \cdot 10^9$	
75	R82	$NO_3 + Br^- \rightarrow NO_3^- + Br$	$3.8 \cdot 10^9$	

76	R83	$Br_2^- + Br_2^- \rightarrow Br_2 + 2\ Br^-$	$1.7 \cdot 10^9$	
70	R84	$Br_2^- + Fe^{2+} \rightarrow 2\ Br^- + Fe^{3+}$	$3.6 \cdot 10^6$	3330
77	R85	$Br_2^- + H_2O_2 \rightarrow 2\ Br^- + H^+ + HO_2$	$1.0 \cdot 10^5$	
78	R86	$Br_2^- + HO_2 \rightarrow 2\ Br^- + H^+ + O_2$	$6.5 \cdot 10^9$	
79	R87	$Br_2^- + HSO_3^- \rightarrow 2\ Br^- + H^+ + SO_3^-$	$5.0 \cdot 10^7$	780
80	R88	$Br_2\ (+ H_2O) \rightarrow Br^- + H^+ + HOBr$	97.0	
20	R89	$BrOH^- \rightarrow Br + OH^-$	$4.2 \cdot 10^6$	

<u>Table VIII:</u> Additional halogen reactions

Number	Reaction	k [$M^{-n}\ s^{-1}$]	reference
A(1)	$ClOH + Cl^- + H^+ \rightarrow Cl_2 + H_2O$	1.8E4	80
A(2)	$BrOH + Br^- + H^+ \rightarrow Br_2 + H_2O$	1.6E10	80
A(3)	$ClOH + Br^- + H^+ \rightarrow BrCl + H_2O$	1.3E6	84
A(4)	$BrOH + Cl^- + H^+ \rightarrow BrCl + H_2O$	5.6E9	89
A(5)	$BrCl \rightarrow BrOH + Cl^- + H^+$	1.0E5	89
A(6)	$BrCl + Br^- \rightarrow Br_2Cl^-$	5.0E9	89
A(7)	$Br_2Cl^- \rightarrow BrCl + Br^-$	2.8E5	89
A(8)	$Br_2 + Cl^- \rightarrow BrCl_2^-$	5.0E9	89
A(9)	$BrCl_2^- \rightarrow Br_2 + Cl^-$	3.9E9	89
A(10)	$Br^- + ClO^- + H^+ \rightarrow BrCl + OH^-$	3.7E10	84
A(11)	$Br^- + O_3\ (+ H^+) \rightarrow BrO^- + O_2$	2.1E2 exp(-4450/T)	83
A(12)	$BrO^- + SO_3^{2-} \rightarrow Br^- + SO_4^{2-}$	1.0E8	87
A(13)	$Br_2^- + HO_2 \rightarrow Br_2 + H_2O_2$	9.1E7	88
A(14)	$BrOH + HSO_3^- \rightarrow Br^- + HSO_4^- + H^+$	5.0E9	(a)
A(15)	$BrOH + SO_3^{2-} \rightarrow Br^- + HSO_4^-$	5.0E9	87
A(16)	$ClOH + HSO_3^- \rightarrow Cl^- + HSO_4^- + H^+$	7.6E8	(b)
A(17)	$ClOH + SO_3^{2-} \rightarrow Cl^- + HSO_4^-$	7.6E8	81
A(18)	$Br^- + HSO_5^- \rightarrow BrOH + SO_4^{2-}$	1.0 exp(-5338/T)	82
A(19)	$Cl^- + HSO_5^- \rightarrow ClOH + SO_4^{2-}$	1.8E-2 exp(-7352/T)	82
A(20)	$HBr \rightarrow H^+ + Br^-$	1.0E13	86
A(21)	$H^+ + Br^- \rightarrow HBr$	1.0E4	86
A(22)	$ClOH \rightarrow H^+ + ClO^-$	3.2E2	86
A(23)	$H^+ + ClO^- \rightarrow ClOH$	1.0E10	86
A(24)	$BrOH \rightarrow H^+ + BrO^-$	23	85
A(25)	$H^+ + BrO^- \rightarrow BrOH$	1.0E10	85

(a) A(15) estimated to be equal to A(16), (b) A(17) estimated to be equal to A(18).

<u>Table IX:</u> Aqueous photolysis

Rates scaled to gas phase absorption curves using the following parameters to obtain absorption curves.

Ref.	No.	Reaction	j_{max} [s^{-1}]	b[b)]	c[b)]
90	P1	$H_2O_2 + h\nu \rightarrow 2\ OH$	$7.64 \cdot 10^{-6}$	2.46425	0.76355
91	P2	$[Fe(OH)]^{2+} + h\nu \rightarrow Fe^{2+} + OH$	$4.76 \cdot 10^{-3}$	2.19894	0.76087
90	P6	$NO_3^- + h\nu \xrightarrow{H^+} NO_2 + OH$	$4.57 \cdot 10^{-7}$	2.59408	0.77213
92	P7	$Fe(C_2O_4)_2^- + h\nu \rightarrow Fe^{2+} + C_2O_4^{2-} + CO_2 + CO_2^-$	$2.47 \cdot 10^{-2}$	1.95825	0.76782

