Electronic Supplementary Material (ESI) for Environmental Science: Atmospheres.

Inorganic compounds

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
HO_x chemistry					
$O_3 + h\nu \rightarrow H_2O_2 + O_2 - H_2O$	R(1)	Calculated		Graedel and Weschler, 1981	
$H_2O_2 + h\nu \rightarrow 2\ HO^\bullet$	R(2)	Calculated		Graedel and Weschler, 1981	
$HO^\bullet + HO^\bullet \rightarrow H_2O_2$	R(3)	$3.6\ 10^9$	930	Elliot and McCracken, 1989	
$HO^\bullet + HO_2^\bullet \rightarrow O_2 + H_2O$	R(4)	$2.8\ 10^{10}$	0	Elliot and Buxton, 1992	
$HO^\bullet + O_2^{\bullet-} \rightarrow O_2 + OH^-$	R(5)	$3.5\ 10^{10}$	720	Elliot and Buxton, 1992	
$HO^\bullet + O_3 \rightarrow HO_2^\bullet + O_2$	R(6)	$1.0\ 10^8$		Sehested et al., 1984	
$H_2O_2 + HO^\bullet \rightarrow HO_2^\bullet + H_2O$	R(7)	$3.2\ 10^7$	1700	Christensen et al., 1982	
$HO_2^\bullet + HO_2^\bullet \rightarrow H_2O_2 + O_2$	R(8)	$8.3\ 10^5$	2700	Bielski et al., 1985	
$HO_2^\bullet + O_2^{\bullet-} \rightarrow H_2O_2 + O_2 + OH^- - H_2O$	R(9)	$9.6\ 10^7$	910	Christensen and Sehested, 1988	
$O_3 + HO_2^\bullet \rightarrow HO^\bullet + 2\ O_2$	R(10)	$<1.0\ 10^4$		Sehested et al., 1984	1
$O_3 + O_2^{\bullet-} \rightarrow HO^\bullet + 2\ O_2 + OH^- - H_2O$	R(11)	$1.5\ 10^9$	2200	Sehested et al., 1983	
$HSO_3^- + HO^\bullet \rightarrow SO_3^{\bullet-} + H_2O$	R(12)	$2.7\ 10^9$		Buxton et al., 1996b	
$SO_3^{2-} + HO^\bullet \rightarrow SO_3^{\bullet-} + OH^-$	R(13)	$4.6\ 10^9$		Buxton et al., 1996b	
TMI chemistry					
$Fe^{3+} + h\nu \rightarrow Fe^{2+} + HO^\bullet + H^+ - H_2O$	R(14)	Calculated		Benkelberg and Warneck, 1995	
$[Fe(OH)]^{2+} + h\nu \rightarrow Fe^{2+} + HO^\bullet$	R(15)	Calculated		Benkelberg and Warneck, 1995	
$[Fe(OH)_2]^+ + h\nu \rightarrow Fe^{2+} + HO^\bullet + OH^-$	R(16)	Calculated		Benkelberg et al., 1991; Weschler et al., 1986	
$[Fe(SO_4)]^+ + h\nu \rightarrow Fe^{2+} + SO_4^{\bullet-}$	R(17)	Calculated		Benkelberg and Warneck, 1995	
$H_2O_2 + Fe^{2+} \rightarrow Fe^{3+} + HO^\bullet + OH^-$	R(18)	$5.2\ 10^1$	5050	Christensen et al., 1993; Kremer, 2003	
$H_2O_2 + FeO^{2+} \rightarrow Fe^{3+} + HO_2^\bullet + OH^-$	R(19)	$9.5\ 10^3$	2800	Jacobsen et al., 1997a	
$O_2^{\bullet-} + Fe^{2+} \rightarrow Fe^{3+} + H_2O_2 - 2\ H^+$	R(20)	$1.0\ 10^7$		Rush and Bielski, 1985	
$O_2^{\bullet-} + Fe^{3+} \rightarrow Fe^{2+} + O_2$	R(21)	$1.5\ 10^8$			$= k(O_2^{\bullet-} + [Fe(OH)]^{2+})$
$O_2^{\bullet-} + [Fe(OH)]^{2+} \rightarrow Fe^{2+} + O_2 + OH^-$	R(22)	$1.5\ 10^8$		Rush and Bielski, 1985	
$O_2^{\bullet-} + [Fe(OH)_2]^+ \rightarrow Fe^{2+} + O_2 + 2\ OH^-$	R(23)	$1.5\ 10^8$			$= k(O_2^{\bullet-} + [Fe(OH)]^{2+})$

