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

C1 compounds

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
Oxidation of HMHP - HydroxyMethyl HydroPeroxide					
$CH_2(OOH)(OH) + h\nu \rightarrow CHO(OH) + HO^\bullet + HO_2^\bullet - O_2$	R(208)	Calculated			= $J(H_2O_2)$
Pathway 1: $CH_2(OOH)(OH) + HO^\bullet \rightarrow CH_2(OH)(OO^\bullet) + H_2O$		$5.0\ 10^8$			BR: 80% - 1
Pathway 2: $CH_2(OOH)(OH) + HO^\bullet \rightarrow C^\bullet H(OOH)(OH) + H_2O$		$1.3\ 10^8$			BR: 20% - 1
$C^\bullet H(OOH)(OH) + O_2 \rightarrow CH(OOH)(OH)(OO^\bullet)$		$2.0\ 10^9$			2
$CH_2(OOH)(OH) + HO^\bullet \rightarrow 0.80\ CH_2(OH)(OO^\bullet) + 0.20\ CH(OOH)(OH)(OO^\bullet) + H_2O - 0.20\ O_2$	R(209)	$6.3\ 10^8$			= $k(CH_3(OOH) + HO^\bullet)$ - 1
Pathway 1: $CH_2(OOH)(OH) + NO_3^\bullet \rightarrow CH_2(OH)(OO^\bullet) + NO_3^- + H^+$					BR: 80%
Pathway 2: $CH_2(OOH)(OH) + NO_3^\bullet \rightarrow C^\bullet H(OOH)(OH) + NO_3^- + H^+$					BR: 20%
$C^\bullet H(OOH)(OH) + O_2 \rightarrow CH(OOH)(OH)(OO^\bullet)$		$2.0\ 10^9$			2
$CH_2(OOH)(OH) + NO_3^\bullet \rightarrow 0.80\ CH_2(OH)(OO^\bullet) + 0.20\ CH(OOH)(OH)(OO^\bullet) + NO_3^- + H^+$	R(210)	$4.9\ 10^6$	2000		= $k(H_2O_2 + NO_3^\bullet)$ - 3
Pathway 1: $CH_2(OOH)(OH) + CO_3^{\bullet-} \rightarrow CH_2(OH)(OO^\bullet) + HCO_3^-$					BR: 80%
Pathway 2: $CH_2(OOH)(OH) + CO_3^{\bullet-} \rightarrow C^\bullet H(OOH)(OH) + HCO_3^-$					BR: 20%
$C^\bullet H(OOH)(OH) + O_2 \rightarrow CH(OOH)(OH)(OO^\bullet)$		$2.0\ 10^9$			2
$CH_2(OOH)(OH) + CO_3^{\bullet-} \rightarrow 0.80\ CH_2(OH)(OO^\bullet) + 0.20\ CH(OOH)(OH)(OO^\bullet) + HCO_3^-$	R(211)	$4.3\ 10^5$			= $k(H_2O_2 + CO_3^{\bullet-})$ - 3
Pathway 1: $CH_2(OOH)(OH) + Cl_2^{\bullet-} \rightarrow CH_2(OH)(OO^\bullet) + 2\ Cl^- + H^+$					BR: 80%
Pathway 2: $CH_2(OOH)(OH) + Cl_2^{\bullet-} \rightarrow C^\bullet H(OOH)(OH) + 2\ Cl^- + H^+$					BR: 20%
$C^\bullet H(OOH)(OH) + O_2 \rightarrow CH(OOH)(OH)(OO^\bullet)$		$2.0\ 10^9$			2
$CH_2(OOH)(OH) + Cl_2^{\bullet-} \rightarrow 0.80\ CH_2(OH)(OO^\bullet) + 0.20\ CH(OOH)(OH)(OO^\bullet) + 2\ Cl^- + H^+$	R(212)	$6.2\ 10^6$			= $k\ (H_2O_2 + Cl_2^{\bullet-})$ - 3
Pathway 1: $CH_2(OOH)(OH) + Cl^\bullet \rightarrow CH_2(OH)(OO^\bullet) + Cl^- + H^+$					BR: 80%
Pathway 2: $CH_2(OOH)(OH) + Cl^\bullet \rightarrow C^\bullet H(OOH)(OH) + Cl^- + H^+$					BR: 20%
$C^\bullet H(OOH)(OH) + O_2 \rightarrow CH(OOH)(OH)(OO^\bullet)$		$2.0\ 10^9$			2
$CH_2(OOH)(OH) + Cl^\bullet \rightarrow 0.80\ CH_2(OH)(OO^\bullet) + 0.20\ CH(OOH)(OH)(OO^\bullet) + Cl^- + H^+$	R(213)	$2.0\ 10^9$			= $k(H_2O_2 + Cl^\bullet)$ - 3
Pathway 1: $CH_2(OOH)(OH) + SO_4^{\bullet-} \rightarrow CH_2(OH)(OO^\bullet) + SO_4^{2-} + H^+$					BR: 80%
Pathway 2: $CH_2(OOH)(OH) + SO_4^{\bullet-} \rightarrow C^\bullet H(OOH)(OH) + SO_4^{2-} + H^+$					BR: 20%
$C^\bullet H(OOH)(OH) + O_2 \rightarrow CH(OOH)(OH)(OO^\bullet)$		$2.0\ 10^9$			2