<u>Table X:</u> Gas phase photolysis

Number	Reaction	Note	Reference
J(1)	NO_2 (+ O_2) + $h\nu$ $\rightarrow$ NO + O_3	a	94
J(2)	O_3 + $h\nu$ $\rightarrow$ O^1(d) + O_2	a	94
J(3)	O_3 + $h\nu$ $\rightarrow$ O^3(p) + O_2	a	Scaled to J(7)
J(4)	HONO + $h\nu$ $\rightarrow$ OH + NO	a	Scaled to J(1)
J(5)	HNO_3 + $h\nu$ $\rightarrow$ NO_2 + OH	a	94
J(6)	HNO_4 + $h\nu$ $\rightarrow$ 0.65HO_2 + 0.65NO_2 + 0.35OH + 0.35NO_3	a	94
J(7)	NO_3 + $h\nu$ $\rightarrow$ NO + O_2	a	94
J(8)	NO_3 (+ O_2) + $h\nu$ $\rightarrow$ NO_2 + O_3	a	94
J(9)	H_2O_2 + $h\nu$ $\rightarrow$ OH + OH	a	94
J(10)	HCHO + $h\nu$ $\rightarrow$ H_2 + CO	a	94
J(11)	HCHO (+ O_2) + $h\nu$ $\rightarrow$ HO_2 + HO_2 + CO	a	94
J(12)	ALD + $h\nu$ $\rightarrow$ CH_3O_2 + HO_2 + OH	a	94
J(13)	CH_3OOH + $h\nu$ $\rightarrow$ HCHO + HO_2 + OH	a	94
J(14)	OP2 + $h\nu$ $\rightarrow$ ALD + HO_2 + OH	a	Scaled to J(10)
J(15)	PAA + $h\nu$ $\rightarrow$ CH_3O_2 + OH	a	Scaled to J(13)
J(16)	KET + $h\nu$ $\rightarrow$ ETHP + ACO_3	a	Scaled to J(5)
J(17)	GLY + $h\nu$ $\rightarrow$ 0.13HCHO + 1.87CO + 0.87H_2	a	Scaled to J(1)
J(18)	GLY + $h\nu$ $\rightarrow$ 0.45HCHO + 1.55CO + 0.80HO_2 + 0.15H_2	a	Scaled to J(1)

J(19)	MGLY + *hv* $\rightarrow$ CO + HO_2 + ACO_3	a	Scaled to J(1)
J(20)	DCB + *hv* $\rightarrow$ TCO_3 + HO_2	a	Scaled to J(10)
J(21)	ONIT + *hv* $\rightarrow$ 0.2ALD + 0.8KET + HO_2 + NO_2	a	Scaled to J(5)
J(22)	MACR + *hv* $\rightarrow$ HCHO + CO + HO_2 + ACO_3	a	Scaled to J(10)
J(23)	HKET + *hv* $\rightarrow$ HCHO + HO_2 + ACO_3	a	Scaled to J(5)
J(24)	ClOH + *hv* $\rightarrow$ Cl + OH	b	95
J(25)	Cl_2O_2 + *hv* $\rightarrow$ Cl + Cl + O_2	b	95
J(26)	$ClNO_2$ + *hv* $\rightarrow$ Cl + NO_2	b	95
J(27)	$ClNO_3$ + *hv* $\rightarrow$ Cl + NO_3	b	95
J(28)	Cl_2 + *hv* $\rightarrow$ Cl + Cl	b	95
J(29)	BrOH + *hv* $\rightarrow$ Br + OH	b	95
J(30)	$BrNO_2$ + *hv* $\rightarrow$ Br + NO_2	b	95
J(31)	$BrNO_3$ + *hv* $\rightarrow$ Br + NO_3	b	95
J(32)	Br_2 + *hv* $\rightarrow$ Br + Br	b	95
J(33)	BrCl + *hv* $\rightarrow$ Br + Cl	b	95
J(34)	BrO (+ O_2) + *hv* $\rightarrow$ Br + O	b	95

[a] Photolysis reactions originating from RACM chemical scheme (Stockwell *et al.*, 1997 – ref 93.)
[b] Additional photolysis rates added to activate halogen species.

<u>Table XI:</u> Additional gas phase reactions added to RACM

Number	Reaction	k [molcules $^{-1}$ cm^3 s^{-1}]	Reference
G(1)	HCl + OH $\rightarrow$ Cl + H_2O	8.0E-13 exp(-350/T)	96
G(2)	Cl + O_3 $\rightarrow$ ClO + O_2	1.2E-11 exp(-260/T)	96
G(3)	Cl + CH_4 (+ O_2) $\rightarrow$ HCl + CH_3O_2	1.0E-13 exp(-1400/T)	96
G(4)	Cl + HCHO (+ O_2) $\rightarrow$ HCl + CO + HO_2	7.3E-11 exp(-30/T)	96
G(5)	ClO + HO_2 $\rightarrow$ ClOH (+ O_2)	5.0E-12 exp(700/T)	96
G(6)	ClO + NO $\rightarrow$ Cl + NO_2	1.7E-11 exp(290/T)	96
G(7)	ClO + NO_2 $\rightarrow$ $ClNO_3$	2.3E-12	96
G(8)	ClO + CH_3O_2 $\rightarrow$ HCHO + Cl + HO_2	2.2E-12 exp(-115/T)	96
G(9)	ClO + ClO $\rightarrow$ Cl_2O_2	3.5E-13	96
G(10)	Cl_2O_2 $\rightarrow$ ClO + ClO	49	96