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$HO_2^\bullet + Fe^{2+} \rightarrow Fe^{3+} + H_2O_2 - H^+$	R(24)	$1.2\ 10^6$	5050	Jayson et al., 1973a	
$HO_2^\bullet + FeO^{2+} \rightarrow Fe^{3+} + O_2 + OH^-$	R(25)	$2.0\ 10^6$		Jacobsen et al., 1997a	
$HO^\bullet + Fe^{2+} \rightarrow [Fe(OH)]^{2+}$	R(26)	$4.6\ 10^8$	1100	Christensen and Sehested, 1981	
$HO^\bullet + FeO^{2+} \rightarrow Fe^{3+} + H_2O_2 - H^+$	R(27)	$1.0\ 10^7$		Logager et al., 1992	
$O_3 + Fe^{2+} \rightarrow FeO^{2+} + O_2$	R(28)	$8.2\ 10^5$		Logager et al., 1992	
$FeO^{2+} \rightarrow Fe^{3+} + HO^\bullet + OH^- - H_2O$	R(29)	$1.3\ 10^{-2}$	4100	Jacobsen et al., 1997a	
$FeO^{2+} + Fe^{2+} \rightarrow 2\ Fe^{3+} + 2\ OH^- - H_2O$	R(30)	$7.2\ 10^4$	840	Jacobsen et al., 1997a	
$FeO^{2+} + Fe^{2+} \rightarrow Fe(OH)_2Fe^{4+} - H_2O$	R(31)	$1.8\ 10^4$	5050	Jacobsen et al., 1997a	
$Fe(OH)_2Fe^{4+} \rightarrow 2\ Fe^{3+} + 2\ OH^-$	R(32)	$4.9\ 10^{-1}$	8800	Jacobsen et al., 1997a	
$Fe(OH)_2Fe^{4+} + H^+ \rightarrow 2\ Fe^{3+} + 2\ H_2O - H^+$	R(33)	2.0	5650	Jacobsen et al., 1997a	
$Cl_2^{\bullet-} + Fe^{2+} \rightarrow Fe^{3+} + 2\ Cl^-$	R(34)	$1.0\ 10^7$	3060	Thornton and Laurence, 1973	
$Cl_2^{\bullet-} + Fe^{2+} \rightarrow [FeCl]^{2+} + Cl^-$	R(35)	$4.0\ 10^6$	3700	Thornton and Laurence, 1973	
$Cl^- + Fe(O)^{2+} \rightarrow Fe^{3+} + ClOH^- - H^+$	R(36)	$1.0\ 10^2$		Jacobsen et al., 1998b	
$NO_3^\bullet + Fe^{2+} \rightarrow Fe^{3+} + NO_3^-$	R(37)	$8.0\ 10^6$		Pikaev et al., 1974	
$NO_2 + Fe^{2+} \rightarrow Fe^{3+} + NO_2^-$	R(38)	$3.1\ 10^4$		Epstein et al., 1982	
$HNO_2 + FeO^{2+} \rightarrow Fe^{3+} + NO_2 + OH^-$	R(39)	$1.1\ 10^4$	4150	Jacobsen et al., 1998b	
$NO_2^- + FeO^{2+} \rightarrow Fe^{3+} + NO_2 + OH^- - H^+$	R(40)	$<1.0\ 10^5$		Jacobsen et al., 1998b	
$HSO_3^- + [Fe(OH)]^{2+} \rightarrow Fe^{2+} + SO_3^{\bullet-} - H_2O$	R(41)	$3.0\ 10^1$		Ziajka et al., 1994	
$SO_5^{\bullet-} + Fe^{2+} \rightarrow [Fe(OH)]^{2+} + HSO_5^- - H_2O$	R(42)	$2.6\ 10^7$		Williams, 1996	
$HSO_5^- + Fe^{2+} \rightarrow [Fe(OH)]^{2+} + SO_4^{\bullet-}$	R(43)	$3.0\ 10^4$		Gilbert and Stell, 1990	
$SO_4^{\bullet-} + Fe^{2+} \rightarrow Fe^{3+} + SO_4^{2-}$	R(44)	$4.1\ 10^9$	-2165	Buxton et al., 1997	
$O_2^{\bullet-} + [Fe(SO_4)]^+ \rightarrow Fe^{2+} + SO_4^{2-} + O_2$	R(45)	$1.5\ 10^8$		Rush and Bielski, 1985	
$S_2O_8^{2-} + Fe^{2+} \rightarrow Fe^{3+} + SO_4^{\bullet-} + SO_4^{2-}$	R(46)	$1.7\ 10^1$		Buxton et al., 1997	
$HSO_3^- + FeO^{2+} \rightarrow Fe^{3+} + SO_3^{\bullet-} + OH^-$	R(47)	$2.5\ 10^5$		Jacobsen et al., 1998b	
$Fe^{3+} + SO_4^{2-} \rightarrow [Fe(SO_4)]^+$	R(48)	$3.2\ 10^3$		Jayson et al., 1973c	
$[Fe(SO_4)]^+ \rightarrow Fe^{3+} + SO_4^{2-}$	R(49)	$2.7\ 10^1$		Jayson et al., 1973c	
$Fe^{3+} + Cl^- \rightarrow [FeCl]^{2+}$	R(50)	4.8		Xu et al., 1985	
$[FeCl]^{2+} \rightarrow Fe^{3+} + Cl^-$	R(51)	$9.2\ 10^{-1}$		Estimated following Nadtochenko and Kiwi, 1998	2
$HO^\bullet + Cu^+ \rightarrow Cu^{2+} + OH^-$	R(52)	$3.0\ 10^9$		Goldstein et al., 1992	
$O_3 + Cu^+ \rightarrow Cu^{2+} + HO^\bullet + O_2 - H^+$	R(53)	$3.0\ 10^7$		Hoigné and Bühler, 1996	
$O_2 + Cu^+ \rightarrow Cu^{2+} + O_2^{\bullet-}$	R(54)	$4.6\ 10^5$		Bjergbakke et al., 1976	
$H_2O_2 + Cu^+ \rightarrow Cu^{2+} + HO^\bullet + OH^-$	R(55)	$7.0\ 10^3$		Berdnikov, 1973	
$HO_2^\bullet + Cu^+ \rightarrow Cu^{2+} + H_2O_2 - H^+$	R(56)	$3.5\ 10^9$		Berdnikov, 1973	