$CH_2(OOH)(OH) + SO_4^{\bullet-} \rightarrow 0.80\ CH_2(OH)(OO^\bullet) + 0.20\ CH(OOH)(OH)(OO^\bullet) + SO_4^{2-} + H^+$	R(214)	$1.2\ 10^7$			= $k(H_2O_2 + SO_4^{\bullet-})$ - 3
$CH_2(OOH)(OH) + Fe^{2+} \rightarrow Fe^{3+} + CHO(OH) + HO_2^\bullet + OH^- - O_2$	R(215)	$1.6\ 10^1$			= $k(CH_3(OOH) + Fe^{2+})$
$CH_2(OH)(OO^\bullet) \rightarrow CH_2O + HO_2^\bullet$	R(216)	$1.0\ 10^1$			4
$CH_2(OH)(OO^\bullet) + OH^- \rightarrow CH_2(O^-)(OO^\bullet) + H_2O$		$2.1\ 10^{10}$	7200	Neta et al., 1990	
$CH_2(O^-)(OO^\bullet) \rightarrow CH_2O + O_2^{\bullet-}$					5
$CH_2(OH)(OO^\bullet) + OH^- \rightarrow CH_2O + O_2^{\bullet-} + H_2O$	R(217)	$2.1\ 10^{10}$	7200	Neta et al., 1990	
$CH_2(OH)(OO^\bullet) + HO_2^\bullet \rightarrow CH_2(OOH)(OH) + O_2$	R(218)	$8.3\ 10^5$	2700		= $k(HO_2^\bullet + HO_2^\bullet)$
$CH_2(OH)(OO^\bullet) + O_2^{\bullet-} \rightarrow CH_2(OOH)(OH) + O_2 + OH^- - H_2O$	R(219)	$9.6\ 10^7$	910		= $k(HO_2^\bullet + O_2^{\bullet-})$
$2\ CH_2(OH)(OO^\bullet) \rightarrow 2\ CHO(OH) + H_2O_2$	R(220)	$7.4\ 10^8$	1400	Huie and Clifton, 1993	
$CH_2(OH)(OO^\bullet) + Fe^{2+} \rightarrow [FeOHCH_2O_2]^{2+}$	R(221)	$5.9\ 10^5$		Khaikin et al., 1996	
$[FeOHCH_2O_2]^{2+} \rightarrow CH_2(OH)(OO^\bullet) + Fe^{2+}$	R(222)	$1.3\ 10^3$		Khaikin et al., 1996	
$[FeOHCH_2O_2]^{2+} \rightarrow Fe^{3+} + CH_2(OOH)(OH) + OH^- - H_2O$	R(223)	$1.0\ 10^2$		Khaikin et al., 1996	
$[FeOHCH_2O_2]^{2+} + H^+ \rightarrow Fe^{3+} + CH_2(OOH)(OH)$	R(224)	$3.0\ 10^4$		Khaikin et al., 1996	
$CH(OOH)(OH)(OO^\bullet) + OH^- \rightarrow CH\ (OOH)(O^-)(OO^\bullet) + H_2O$		$4.0\ 10^9$			
$CH(O^-)(OOH)(OO^\bullet) \rightarrow CHO(OOH) + O_2^{\bullet-}$					5
$CH(OOH)(OH)(OO^\bullet) + OH^- \rightarrow CHO(OOH) + O_2^{\bullet-} + H_2O$	R(225)	$4.0\ 10^9$			= $k(CH_3CH(OH)(OO^\bullet) + OH^-)$
$CH(OOH)(OH)(OO^\bullet) \rightarrow CHO(OOH) + HO_2^\bullet$	R(226)	$1.0\ 10^6$			6

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
Oxidation of Performic acid					
$CHO(OH) + H_2O_2 + H^+ \rightarrow CHO(OOH) + H_2O + H^+$	R(227)	$3.1\ 10^{-4}$	5235	De Filippis et al., 2009	7
$CHO(OOH) + H_2O + H^+ \rightarrow CHO(OH) + H_2O_2 + H^+$	R(228)	$3.8\ 10^{-4}$	5235	De Filippis et al., 2009	7
$CHO(OOH) + H^+ \rightarrow CO_2 + H_2O + H^+$	R(229)	$1.2\ 10^{-3}$	8735	De Filippis et al., 2009	7
Oxidation of MHP (Methyl HydroPeroxide)					
$CH_3(OOH) + h\nu \rightarrow CH_2O + HO^\bullet + HO_2^\bullet - O_2$	R(230)	Calculated			= $J(H_2O_2)$
Pathway 1: $CH_3(OOH) + HO^\bullet \rightarrow CH_3(OO^\bullet) + H_2O$		$5.0\ 10^{8}$			BR: 80% - 8
Pathway 2: $CH_3(OOH) + HO^\bullet \rightarrow C^\bullet H_2(OOH) + H_2O$		$1.3\ 10^{8}$			BR: 20% - 8
$C^\bullet H_2(OOH) + O_2 \rightarrow CH_2(OOH)(OO^\bullet)$		$2.0\ 10^{9}$			2
$CH_3(OOH) + HO^\bullet \rightarrow 0.80\ CH_3(OO^\bullet) + 0.20\ CH_2(OOH)(OO^\bullet) + H_2O - 0.20\ O_2$	R(231)	$6.3\ 10^{8}$		Monod et al., 2007	8
Pathway 1: $CH_3(OOH) + NO_3^\bullet \rightarrow CH_3(OO^\bullet) + NO_3^- + H^+$					BR: 80%
Pathway 2: $CH_3(OOH) + NO_3^\bullet \rightarrow C^\bullet H_2(OOH) + NO_3^- + H^+$					BR: 20%