G(11)	$Cl + H_2O_2 \rightarrow HCl + HO_2$	4.1E-13 exp(-980/T)	96
G(12)	$Cl + CH_3OOH \rightarrow HCl + CH_3O_2$	5.7E-11	(E)
G(13)	$Cl + C_2H_6\ (+ O_2) \rightarrow HCl + ETHP$	5.7E-11 exp(-90/T)	96
G(14)	$Cl + C_2H_4\ (+ O_2) \rightarrow HCl + XO_2$	1.0E-10	96
G(15)	$HBr + OH \rightarrow Br + H_2O$	1.1E-11	96
G(16)	$Br + O_3 \rightarrow BrO + O_2$	1.2E-12 exp(-800/T)	96
G(17)	$Br + HCHO\ (+ O_2) \rightarrow HBr + CO + HO_2$	1.1E-12 exp(-800/T)	96
G(18)	$BrO + HO_2 \rightarrow BrOH + O_2$	2.1E-11 exp(540/T)	96
G(19)	$BrO + NO \rightarrow Br + NO_2$	2.1E-11 exp(260/T)	96
G(20)	$BrO + NO_2 \rightarrow BrNO_3$	2.8E-12	96
G(21)	$BrO + CH_3O_2 \rightarrow HCHO + Br + HO_2$	4.1E-12	98
G(22)	$BrO + CH_3O_2 \rightarrow BrOH + HCHO$	1.6E-12	98
G(23)	$Br + CH_3OOH \rightarrow HBr + CH_3O_2$	1.4E-14 exp(-1610/T)	
G(24)	$Br + HO_2 \rightarrow HBr + O_2$	2.0E-12 exp(-600/T)	96
G(25)	$Br + C_2H_4\ (+ O_2) \rightarrow HBr + XO_2$	2.2E-13	99
G(26)	$Cl + Br_2 \rightarrow BrCl + Br$	1.2E-10	97
G(27)	$BrCl + Br \rightarrow Br_2 + Cl$	3.3E-15	97
G(28)	$Cl_2 + Br \rightarrow BrCl + Cl$	1.1E-15	97
G(29)	$BrCl + Cl \rightarrow Cl_2 + Br$	1.5E-11	97
G(30)	$BrO + ClO \rightarrow Br + ClO\ (+ O)$	6.8E-12 exp(430/T)	96
G(31)	$BrO + ClO \rightarrow Br + Cl + O_2$	6.1E-12 exp(220/T)	96
G(32)	$BrO + ClO \rightarrow BrCl + O_2$	1.0E-12 exp(170/T)	96
G(33)	$BrO + BrO \rightarrow Br + Br + O_2$	2.7E-12 exp(40/T)	96
G(34)	$BrO + BrO \rightarrow Br_2 + O_2$	5.0E-13 exp(860/T)	96
G(35)	$DMS + OH \rightarrow SO_2 + HCHO + HCHO$	4.4E-12 exp(-234/T)	100
G(36)	$DMS + NO_3 \rightarrow SO_2 + HCHO + HCHO + HNO_3$	1.1E-12 exp(520/T)	100
G(37)	$DMS + Cl\ (+ O_2) \rightarrow SO_2 + HCHO + HCHO + HCl$	3.3E-10	101
G(38)	$DMS + Br\ (+ O_2) \rightarrow SO_2 + HCHO + HCHO + HBr$	3.0E-14 exp(-2386/T)	102

<u>Table XII:</u> Additional uptake parameters to CAPRAM 2.4

Species	K [mol dm^{-3} atm^{-1}]	-E/R [K]	α [-]	D_g [10^{-5} m^2 s^{-1}]	reference
HBr	0.72	6077	0.05	1.0	80
ClOH	480	1633	0.05	1.0	80
BrOH	48	–	0.05	1.0	80
$H_2C_2O_4$	5.0e8	–	0.05[a]	1.0[a]	103

[a] Estimated value

Table XIII: **Emission Rates**

Species	J_e(Marine) cm^{-2} s^{-1}	Reference
O_3	5.0e10	80
NH_3	2.0e9	80
CO	2.0e10	80
NO	2.5e8	80
ETH	3.6e7	104
ETE	1.8e8	104
CH_3SCH_3	2.0e9	80

Table XIV: **Deposition Velocities**

Species	ν_d cm s^{-1}
O_3	0.04
NH_3	1.0
CO	0.1
SO_2	0.5
NO_2	0.1
HCl	0.5
H_2SO_4	0.5
HNO_3	0.5
HCHO	0.5
OP1	0.5
ORA1	0.5
CH_3OH	0.5
EtOH	0.5

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