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$O_2^{\bullet-} + Cu^+ \rightarrow Cu^{2+} + H_2O_2$ - 2 H^+	R(57)	9.4 10^9		Piechowski et al., 1993	
$HO_2^{\bullet} + Cu^{2+} \rightarrow Cu^+ + O_2 + H^+$	R(58)	1.0 10^8		Rabani et al., 1973	
$O_2^{\bullet-} + Cu^{2+} \rightarrow Cu^+ + O_2$	R(59)	8.0 10^9		Rabani et al., 1973	
$Cl_2^{\bullet-} + Cu^+ \rightarrow Cu^{2+} + 2\ Cl^-$	R(60)	1.0 10^7	3060		= k($Cl_2^{\bullet-}$ + Fe^{2+})
$SO_4^{\bullet-} + Cu^+ \rightarrow Cu^{2+} + SO_4^{2-}$	R(61)	4.1 10^9	-2165		= k($SO_4^{\bullet-}$ + Fe^{2+})
$Cu^{2+} + HO^{\bullet} \rightarrow [Cu(OH)]^{2+}$	R(62)	3.5 10^8		Meyerstein, 1971	
$[Cu(OH)]^{2+} \rightarrow Cu^{2+} + HO^{\bullet}$	R(63)	3.0 10^4		Meyerstein, 1971	
$Fe^{3+} + Cu^+ \rightarrow Fe^{2+} + Cu^{2+}$	R(64)	1.3 10^7		Buxton et al., 1995	
$[Fe(OH)]^{2+} + Cu^+ \rightarrow Fe^{2+} + Cu^{2+} + OH^-$	R(65)	1.3 10^7			= k(Fe^{3+} + Cu^+)
$[Fe(OH)_2]^+ + Cu^+ \rightarrow Fe^{2+} + Cu^{2+} + 2\ OH^-$	R(66)	1.3 10^7			= k(Fe^{3+} + Cu^+)
$HO^{\bullet} + Mn^{2+} \rightarrow [Mn(OH)]^{2+}$	R(67)	2.0 10^7		Jacobsen et al., 1997b	
$O_3 + Mn^{2+} \rightarrow MnO^{2+} + O_2$	R(68)	1.6 10^3	4750	Jacobsen et al., 1998a	
$MnO^{2+} + Mn^{2+} \rightarrow 2\ Mn^{3+} + H_2O$ - 2 H^+	R(69)	1.0 10^5		Jacobsen et al., 1998a	
$MnO_2^+ + MnO_2^+ \rightarrow 2\ Mn^{2+} + H_2O_2 + O_2$ - 2 H^+	R(70)	6.0 10^6		Jacobsen et al., 1997b	
$HO_2^{\bullet} + MnO_2^+ \rightarrow Mn^{2+} + H_2O_2 + O_2$ - H^+	R(71)	1.0 10^7		Jacobsen et al., 1997b	
$H_2O_2 + Mn^{3+} \rightarrow Mn^{2+} + HO_2^{\bullet} + H^+$	R(72)	7.3 10^4		Davies, 1969	
$H_2O_2 + [Mn(OH)]^{2+} \rightarrow MnO_2^+ + H^+ + H_2O$	R(73)	2.8 10^3		Jacobsen et al., 1997b	
$H_2O_2 + Mn^{4+} \rightarrow Mn^{2+} + O_2 + 2\ H^+$	R(74)	1.2 10^8		Jacobsen et al., 1998a	
$NO_3^{\bullet} + Mn^{2+} \rightarrow Mn^{3+} + NO_3^-$	R(75)	1.1 10^6		Neta and Huie, 1986	
$Cl_2^{\bullet-} + Mn^{2+} \rightarrow Mn^{3+} + 2\ Cl^-$	R(76)	8.5 10^6	4090	Laurence and Thornton, 1973	
$Cl_2^{\bullet-} + Mn^{2+} \rightarrow MnCl_2^+$	R(77)	2.0 10^7	4090	Laurence and Thornton, 1973	
$[MnCl_2]^+ \rightarrow Mn^{2+} + Cl_2^{\bullet-}$	R(78)	3.0 10^5		Laurence and Thornton, 1973	
$[MnCl_2]^+ \rightarrow Mn^{3+} + 2\ Cl^-$	R(79)	2.1 10^5	2100	Laurence and Thornton, 1973	
$HSO_5^- + Mn^{2+} \rightarrow Mn^{3+} + SO_4^- + OH^-$	R(80)	3.0 10^4			= k(HSO_5^- + Fe^{2+})
$SO_4^{\bullet-} + Mn^{2+} \rightarrow Mn^{3+} + SO_4^{2-}$	R(81)	1.8 10^7	4100	Buxton et al., 1997	
$SO_5^{\bullet-} + Mn^{2+} \rightarrow Mn^{3+} + HSO_5^- + OH^-$ - H_2O	R(82)	1.0 10^8		Fronaeus et al., 1998	
$[MnHSO_3]^+ + Mn^{3+} \rightarrow 2\ Mn^{2+} + SO_3^- + H^+$	R(83)	1.3 10^6		Berglund et al., 1993	
$CO_3^{\bullet-} + Mn^{2+} \rightarrow Mn^{3+} + CO_3^{2-}$	R(84)	1.5 10^7		Cope et al., 1978	
$Mn^{3+} + Fe^{2+} \rightarrow Mn^{2+} + Fe^{3+}$	R(85)	1.3 10^4		Davies, 1969	
$[Mn(OH)]^{2+} + Fe^{2+} \rightarrow Mn^{2+} + [Fe(OH)]^{2+}$	R(86)	2.1 10^4		Davies, 1969	
$Mn^{2+} + FeO^{2+} \rightarrow Mn^{3+} + Fe^{3+} + H_2O$ - 2 H^+	R(87)	1.0 10^4	2700	Jacobsen et al., 1998a	
$Mn^{2+} + O_2^{\bullet-} \rightarrow MnO_2^+$	R(88)	9.5 10^7		Jacobsen et al., 1997b	
$MnO_2^+ \rightarrow Mn^{2+} + O_2^{\bullet-}$	R(89)	7.5 10^3		Jacobsen et al., 1997b	
$Mn^{2+} + HO_2^{\bullet} \rightarrow MnO_2^+ + H^+$	R(90)	1.4 10^6		Jacobsen et al., 1997b	