$C^\bullet H_2(OOH) + O_2 \rightarrow CH_2(OOH)(OO^\bullet)$		$2.0\ 10^{9}$			2
$CH_3(OOH) + NO_3^\bullet \rightarrow 0.80\ CH_3(OO^\bullet) + 0.20\ CH_2(OOH)(OO^\bullet) + NO_3^- + H^+$	R(232)	$4.9\ 10^{6}$	2000		= $k(H_2O_2 + NO_3^\bullet)$ - 3
Pathway 1: $CH_3(OOH) + CO_3^{\bullet-} \rightarrow CH_3(OO^\bullet) + HCO_3^-$					BR: 80%
Pathway 2: $CH_3(OOH) + CO_3^{\bullet-} \rightarrow C^\bullet H_2(OOH) + HCO_3^-$					BR: 20%
$C^\bullet H_2(OOH) + O_2 \rightarrow CH_2(OOH)(OO^\bullet)$		$2.0\ 10^{9}$			2
$CH_3(OOH) + CO_3^{\bullet-} \rightarrow 0.80\ CH_3(OO^\bullet) + 0.20\ CH_2(OOH)(OO^\bullet) + HCO_3^-$	R(233)	$4.3\ 10^{5}$			= $k(H_2O_2 + CO_3^{\bullet-})$ - 3
Pathway 1: $CH_3(OOH) + Cl_2^{\bullet-} \rightarrow CH_3(OO^\bullet) + 2\ Cl^- + H^+$					BR: 80%
Pathway 2: $CH_3(OOH) + Cl_2^{\bullet-} \rightarrow C^\bullet H_2(OOH) + 2\ Cl^- + H^+$					BR: 20%
$C^\bullet H_2(OOH) + O_2 \rightarrow CH_2(OOH)(OO^\bullet)$		$2.0\ 10^{9}$			2
$CH_3(OOH) + Cl_2^{\bullet-} \rightarrow 0.80\ CH_3(OO^\bullet) + 0.20\ CH_2(OOH)(OO^\bullet) + 2\ Cl^- + H^+$	R(234)	$6.2\ 10^{6}$			= $k(H_2O_2 + Cl_2^{\bullet-})$ - 3
Pathway 1: $CH_3(OOH) + Cl^\bullet \rightarrow CH_3(OO^\bullet) + Cl^- + H^+$					BR: 80%
Pathway 2: $CH_3(OOH) + Cl^\bullet \rightarrow C^\bullet H_2(OOH) + Cl^- + H^+$					BR: 20%
$C^\bullet H_2(OOH) + O_2 \rightarrow CH_2(OOH)(OO^\bullet)$		$2.0\ 10^{9}$			2
$CH_3(OOH) + Cl^\bullet \rightarrow 0.80\ CH_3(OO^\bullet) + 0.20\ CH_2(OOH)(OO^\bullet) + Cl^- + H^+$	R(235)	$2.0\ 10^{9}$			= $k(H_2O_2 + Cl^\bullet)$ - 3
Pathway 1: $CH_3(OOH) + SO_4^{\bullet-} \rightarrow CH_3(OO^\bullet) + SO_4^{2-} + H^+$					BR: 80%
Pathway 2: $CH_3(OOH) + SO_4^{\bullet-} \rightarrow C^\bullet H_2(OOH) + SO_4^{2-} + H^+$					BR: 20%
$C^\bullet H_2(OOH) + O_2 \rightarrow CH_2(OOH)(OO^\bullet)$		$2.0\ 10^{9}$			2
$CH_3(OOH) + SO_4^{\bullet-} \rightarrow 0.80\ CH_3(OO^\bullet) + 0.20\ CH_2(OOH)(OO^\bullet) + SO_4^{2-} + H^+$	R(236)	$1.2\ 10^{7}$			= $k(H_2O_2 + SO_4^{\bullet-})$ - 3
$CH_3(OOH) + HSO_3^- \rightarrow CH_3(OH) + SO_4^{2-} + H^+$	R(237)	$1.8\ 10^{7}$	3800	Lind et al., 1987	
$CH_3(OOH) + Fe^{2+} \rightarrow Fe^{3+} + CH_2(OH)(OO^\bullet) + OH^- - O_2$	R(238)	$1.6\ 10^{1}$		Chevallier et al., 2004	
$CH_3(OO^\bullet) + HO_2^\bullet \rightarrow CH_3(OOH) + O_2$	R(239)	$4.2\ 10^{5}$	2700		= $k(HO_2^\bullet + HO_2^\bullet)/2$
$CH_3(OO^\bullet) + O_2^{\bullet-} \rightarrow CH_3(OOH) + O_2 + OH^- - H_2O$	R(240)	$4.8\ 10^{7}$	910		= $k(HO_2^\bullet + O_2^{\bullet-})/2$
Pathway 1: $2\ CH_3(OO^\bullet) \rightarrow 2\ CH_2O + H_2O_2$		$2.2\ 10^{7}$			BR: 20% - 9
Pathway 2: $2\ CH_3(OO^\bullet) \rightarrow 2\ CH_3O^\bullet + O_2$		$8.8\ 10^{7}$			BR: 80% - 9
$CH_3O^\bullet \rightarrow C^\bullet H_2OH$					10
$C^\bullet H_2OH + O_2 \rightarrow CH_2OH(OO^\bullet)$		$2.0\ 10^{9}$			2
$2\ CH_3(OO^\bullet) \rightarrow 0.40\ CH_2O + 1.60\ CH_2OH(OO^\bullet) + 0.20\ H_2O_2 - 0.80\ O_2$	R(241)	$1.1\ 10^{8}$	2200	Herrmann et al., 1999	9