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$MnO_2^+ + H^+ \rightarrow Mn^{2+} + HO_2^\bullet$	R(91)	$1.4\ 10^7$		Jacobsen et al., 1997b	
$Mn^{3+} + Mn^{3+} \rightarrow Mn^{2+} + Mn^{4+}$	R(92)	$1.0\ 10^7$			3
$Mn^{2+} + Mn^{4+} \rightarrow Mn^{3+} + Mn^{3+}$	R(93)	$1.0\ 10^7$			3
$Mn^{2+} + HSO_3^- \rightarrow [MnHSO_3]^+$	R(94)	$3.0\ 10^7$		Berglund et al., 1993	
$[MnHSO_3]^+ \rightarrow Mn^{2+} + HSO_3^-$	R(95)	$1.0\ 10^3$		Berglund et al., 1993	
Chlorine chemistry					
$HO^\bullet + Cl^- \rightarrow OHCl^-$	R(96)	$4.3\ 10^9$		Jayson et al., 1973b	
$OHCl^- \rightarrow Cl^- + HO^\bullet$	R(97)	$6.1\ 10^9$		Jayson et al., 1973b	
$Cl^\bullet \rightarrow OHCl^- + H^+ - H_2O$	R(98)	$1.7\ 10^5$		Yu, 2004	
$OHCl^- + H^+ \rightarrow Cl^\bullet + H_2O$	R(99)	$3.3\ 10^{10}$		Yu and Barker, 2003	
$Cl^\bullet + Cl^- \rightarrow Cl_2^{\bullet-}$	R(100)	$7.8\ 10^9$		Yu and Barker, 2003	
$Cl_2^{\bullet-} \rightarrow Cl^\bullet + Cl^-$	R(101)	$5.7\ 10^4$		Yu and Barker, 2003	
$Cl_2^{\bullet-} \rightarrow OHCl^- + Cl^- + H^+ - H_2O$	R(102)	$1.3.10^3$		Yu, 2004	
$Cl_2^{\bullet-} + OH^- \rightarrow OHCl^- + Cl^-$	R(103)	$2.0\ 10^7$		Grigor'ev et al., 1987	
$OHCl^- + Cl^- \rightarrow Cl_2^{\bullet-} + OH^-$	R(104)	$1.0\ 10^4$		Grigor'ev et al., 1987	
$Cl_2^{\bullet-} + Cl_2^{\bullet-} \rightarrow Cl_2 + 2\ Cl^-$	R(105)	$9.0\ 10^8$		Yu, 2004	
$Cl_2^{\bullet-} + Cl^\bullet \rightarrow Cl_2 + Cl^-$	R(106)	$2.1\ 10^9$		Yu, 2004	
$Cl_2 \rightarrow Cl^- + HOCl + H^+ - H_2O$	R(107)	$2.2\ 10^1$	7600	Wang and Margerum, 1994	
$Cl^- + HOCl + H^+ \rightarrow Cl_2 + H_2O$	R(108)	$2.1\ 10^4$	3500	Wang and Margerum, 1994	
$HOCl + HO_2^\bullet \rightarrow Cl^\bullet + O_2 + H_2O$	R(109)	$7.5\ 10^6$			= k($HOCl + O_2^{\bullet-}$)
$HOCl + O_2^{\bullet-} \rightarrow Cl^\bullet + O_2 + OH^-$	R(110)	$7.5\ 10^6$		Long and Bielski, 1980	
$Cl_2 + HO_2^\bullet \rightarrow Cl_2^{\bullet-} + O_2 + H^+$	R(111)	$1.0\ 10^9$		Bjergbakke et al., 1981	
$Cl_2 + O_2^{\bullet-} \rightarrow Cl_2^{\bullet-} + O_2$	R(112)	$1.0\ 10^9$			= k($Cl_2 + HO_2^\bullet$)
$HO_2^\bullet + Cl^\bullet \rightarrow Cl^- + O_2 + H^+$	R(113)	$3.1\ 10^9$	1500	Graedel and Goldberg, 1983	
$H_2O_2 + Cl^\bullet \rightarrow Cl^- + HO_2^\bullet + H^+$	R(114)	$2.0\ 10^9$		Yu and Barker, 2003	
$Cl^- + NO_3^\bullet \rightarrow NO_3^- + Cl^\bullet$	R(115)	$1.0\ 10^7$	4300	Exner et al., 1992	
$NO_3^- + Cl^\bullet \rightarrow Cl^- + NO_3^\bullet$	R(116)	$1.0\ 10^8$		Buxton et al., 2000	
$SO_4^{\bullet-} + Cl^- + \rightarrow SO_4^{2-} + Cl^\bullet$	R(117)	$2.5\ 10^8$		Buxton et al., 1999	
$SO_4^{2-} + Cl^\bullet \rightarrow SO_4^{\bullet-} + Cl^-$	R(118)	$2.1\ 10^8$		Buxton et al., 1999	
$HO^\bullet + Cl_2^{\bullet-} \rightarrow OHCl + Cl^-$	R(119)	$1.0\ 10^9$		Wagner et al., 1986	
$HO_2^\bullet + Cl_2^{\bullet-} \rightarrow O_2 + 2\ Cl^- + H^+$	R(120)	$1.3\ 10^{10}$		Jacobi et al., 1996	
$O_2^{\bullet-} + Cl_2^{\bullet-} \rightarrow O_2 + 2\ Cl^-$	R(121)	$6.0\ 10^9$		Jacobi et al., 1996	
$H_2O_2 + Cl_2^{\bullet-} \rightarrow 2\ Cl^- + HO_2^\bullet + H^+$	R(122)	$6.2\ 10^6$		Yu, 2004	
$O_3 + Cl_2^{\bullet-} \rightarrow OHCl + Cl^\bullet + O_2 + OH^- - H_2O$	R(123)	$9.0\ 10^7$		Bielski, 1993	
$HSO_3^- + Cl_2^{\bullet-} \rightarrow SO_3^{\bullet-} + 2\ Cl^- + H^+$	R(124)	$1.7\ 10^8$	400	Jacobi et al., 1996	