$CH_3(OO^\bullet) + HSO_3^- \rightarrow CH_3(OOH) + SO_3^{\bullet-}$	R(242)	$5.0\ 10^{5}$		Herrmann et al., 1999	
$CH_3(OO^\bullet) + Fe^{2+} \rightarrow [FeCH_3O_2]^{2+}$	R(243)	$8.6\ 10^{5}$		Khaikin et al., 1996	
$[FeCH_3O_2]^{2+} \rightarrow CH_3(OO^\bullet) + Fe^{2+}$	R(244)	$1.3\ 10^{3}$		Khaikin et al., 1996	
$[FeCH_3O_2]^{2+} \rightarrow Fe^{3+} + CH_3(OOH) + OH^- - H_2O$	R(245)	$1.0\ 10^{2}$		Khaikin et al., 1996	
$[FeCH_3O_2]^{2+} + H^+ \rightarrow Fe^{3+} + CH_3(OOH)$	R(246)	$3.0\ 10^{4}$		Khaikin et al., 1996	

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$CH_2(OOH)(OO^\bullet) + OH^- \rightarrow CH_2(OO^-)(OO^\bullet) + H_2O$		$4.0\ 10^9$			
$CH_2(OO^-)(OO^\bullet) \rightarrow CHO(OH) + O_2^{\bullet-}$					11
$CH_2(OOH)(OO^\bullet) + OH^- \rightarrow CHO(OH) + O_2^{\bullet-} + H_2O$	R(247)	$4.0\ 10^9$			= $k(CH_3CH(OH)(OO^\bullet) + OH^-)$ - 12
$CH_2(OOH)(OO^\bullet) \rightarrow CHO(OH) + HO_2^\bullet$	R(248)	$1.0\ 10^1$			= $k(CH_2(OH)(OO^\bullet) \rightarrow CH_2O + HO_2^\bullet)$ - 13
Oxidation of Methanol					
$CH_3(OH) + HO^\bullet \rightarrow C^\bullet H_2(OH) + H_2O$		$1.0\ 10^9$	600	Elliot and McCracken, 1989	
$C^\bullet H_2(OH) + O_2 \rightarrow CH_2(OH)(OO^\bullet)$		$4.2\ 10^9$		Schaefer et al., 2014	
$CH_3(OH) + HO^\bullet \rightarrow CH_2(OH)(OO^\bullet) + H_2O - O_2$	R(249)	$1.0\ 10^9$	600	Elliot and McCracken, 1989	
$CH_3(OH) + NO_3^\bullet \rightarrow C^\bullet H_2(OH) + NO_3^- + H^+$					
$C^\bullet H_2(OH) + O_2 \rightarrow CH_2(OH)(OO^\bullet)$		$4.2\ 10^9$		Schaefer et al., 2014	
$CH_3(OH) + NO_3^\bullet \rightarrow CH_2(OH)(OO^\bullet) + NO_3^- + H^+ - O_2$	R(250)	$5.4\ 10^5$	4300	Herrmann and Zellner, 1998	
$CH_3(OH) + CO_3^{\bullet-} \rightarrow C^\bullet H_2(OH) + HCO_3^-$					
$C^\bullet H_2(OH) + O_2 \rightarrow CH_2(OH)(OO^\bullet)$		$4.2\ 10^9$		Schaefer et al., 2014	
$CH_3(OH) + CO_3^{\bullet-} \rightarrow CH_2(OH)(OO^\bullet) + HCO_3^- - O_2$	R(251)	$5.7\ 10^3$	3100	Clifton and Huie, 1993	
$CH_3(OH) + Cl_2^{\bullet-} \rightarrow C^\bullet H_2(OH) + 2\ Cl^- + H^+$					
$C^\bullet H_2(OH) + O_2 \rightarrow CH_2(OH)(OO^\bullet)$		$4.2\ 10^9$		Schaefer et al., 2014	
$CH_3(OH) + Cl_2^{\bullet-} \rightarrow CH_2(OH)(OO^\bullet) + 2\ Cl^- + H^+ - O_2$	R(252)	$5.0\ 10^4$	5500	Jacobi et al., 1999	
$CH_3(OH) + Cl^\bullet \rightarrow C^\bullet H_2(OH) + Cl^- + H^+$					
$C^\bullet H_2(OH) + O_2 \rightarrow CH_2(OH)(OO^\bullet)$		$4.2\ 10^9$		Schaefer et al., 2014	
$CH_3(OH) + Cl^\bullet \rightarrow CH_2(OH)(OO^\bullet) + Cl^- + H^+ - O_2$	R(253)	$1.0\ 10^9$	1450	Buxton et al., 2000	
$CH_3(OH) + SO_4^{\bullet-} \rightarrow C^\bullet H_2(OH) + SO_4^{2-} + H^+$					
$C^\bullet H_2(OH) + O_2 \rightarrow CH_2(OH)(OO^\bullet)$		$4.2\ 10^9$		Schaefer et al., 2014	
$CH_3(OH) + SO_4^{\bullet-} \rightarrow CH_2(OH)(OO^\bullet) + SO_4^{2-} + H^+ - O_2$	R(254)	$9.0\ 10^6$	2200	Clifton and Huie, 1989	
Oxidation of Formaldehyde					14