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$SO_3^{2-} + Cl_2^{\bullet-} \rightarrow SO_3^{\bullet-} + 2\ Cl^-$	R(125)	$6.2\ 10^7$		Jacobi et al., 1996	
Carbonate chemistry					
$HCO_3^- + HO^\bullet \rightarrow CO_3^{\bullet-} + H_2O$	R(126)	$4.2\ 10^8$	2840		= $k(CO_3^{2-} + HO^\bullet)$
$CO_3^{2-} + HO^\bullet \rightarrow CO_3^{\bullet-} + OH^-$	R(127)	$4.2\ 10^8$	2840	Buxton et al., 1988	
$HCO_3^- + SO_4^{\bullet-} \rightarrow SO_4^{2-} + CO_3^{\bullet-} + H^+$	R(128)	$2.8\ 10^6$	2100	Huie and Clifton, 1990	
$CO_3^{2-} + SO_4^{\bullet-} \rightarrow SO_4^{2-} + CO_3^{\bullet-}$	R(129)	$4.1\ 10^6$	3200	Padmaja et al., 1993	
$HCO_3^- + Cl^\bullet \rightarrow Cl^- + CO_3^{\bullet-} + H^+$	R(130)	$2.4\ 10^9$		Buxton et al., 2000	
$CO_3^{2-} + Cl^\bullet \rightarrow Cl^- + CO_3^{\bullet-}$	R(131)	$5.0\ 10^8$		Mertens and Von Sonntag, 1995	
$CO_3^{\bullet-} + CO_3^{\bullet-} \rightarrow 2\ O_2^{\bullet-} + 2\ CO_2 - O_2$	R(132)	$2.2\ 10^6$		Huie and Clifton, 1990	
$CO_3^{\bullet-} + HO_2^\bullet \rightarrow HCO_3^- + O_2$	R(133)	$5.6\ 10^7$		Behar et al., 1970	
$CO_3^{\bullet-} + O_2^{\bullet-} \rightarrow CO_3^{2-} + O_2$	R(134)	$6.5\ 10^8$		Eriksen et al., 1985	
$CO_3^{\bullet-} + H_2O_2 \rightarrow HO_2^\bullet + HCO_3^-$	R(135)	$4.3\ 10^5$		Draganic et al., 1991	
$CO_3^{\bullet-} + SO_3^{2-} \rightarrow CO_3^{2-} + SO_3^{\bullet-}$	R(136)	$2.9\ 10^7$	470	Huie et al., 1991	
$CO_3^{\bullet-} + O_3 \rightarrow CO_2 + O_2^{\bullet-} + O_2$	R(137)	$1.0\ 10^5$		Sehested et al., 1983	
$CO_3^{\bullet-} + NO_2 \rightarrow CO_2 + NO_3^-$	R(138)	$1.0\ 10^9$		Lilie et al., 1978	
N chemistry					
$HNO_2 + h\nu \rightarrow NO + HO^\bullet$	R(139)	Calculated		Graedel and Weschler, 1981	
$NO_2^- + h\nu + H_2O \rightarrow NO + HO^\bullet + OH^-$	R(140)	Calculated		Graedel and Weschler, 1981 ; Zellner et al., 1990	
$HNO_2 + HO^\bullet \rightarrow NO_2 + H_2O$	R(141)	$1.0\ 10^{10}$		Barker et al., 1970	
$NO_2^- + HO^\bullet \rightarrow NO_2 + OH^-$	R(142)	$9.1\ 10^9$		Barker et al., 1970	
$HNO_2 + H_2O_2 + H^+ \rightarrow NO_3^- + 2\ H^+ + H_2O$	R(143)	$6.3\ 10^3$	6700	Lee and Lind, 1986	
$NO_2^- + O_3 \rightarrow NO_3^- + O_2$	R(144)	$5.0\ 10^5$	6900	Damschen and Martin, 1983	
$HNO_2 + NO_3^\bullet \rightarrow NO_2 + NO_3^- + H^+$	R(145)	$8.0\ 10^6$		Katsumura, 1998	
$NO_2^- + NO_3^\bullet \rightarrow NO_2 + NO_3^-$	R(146)	$1.4\ 10^9$		Herrmann and Zellner, 1998	
$NO_2^- + CO_3^{\bullet-} \rightarrow NO_2 + CO_3^{2-}$	R(147)	$6.6\ 10^5$	850	Huie et al., 1991	
$NO_2^- + Cl^\bullet \rightarrow NO_2 + Cl^-$	R(148)	$5.0\ 10^9$		Buxton et al., 2000	
$NO_2 + HO^\bullet \rightarrow NO_3^- + H^+$	R(149)	$1.2\ 10^{10}$		Wagner et al., 1980	
$NO_2 + HO_2^\bullet \rightarrow HNO_4$	R(150)	$1.8\ 10^9$		Logager and Sehested, 1993	
$NO_2 + O_2^{\bullet-} \rightarrow NO_4^-$	R(151)	$4.5\ 10^9$		Logager and Sehested, 1993	
$HNO_4 \rightarrow HO_2^\bullet + NO_2$	R(152)	$2.6\ 10^{-2}$		Goldstein and Czapski, 1997	
$HNO_4 \rightarrow HNO_2 + O_2$	R(153)	$7.0\ 10^{-4}$		Logager and	

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
				Sehested, 1993	
$NO_4^- \rightarrow NO_2^- + O_2$	R(154)	1.1		Goldstein and Czapski, 1997	
$NO_4^- \rightarrow NO_2 + O_2^{\bullet-}$	R(155)	1.3		Goldstein and Czapski, 1997	
$HNO_4 + HSO_3^- \rightarrow SO_4^{2-} + NO_3^- + 2\ H^+$	R(156)	$3.3\ 10^5$		Amels et al., 1996	
$NO_2 + NO_2 \rightarrow HNO_2 + NO_3^- + H^+ - H_2O$	R(157)	$8.4\ 10^7$	-2900	Park and Lee, 1988	
$NO_2 + NO \rightarrow 2\ NO_2^- + 2H^+ - H_2O$	R(158)	$3.0\ 10^8$		Hoffmann and Calvert, 1985	
$NO + HO^{\bullet} \rightarrow NO_2^- + H^+$	R(159)	$2.0\ 10^{10}$	1500	Strehlow and Wagner, 1982	
$NO_3^- + h\nu \rightarrow NO_2 + HO^{\bullet} + OH^- - H_2O$	R(160)	Calculated		Graedel and Weschler, 1981 ; Zellner et al., 1990	
$N_2O_5 \rightarrow 2\ HNO_3 - H_2O$	R(161)	$1.0\ 10^6$		Estimated	4
$NO_3^{\bullet} + h\nu \rightarrow NO + O_2$	R(162)	Calculated		Graedel and Weschler, 1981	
$NO_3^{\bullet} + HO_2^{\bullet} \rightarrow NO_3^- + H^+ + O_2$	R(163)	$3.0\ 10^9$		Sehested et al., 1994	
$NO_3^{\bullet} + O_2^{\bullet-} \rightarrow NO_3^- + O_2$	R(164)	$3.0\ 10^9$			= $k(NO_3^{\bullet} + HO_2^{\bullet})$
$NO_3^{\bullet} + OH^- \rightarrow NO_3^- + HO^{\bullet}$	R(165)	$9.4\ 10^7$	2700	Exner et al., 1992	
$NO_3^{\bullet} + H_2O_2 \rightarrow NO_3^- + H^+ + HO_2^{\bullet}$	R(166)	$4.9\ 10^6$	2000	Herrmann et al., 1994	
$NO_3^{\bullet} + HSO_4^- \rightarrow NO_3^- + H^+ + SO_4^{\bullet-}$	R(167)	$2.6\ 10^5$		Raabe, 1996	
$NO_3^{\bullet} + SO_4^{2-} \rightarrow NO_3^- + SO_4^{\bullet-}$	R(168)	$1.0\ 10^5$		Logager and Sehested, 1993	
$NO_3^{\bullet} + HSO_3^- \rightarrow SO_3^{\bullet-} + NO_3^- + H^+$	R(169)	$1.3\ 10^9$	2200	Exner et al., 1992	
$NO_3^{\bullet} + SO_3^{2-} \rightarrow NO_3^- + SO_3^{\bullet-}$	R(170)	$3.0\ 10^8$		Exner et al., 1992	
S chemistry					
$HSO_3^- + CH_2O \rightarrow CH_2(OH)SO_3^-$	R(171)	$7.9\ 10^2$	2990	Olson and Hoffmann, 1989	
$SO_3^{2-} + CH_2(OH)(OH) \rightarrow CH_2(OH)SO_3^- + OH^-$	R(172)	$2.5\ 10^7$	2450	Olson and Hoffmann, 1989	
$CH_2(OH)SO_3^- \rightarrow HSO_3^- + CH_2O$	R(173)	$7.7\ 10^{-3}$	9200	Möller and Mauersberger, 1995	
$CH_2(OH)SO_3^- + OH^- \rightarrow SO_3^{2-} + CH_2(OH)(OH)$	R(174)	$3.7\ 10^3$		Deister et al., 1986	
$CH_2(OH)SO_3^- + HO^{\bullet} \rightarrow HO_2^{\bullet} + CHO(OH) + HSO_3^- - O_2$	R(175)	$3.0\ 10^8$		Buxton, 1994	
$CH_2(OH)SO_3^- + NO_3^{\bullet} \rightarrow NO_3^- + SO_4^{2-} + 2\ H^+ + CH_2(OH)(OO^{\bullet}) - H_2O - O_2$	R(176)	$4.2\ 10^6$		Herrmann et al., 1996	
$CH_2(OH)SO_3^- + Cl_2^{\bullet-} \rightarrow 2\ Cl^- + SO_4^{2-} + 2\ H^+ + CH_2(OH)(OO^{\bullet}) - H_2O - O_2$	R(177)	$5.0\ 10^5$		Jacobi et al., 1996	
$CH_2(OH)SO_3^- + SO_4^{\bullet-} \rightarrow 2\ SO_4^{2-} + 2\ H^+ + CH_2(OH)(OO^{\bullet}) - H_2O - O_2$	R(178)	$2.8\ 10^6$		Buxton, 1994	
$SO_3^{\bullet-} + O_2 \rightarrow SO_5^{\bullet-}$	R(179)	$1.1\ 10^9$		Das, 2001	
$SO_3^{\bullet-} + SO_3^{\bullet-} \rightarrow S_2O_6^{2-}$	R(180)	$1.6\ 10^7$	1200	Buxton et al., 1996c	