Pathway 1: $CH_2(OH)(OH) + HO^\bullet \rightarrow CH^\bullet(OH)(OH) + H_2O$		$5.4\ 10^8$			BR: 70% - 15
$CH^\bullet(OH)(OH) + O_2 \rightarrow CH(OH)(OH)(OO^\bullet)$		$2.0\ 10^9$			2
Pathway 2: $CH_2(OH)(OH) + HO^\bullet \rightarrow CH_2(OH)(O^\bullet) + H_2O$		$2.4\ 10^8$			BR: 30% - 15
$CH_2(OH)(O^\bullet) \rightarrow C^\bullet H(OH)(OH)$					10
$CH^\bullet(OH)(OH) + O_2 \rightarrow CH(OH)(OH)(OO^\bullet)$		$2.0\ 10^9$			2
$CH_2(OH)(OH) + HO^\bullet \rightarrow CH(OH)(OH)(OO^\bullet) + H_2O - O_2$	R(255)	$7.8\ 10^8$	1000	Chin and Wine, 1994	16
Pathway 1: $CH_2(OH)(OH) + NO_3^\bullet \rightarrow CH^\bullet(OH)(OH) + NO_3^- + H^+ - O_2$					BR: 70%
$CH^\bullet(OH)(OH) + O_2 \rightarrow CH(OH)(OH)(OO^\bullet)$		$2.0\ 10^9$			2
Pathway 2: $CH_2(OH)(OH) + NO_3^\bullet \rightarrow CH_2(OH)(O^\bullet) + NO_3^- + H^+ - O_2$					BR: 30%
$CH_2(OH)(O^\bullet) \rightarrow C^\bullet H(OH)(OH)$					10
$CH^\bullet(OH)(OH) + O_2 \rightarrow CH(OH)(OH)(OO^\bullet)$		$2.0\ 10^9$			2
$CH_2(OH)(OH) + NO_3^\bullet \rightarrow CH(OH)(OH)(OO^\bullet) + NO_3^- + H^+ - O_2$	R(256)	$1.0\ 10^6$	4500	Exner et al., 1993	3
Pathway 1: $CH_2(OH)(OH) + CO_3^{\bullet-} \rightarrow CH^\bullet(OH)(OH) + HCO_3^- - O_2$					BR: 70%
$CH^\bullet(OH)(OH) + O_2 \rightarrow CH(OH)(OH)(OO^\bullet)$		$2.0\ 10^9$			2
Pathway 2: $CH_2(OH)(OH) + CO_3^{\bullet-} \rightarrow CH_2(OH)(O^\bullet) + HCO_3^- - O_2$					BR: 30%
$CH_2(OH)(O^\bullet) \rightarrow C^\bullet H(OH)(OH)$					10
$CH^\bullet(OH)(OH) + O_2 \rightarrow CH(OH)(OH)(OO^\bullet)$		$2.0\ 10^9$			2
$CH_2(OH)(OH) + CO_3^{\bullet-} \rightarrow CH(OH)(OH)(OO^\bullet) + HCO_3^- - O_2$	R(257)	$1.3\ 10^4$		Zellner et al., 1996	3

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
Pathway 1: $CH_2(OH)(OH) + Cl_2^{\bullet-} \rightarrow CH^{\bullet}(OH)(OH) + 2\ Cl^- + H^+ - O_2$					BR: 70%
$CH^{\bullet}(OH)(OH) + O_2 \rightarrow CH(OH)(OH)(OO^{\bullet})$		$2.0\ 10^9$			2
Pathway 2: $CH_2(OH)(OH) + Cl_2^{\bullet-} \rightarrow CH_2(OH)(O^{\bullet}) + 2\ Cl^- + H^+ - O_2$					BR: 30%
$CH_2(OH)(O^{\bullet}) \rightarrow C^{\bullet}H(OH)(OH)$					10
$CH^{\bullet}(OH)(OH) + O_2 \rightarrow CH(OH)(OH)(OO^{\bullet})$		$2.0\ 10^9$			2
$CH_2(OH)(OH) + Cl_2^{\bullet-} \rightarrow CH(OH)(OH)(OO^{\bullet}) + 2\ Cl^- + H^+ - O_2$	R(258)	$3.6\ 10^4$	4400	Jacobi et al., 1999	3
Pathway 1: $CH_2(OH)(OH) + Cl^{\bullet} \rightarrow CH^{\bullet}(OH)(OH) + Cl^- + H^+ - O_2$					BR: 70%
$CH^{\bullet}(OH)(OH) + O_2 \rightarrow CH(OH)(OH)(OO^{\bullet})$		$2.0\ 10^9$			2
Pathway 2: $CH_2(OH)(OH) + Cl^{\bullet} \rightarrow CH_2(OH)(O^{\bullet}) + Cl^- + H^+ - O_2$					BR: 30%
$CH_2(OH)(O^{\bullet}) \rightarrow C^{\bullet}H(OH)(OH)$					10
$CH^{\bullet}(OH)(OH) + O_2 \rightarrow CH(OH)(OH)(OO^{\bullet})$		$2.0\ 10^9$			2
$CH_2(OH)(OH) + Cl^{\bullet} \rightarrow CH(OH)(OH)(OO^{\bullet}) + Cl^- + H^+ - O_2$	R(259)	$1.4\ 10^9$		Buxton et al., 2000	3
Pathway 1: $CH_2(OH)(OH) + SO_4^{\bullet-} \rightarrow CH^{\bullet}(OH)(OH) + SO_4^{2-} + H^+ - O_2$					BR: 70%