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$SO_5^{\bullet-} + HSO_3^- \rightarrow HSO_5^- + SO_3^{\bullet-}$	R(181)	$8.6\ 10^3$		Buxton et al., 1996c	
$SO_5^{\bullet-} + HSO_3^- \rightarrow SO_4^{\bullet-} + SO_4^{2-} + H^+$	R(182)	$3.6\ 10^2$		Buxton et al., 1996c	
$SO_5^{\bullet-} + SO_3^{2-} \rightarrow HSO_5^- + SO_3^- + OH^- - H_2O$	R(183)	$2.1\ 10^5$		Buxton et al., 1996c	
$SO_5^{\bullet-} + SO_3^{2-} \rightarrow SO_4^{\bullet-} + SO_4^{2-}$	R(184)	$5.5\ 10^5$		Buxton et al., 1996c	
$SO_5^{\bullet-} + HO_2^{\bullet} \rightarrow HSO_5^- + O_2$	R(185)	$1.7\ 10^9$		Buxton et al., 1996a	
$SO_5^{\bullet-} + O_2^{\bullet-} \rightarrow HSO_5^- + O_2 + OH^- - H_2O$	R(186)	$2.3\ 10^8$		Buxton et al., 1996c	
$SO_5^{\bullet-} + SO_5^{\bullet-} \rightarrow 2\ SO_4^{\bullet-} + O_2$	R(187)	$2.1\ 10^8$		Das, 2001	
$SO_5^{\bullet-} + SO_5^{\bullet-} \rightarrow S_2O_8^{2-} + O_2$	R(188)	$2.2\ 10^8$		Das, 2001	
$HSO_5^- + HSO_3^- + H^+ \rightarrow 2\ SO_4^{2-} + 3\ H^+$	R(189)	$1.0\ 10^7$		Das, 2001	
$HSO_5^- + SO_3^{2-} + H^+ \rightarrow 2\ SO_4^{2-} + 2\ H^+$	R(190)	$1.0\ 10^7$			$= k(HSO_5^- + HSO_3^-)$
$HSO_5^- + HO^{\bullet} \rightarrow SO_5^{\bullet-} + H_2O$	R(191)	$5.0\ 10^6$		Das, 2001	
$HSO_5^- + SO_4^{\bullet-} \rightarrow SO_5^{\bullet-} + HSO_4^-$	R(192)	$1.0\ 10^6$		Das, 2001	
$SO_4^{\bullet-} + SO_4^{\bullet-} \rightarrow S_2O_8^{2-}$	R(193)	$7.0\ 10^8$		Das, 2001	
$SO_4^{\bullet-} \rightarrow HSO_4^- + HO^{\bullet} - H_2O$	R(194)	$4.6\ 10^2$	1100	Herrmann et al., 1995	
$SO_4^{\bullet-} + HSO_3^- \rightarrow SO_4^{2-} + H^+ + SO_3^{\bullet-}$	R(195)	$6.8\ 10^8$		Buxton et al., 1996c	
$SO_4^{\bullet-} + SO_3^{2-} \rightarrow SO_4^{2-} + SO_3^{\bullet-}$	R(196)	$3.1\ 10^8$	1200	Buxton et al., 1996c	
$SO_4^{\bullet-} + HO^{\bullet} \rightarrow HSO_5^-$	R(197)	$9.0\ 10^9$		Buxton et al., 1996c	
$SO_4^{\bullet-} + HO_2^{\bullet} \rightarrow SO_4^{2-} + H^+ + O_2$	R(198)	$3.5\ 10^9$		Jiang et al., 1992	
$SO_4^{\bullet-} + O_2^{\bullet-} \rightarrow SO_4^{2-} + O_2$	R(199)	$4.0\ 10^9$		Buxton et al., 1996c	
$SO_4^{\bullet-} + OH^- \rightarrow SO_4^{2-} + HO^{\bullet}$	R(200)	$2.0\ 10^7$		Ross et al., 1994	
$SO_4^{\bullet-} + H_2O_2 \rightarrow SO_4^{2-} + HO_2^{\bullet} + H^+$	R(201)	$1.2\ 10^7$		Maruthamuthu and Neta, 1978	
$SO_4^{\bullet-} + NO_3^- \rightarrow SO_4^{2-} + NO_3^{\bullet}$	R(202)	$5.0\ 10^4$		Exner et al., 1992	
$HSO_4^- + HO^{\bullet} \rightarrow H_2O + SO_4^{\bullet-}$	R(203)	$3.5\ 10^5$		Tang et al., 1988	
$SO_4^{\bullet-} \rightarrow HSO_4^- + HO^{\bullet} - H_2O$	R(204)	$3.6\ 10^2$		Tang et al., 1988	
$HSO_3^- + O_3 \rightarrow HSO_4^- + O_2$	R(205)	$3.7\ 10^5$	5500	Hoffmann, 1986	
$SO_3^{2-} + O_3 \rightarrow SO_4^{2-} + O_2$	R(206)	$1.5\ 10^9$	5300	Hoffmann, 1986	
$HSO_3^- + H_2O_2 \rightarrow SO_4^{2-} + 2\ H^+ + H_2O - H^+$	R(207)	$9.1\ 10^7$	3600	Maaß et al., 1999	

1 - Sehested et al. (1984) argue that this reaction is very slow with a rate constant lower than 10^4 M^{-1} s^{-1}.

2 - Xu et al. (1985) calculated $k(Fe^{3+} + Cl^-) = 4.8$ M^{-1} s^{-1}. The equilibrium constant from Nadtochenko and Kiwi (1998) is equal to 5.3 M^{-1}. Therefore we calculate the backward rate constant by 4.8/5.3 = $9.1\ 10^{-1}$ s^{-1}.

3 - The equilibrium constant $2\ Mn^{3+} \leftrightarrow Mn^{2+} + Mn^{4+}$ is evaluated by Jacobsen et al. (1998b) and Rosseinski (1963) between 100 and 10^{-2}. We decide to suppose a value of 1. The forward and backward rate constants are supposed to be rapid following Rosseinski (1963) and are set at 10^7 M^{-1} s^{-1}.

4 - We suppose that the N_2O_5 hydrolysis is fast with a first order rate constant equal to 10^6 s^{-1} (Bertram and Thornton, 2009).

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Equilibria

Species		K_a or K_h	-ΔH/R (K)	References	Notes
$H_2O_2 \leftrightarrow HO_2^- + H^+$	T(1)	$2.2\ 10^{-12}$	-3730	Smith and Martell, 1976	
$HO_2^\bullet \leftrightarrow O_2^{\bullet-} + H^+$	T(2)	$1.6\ 10^{-5}$		Bielski et al., 1985	
$HNO_2 \leftrightarrow NO_2^- + H^+$	T(3)	$1.6\ 10^{-3}$	1760	Park and Lee, 1988; Riordan et al., 2005	
$HNO_3 \leftrightarrow NO_3^- + H^+$	T(4)	$2.2\ 10^{1}$		N.B.S, 1965	
$HNO_4 \leftrightarrow NO_4^- + H^+$	T(5)	$1.3\ 10^{-6}$		Goldstein and Czapski, 1997	
$NH_3 + H_2O \leftrightarrow NH_4^+ + OH^-$	T(6)	$1.7\ 10^{-5}$	560	N.B.S, 1965	
$HCl \leftrightarrow Cl^- + H^+$	T(7)	$1.7\ 10^{6}$	-6890	Marsh and McElroy, 1985	
$SO_2 + H_2O \leftrightarrow HSO_3^- + H^+$	T(8)	$1.3\ 10^{-2}$	-1960	Maash, 1982	
$HSO_3^- \leftrightarrow SO_3^{2-} + H^+$	T(9)	$6.4\ 10^{-8}$	-1430	Maash, 1982	
$H_2SO_4 \leftrightarrow HSO_4^- + H^+$	T(10)	$1.0\ 10^{3}$		Cotton and Wilkinson, 1980	
$HSO_4^- \leftrightarrow SO_4^{2-} + H^+$	T(11)	$1.0\ 10^{-2}$		Eigen et al., 1964	
$Fe^{3+} + H_2O \leftrightarrow [Fe(OH)]^{2+} + H^+$	T(12)	$6.0\ 10^{-3}$		Brandt and van Eldik, 1995	
$[Fe(OH)]^{2+} + H_2O \leftrightarrow [Fe(OH)_2]^+ + H^+$	T(13)	$7.6\ 10^{-4}$		Brandt and van Eldik, 1995	
$Mn^{3+} + H_2O \leftrightarrow [Mn(OH)]^{2+} + H^+$	T(14)	$9.1\ 10^{-1}$		Wells and Davies, 1967	
$[Mn(OH)]^{2+} + H_2O \leftrightarrow [Mn(OH)_2]^+ + H^+$	T(15)	$1.0\ 10^{-5}$		Baral et al., 1986	
$CO_2 + H_2O \leftrightarrow HCO_3^- + H^+$	T(16)	$4.2\ 10^{-7}$		Cotton and Wilkinson, 1980	
$HCO_3^- \leftrightarrow CO_3^{2-} + H^+$	T(17)	$4.8\ 10^{-11}$		Cotton and Wilkinson, 1980	

Henry's law constants

Species		H (298K) ($M\ atm^{-1}$)	-ΔH/R (K)	References	Notes
Inorganic compounds					
O_2	T(1)	$1.3\ 10^{-3}$	1500	Lide and Frederikse, 1995	
O_3	T(2)	$1.0\ 10^{-2}$	2830	Sander, 2014	
$HO_2^{\bullet}$	T(3)	$6.9\ 10^{2}$	6640	Sander, 2014	
$HO^{\bullet}$	T(4)	$3.9\ 10^{1}$		Sander, 2014	
H_2O_2	T(5)	$7.7\ 10^{4}$	7310	Sander, 2014	
NO_2	T(6)	$1.4\ 10^{-2}$	2520	Sander, 2014	
NO	T(7)	$1.9\ 10^{-3}$	1790	Sander, 2014	
$NO_3^{\bullet}$	T(8)	$3.8\ 10^{-2}$		Sander, 2014	
N_2O_5	T(9)	2.1	3400	Fried et al., 1994	
HNO_2	T(10)	$4.9\ 10^{1}$	4880	Becker et al., 1996	
HNO_3	T(11)	$2.1\ 10^{5}$	8700	Schwartz and White, 1981	
HNO_4	T(12)	$1.2\ 10^{4}$	6900	Régimbal and Mozurkewich, 1997	
NH_3	T(13)	$6.0\ 10^{1}$	4160	Sander, 2014	
HCl	T(14)	1.1	2020	Marsh and McElroy, 1985	
SO_2	T(15)	1.4	2900	Lide and Frederikse, 1995	
H_2SO_4	T(16)	$2.1\ 10^{5}$	8700		= $H_{298}(HNO_3)$
CO_2	T(17)	$3.4\ 10^{-2}$	2710	Sander, 2014	

Accommodation coefficients

Species		α (298K)	-ΔH (J/mol)	--ΔS (J/mol/K)	References	Notes
O_2	T(1)	$5.0\ 10^{-2}$			Estimated	1
O_3	T(2)	$4.0\ 10^{-2}$			Müller and Heal, 2002	
$HO_2^{\bullet}$	T(3)	$2.0\ 10^{-1}$			Sander, 2014	
$HO^{\bullet}$	T(4)	$5.0\ 10^{-2}$			Estimated	1
H_2O_2	T(5)	$1.1\ 10^{-1}$	$2.3\ 10^{4}$	$9.4\ 10^{1}$	Davidovits et al., 2011	
HCl	T(6)	$6.7\ 10^{-2}$	$3.0\ 10^{4}$	$1.2\ 10^{2}$	Davidovits et al., 2011	
NO_2	T(7)	$1.5\ 10^{-3}$			Ponche et al., 1993	
NO	T(8)	$1.0\ 10^{-4}$			Saastad et al., 1993	
$NO_3^{\bullet}$	T(9)	$5.0\ 10^{-2}$			Sander, 2014	1
N_2O_5	T(10)	$3.7\ 10^{-3}$			George et al., 1994	
NH_3	T(11)	$4.0\ 10^{-2}$			Bongartz et al., 1995	
HNO_2	T(12)	$5.0\ 10^{-2}$			Bongartz et al., 1995a	
HNO_3	T(13)	$6.1\ 10^{-2}$	$2.8\ 10^{4}$	$1.2\ 10^{2}$	Davidovits et al., 2011	
HNO_4	T(14)	$5.0\ 10^{-2}$			Estimated	1
SO_2	T(15)	$1.3\ 10^{-1}$	$3.2\ 10^{4}$	$1.2\ 10^{2}$	Davidovits et al., 2011	
H_2SO_4	T(16)	$7.0\ 10^{-2}$			Davidovits et al., 1995	
CO_2	T(17)	$2.0\ 10^{-4}$			Schurath et al., 1996	

1 - Estimated equal to 0.05 following Lelieveld and Crutzen, (1991) and Davidovits et al., (2011).

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