$CH^{\bullet}(OH)(OH) + O_2 \rightarrow CH(OH)(OH)(OO^{\bullet})$		$2.0\ 10^9$			2
Pathway 2: $CH_2(OH)(OH) + SO_4^{\bullet-} \rightarrow CH_2(OH)(O^{\bullet}) + SO_4^{2-} + H^+ - O_2$					BR: 30%
$CH_2(OH)(O^{\bullet}) \rightarrow C^{\bullet}H(OH)(OH)$					10
$CH^{\bullet}(OH)(OH) + O_2 \rightarrow CH(OH)(OH)(OO^{\bullet})$		$2.0\ 10^9$			2
$CH_2(OH)(OH) + SO_4^{\bullet-} \rightarrow CH(OH)(OH)(OO^{\bullet}) + SO_4^{2-} + H^+ - O_2$	R(260)	$1.4\ 10^7$	1300	Buxton et al., 1990	3
$CH_2(OH)(OH) + FeO^{2+} \rightarrow CHO(OH) + Fe^{3+} + HO_2^{\bullet} + OH^- - O_2$	R(261)	$4.0\ 10^2$	5350	Jacobsen et al., 1998	
$CH(OH)(OH)(OO^{\bullet}) + OH^- \rightarrow CH(OH)(O^-)(OO^{\bullet}) + H_2O$		$4.0\ 10^9$			
$CH(OH)(O^-)(OO^{\bullet}) \rightarrow CHO(OH) + O_2^{\bullet-}$					5
$CH(OH)(OH)(OO^{\bullet}) + OH^- \rightarrow CHO(OH) + O_2^{\bullet-} + H_2O$	R(262)	$4.0\ 10^9$			= $k(CH_3CH(OH)(OO^{\bullet}) + OH^-)$
$CH(OH)(OH)(OO^{\bullet}) \rightarrow CHO(OH) + HO_2^{\bullet}$	R(263)	$1.0\ 10^6$			17
Oxidation of Formic acid					
$CHO(OH) + HO^{\bullet} \rightarrow CO(OH)(OO^{\bullet}) + H_2O - O_2$	R(264)	$1.0\ 10^8$	1000	Chin and Wine, 1994	
$CHO(O^-) + HO^{\bullet} \rightarrow CO(O^-)(OO^{\bullet}) + H_2O - O_2$	R(265)	$3.4\ 10^9$	1200	Chin and Wine, 1994	
$CHO(OH) + NO_3^{\bullet} \rightarrow CO(OH)(OO^{\bullet}) + NO_3^- + H^+ - O_2$	R(266)	$3.8\ 10^5$	3400	Exner et al., 1994	
$CHO(O^-) + NO_3^{\bullet} \rightarrow CO(O^-)(OO^{\bullet}) + NO_3^- + H^+ - O_2$	R(267)	$5.1\ 10^7$	2200	Exner et al., 1994	
$CHO(O^-) + CO_3^{\bullet-} \rightarrow CO(O^-)(OO^{\bullet}) + HCO_3^- - O_2$	R(268)	$1.6\ 10^5$		Zellner et al., 1996	
$CHO(OH) + Cl_2^{\bullet-} \rightarrow CO(OH)(OO^{\bullet}) + 2\ Cl^- + H^+ - O_2$	R(269)	$8.0\ 10^4$	4500	Jacobi et al., 1999	
$CHO(O^-) + Cl_2^{\bullet-} \rightarrow CO(O^-)(OO^{\bullet}) + 2\ Cl^- + H^+ - O_2$	R(270)	$1.3\ 10^6$		Jacobi et al., 1996	
$CHO(OH) + Cl^{\bullet} \rightarrow CO(OH)(OO^{\bullet}) + Cl^- + H^+ - O_2$	R(271)	$1.3\ 10^8$	1100	Buxton et al., 2000	
$CHO(O^-) + Cl^{\bullet} \rightarrow CO(O^-)(OO^{\bullet}) + Cl^- + H^+ - O_2$	R(272)	$4.2\ 10^9$	1900	Buxton et al., 2000	
$CHO(OH) + FeO^{2+} \rightarrow CO(OH)(OO^{\bullet}) + Fe^{3+} + H_2O - H^+ - O_2$	R(273)	$1.6\ 10^2$	2680	Jacobsen et al., 1998	
$CHO(O^-) + FeO^{2+} \rightarrow CO(O^-)(OO^{\bullet}) + Fe^{3+} + H_2O - H^+ - O_2$	R(274)	$3.0\ 10^5$		Jacobsen et al., 1998	
$CO(OH)(OO^{\bullet}) + OH^- \rightarrow CO(O^-)(OO^{\bullet}) + H_2O$		$4.0\ 10^9$			
$CO(O^-)(OO^{\bullet}) \rightarrow CO_2 + O_2^{\bullet-}$					5
$CO(OH)(OO^{\bullet}) + OH^- \rightarrow CO_2 + O_2^{\bullet-} + H_2O$	R(275)	$4.0\ 10^9$			= $k(CH_3CH(OH)(OO^{\bullet}) + OH^-)$
$CO(OH)(OO^{\bullet}) \rightarrow CO_2 + HO_2^{\bullet}$	R(276)	$1.0\ 10^6$			18
$CO(O^-)(OO^{\bullet}) \rightarrow CO_2 + O_2^{\bullet-}$	R(277)	$1.0\ 10^6$			19

C2 compounds

For C2 oxidation, chemical pathways with branching ratio < 10% are not considered.

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
Oxidation of Ethanol					
Pathway 1:$CH_3CH_2(OH) + HO^\bullet \rightarrow CH_3C^\bullet H(OH) + H_2O$		$1.9\ 10^9$			BR: 90% - 20
$CH_3C^\bullet H(OH) + O_2 \rightarrow CH_3CH(OH)(OO^\bullet)$		$4.6\ 10^9$		Adams and Willson, 1969	
Pathway 2: $CH_3CH_2(OH) + HO^\bullet \rightarrow CH_2{}^\bullet CH_2(OH) + H_2O$		$2.0\ 10^8$			BR: 10% - 20
$CH_2{}^\bullet CH_2(OH) + O_2 \rightarrow CH_2(OH)CH_2(OO^\bullet)$		$4.6\ 10^9$		Adams and Willson, 1969	
$CH_3CH_2(OH) + HO^\bullet \rightarrow 0.90\ CH_3CH(OH)(OO^\bullet) + 0.10\ CH_2(OH)CH_2(OO^\bullet) + H_2O - O_2$	R(278)	$2.1\ 10^9$	830	Monod et al., 2005	
Pathway 1: $CH_3CH_2(OH) + NO_3^\bullet \rightarrow CH_3C^\bullet H(OH) + NO_3^- + H^+$		$2.0\ 10^6$			BR: 90%
$CH_3C^\bullet H(OH) + O_2 \rightarrow CH_3CH(OH)(OO^\bullet)$		$4.6\ 10^9$		Adams and Willson, 1969	
Pathway 2: $CH_3CH_2(OH) + NO_3^\bullet \rightarrow CH_2{}^\bullet CH_2(OH) + NO_3^- + H^+$		$2.0\ 10^5$			BR: 10%
$CH_2{}^\bullet CH_2(OH) + O_2 \rightarrow CH_2(OH)CH_2(OO^\bullet)$		$4.6\ 10^9$		Adams and Willson, 1969	
$CH_3CH_2(OH) + NO_3^\bullet \rightarrow 0.90\ CH_3CH(OH)(OO^\bullet) + 0.10\ CH_2(OH)CH_2(OO^\bullet) + NO_3^- + H^+ - O_2$	R(279)	$2.2\ 10^6$	3300	Herrmann and Zellner, 1998	3
Pathway 1: $CH_3CH_2(OH) + FeO^{2+} \rightarrow CH_3C^\bullet H(OH) + Fe^{3+} + OH^-$		$2.2\ 10^3$			BR: 90%
$CH_3C^\bullet H(OH) + O_2 \rightarrow CH_3CH(OH)(OO^\bullet)$		$4.6\ 10^9$		Adams and Willson, 1969	
Pathway 2: $CH_3CH_2(OH) + FeO^{2+} \rightarrow CH_2{}^\bullet CH_2(OH) + Fe^{3+} + OH^-$		$3.0\ 10^2$			BR: 10%
$CH_2{}^\bullet CH_2(OH) + O_2 \rightarrow CH_2(OH)CH_2(OO^\bullet)$		$4.6{\cdot}10^9$		Adams and Willson, 1969	
$CH_3CH_2(OH) + FeO^{2+} \rightarrow 0.90\ CH_3CH(OH)(OO^\bullet) + 0.10\ CH_2(OH)CH_2(OO^\bullet) + Fe^{3+} + OH^- - O_2$	R(280)	$2.5{\cdot}10^3$		Jacobsen et al., 1998	3
Pathway 1: $CH_3CH_2(OH) + SO_4^{\bullet-} \rightarrow CH_3C^\bullet H(OH) + SO_4^{2-} + H^+$		$3.7\ 10^7$			BR: 90%
$CH_3C^\bullet H(OH) + O_2 \rightarrow CH_3CH(OH)(OO^\bullet)$		$4.6\ 10^9$		Adams and Willson, 1969	
Pathway 2: $CH_3CH_2(OH) + SO_4^{\bullet-} \rightarrow CH_2{}^\bullet CH_2(OH) + SO_4^{2-} + H^+$		$4.0\ 10^6$			BR: 10%
$CH_2{}^\bullet CH_2(OH) + O_2 \rightarrow CH_2(OH)CH_2(OO^\bullet)$		$4.6\ 10^9$		Adams and Willson, 1969	
$CH_3CH_2(OH) + SO_4^{\bullet-} \rightarrow 0.90\ CH_3CH(OH)(OO^\bullet) + 0.10\ CH_2(OH)CH_2(OO^\bullet) + SO_4^{2-} + H^+ - O_2$	R(281)	$4.1\ 10^7$	1760	Clifton and Huie, 1989	3
Patway 1: $CH_3CH_2(OH) + Cl_2^{\bullet-} \rightarrow CH_3C^\bullet H(OH) + 2\ Cl^- + H^+$		$1.1\ 10^5$			BR: 90%
$CH_3C^\bullet H(OH) + O_2 \rightarrow CH_3CH(OH)(OO^\bullet)$		$4.6\ 10^9$		Adams and Willson, 1969	
Pathway 2: $CH_3CH_2(OH) + Cl_2^{\bullet-} \rightarrow CH_2{}^\bullet CH_2(OH) + 2\ Cl^- + H^+$		$1.0\ 10^4$			BR: 10%
$CH_2{}^\bullet CH_2(OH) + O_2 \rightarrow CH_2(OH)CH_2(OO^\bullet)$		$4.6\ 10^9$		Adams and Willson, 1969	
$CH_3CH_2(OH) + Cl_2^{\bullet-} \rightarrow 0.90\ CH_3CH(OH)(OO^\bullet) + 0.10\ CH_2(OH)CH_2(OO^\bullet) + 2\ Cl^- + H^+ - O_2$	R(282)	$1.2\ 10^5$		Zellner et al., 1996	3
Pathway 1: $CH_3CH_2(OH) + CO_3^{\bullet-} \rightarrow CH_3C^\bullet H(OH) + CO_3^{2-} + H^+$		$1.3\ 10^4$			BR: 90%
$CH_3C^\bullet H(OH) + O_2 \rightarrow CH_3CH(OH)(OO^\bullet)$		$4.6\ 10^9$		Adams and Willson, 1969	
Pathway 2: $CH_3CH_2(OH) + CO_3^{\bullet-} \rightarrow CH_2{}^\bullet CH_2(OH) + CO_3^{2-} + H^+$		$2.0\ 10^3$			BR: 10%
$CH_2{}^\bullet CH_2(OH) + O_2 \rightarrow CH_2(OH)CH_2(OO^\bullet)$		$4.6\ 10^9$		Adams and Willson, 1969	
$CH_3CH_2(OH) + CO_3^{\bullet-} \rightarrow 0.90\ CH_3CH(OH)(OO^\bullet) + 0.10\ CH_2(OH)CH_2(OO^\bullet) + CO_3^{2-} + H^+ - O_2$	R(283)	$1.5\ 10^4$		Kuz'min, 1972	3
$CH_3CH(OH)(OO^\bullet) + OH^- \rightarrow CH_3CH(O^-)(OO^\bullet) + H_2O$		$4.0\ 10^9$			
$CH_3CH(O^-)(OO^\bullet) \rightarrow CH_3CHO + O_2^{\bullet-}$					5
$CH_3CH(OH)(OO^\bullet) + OH^- \rightarrow CH_3CHO + O_2^{\bullet-} + H_2O$	R(284)	$4.0\ 10^9$		Neta et al., 1990	
$CH_3CH(OH)(OO^\bullet) \rightarrow CH_3CHO + HO_2^\bullet$	R(285)	$5.2\ 10^1$	7217	Von Sonntag, 1987	
Pathway 1: $2\ CH_2(OH)CH_2(OO^\bullet) \rightarrow 2\ CH_2(OH)CHO + H_2O_2$		$5.0\ 10^7$			BR: 50%
Pathway 2: $2\ CH_2(OH)CH_2(OO^\bullet) \rightarrow CH_2(OH)CH_2(OH) + CH_2(OH)CHO + O_2$		$3.3\ 10^7$			BR: 33%
Pathway 3: $2\ CH_2(OH)CH_2(OO^\bullet) \rightarrow 2\ CH_2(O^\bullet)CH_2(OH) + O_2$		$1.7\ 10^7$			BR: 17%
$CH_2(O^\bullet)CH_2(OH) \rightarrow C^\bullet H_2(OH) + CH_2O$					21 - 22
$C^\bullet H_2(OH) + O_2 \rightarrow CH_2(OH)(OO^\bullet)$		$2.0\ 10^9$			2
$2\ CH_2(OH)CH_2(OO^\bullet) \rightarrow 1.33\ CH_2(OH)CHO + 0.33\ CH_2(OH)CH_2(OH) + 0.34\ CH_2(OH)(OO^\bullet) + 0.34\ CH_2O + 0.5\ H_2O_2 + 0.16\ O_2$	R(286)	$1.0\ 10^8$		Piesiak et al., 1984	23

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
Oxidation of Ethylene glycol					
$CH_2(OH)CH_2(OH) + HO^\bullet \rightarrow CH_2(OH)CH^\bullet(OH) + H_2O$		$1.7\ 10^9$	1191		
$CH_2(OH)CH^\bullet(OH) + O_2 \rightarrow CH_2(OH)CH(OH)(OO^\bullet)$		$3.2\ 10^9$		Adams and Willson, 1969	
$CH_2(OH)CH_2(OH) + HO^\bullet \rightarrow CH_2(OH)CH(OH)(OO^\bullet) + H_2O - O_2$	R(287)	$1.7\ 10^9$	1191	Hoffmann et al., 2009	
$CH_2(OH)CH_2(OH) + NO_3^\bullet \rightarrow CH_2(OH)CH^\bullet(OH) + NO_3^- + H^+$		$6.6\ 10^6$	2117		
$CH_2(OH)CH^\bullet(OH) + O_2 \rightarrow CH_2(OH)CH(OH)(OO^\bullet)$		$3.2\ 10^9$		Adams and Willson, 1969	
$CH_2(OH)CH_2(OH) + NO_3^\bullet \rightarrow CH_2(OH)CH(OH)(OO^\bullet) + NO_3^- + H^+ - O_2$	R(288)	$6.6\ 10^6$	2117	Hoffmann et al., 2009	
$CH_2(OH)CH(OH)(OO^\bullet) + OH^- \rightarrow CH_2(OH)CH(O^-)(OO^\bullet) + H_2O$		$4.0\ 10^9$			
$CH_2(OH)CH(O^-)(OO^\bullet) \rightarrow CH_2(OH)CHO + O_2^{\bullet-}$					5
$CH_2(OH)CH(OH)(OO^\bullet) + OH^- \rightarrow CH_2(OH)CHO + O_2^{\bullet-} + H_2O$	R(289)	$4.0\ 10^9$			= $k(CH_3CH(OH)(OO^\bullet) + OH^-)$
$CH_2(OH)CH(OH)(OO^\bullet) \rightarrow CH_2(OH)CHO + HO_2^\bullet$	R(290)	$1.9\ 10^2$			4
Oxidation of Acetaldehyde					24
$CH_3CHO + HO^\bullet \rightarrow CH_3C^\bullet O + H_2O$		$3.6\ 10^9$			25
$CH_3C^\bullet O + O_2 \rightarrow CH_3CO(OO^\bullet)$		$2.0\ 10^9$			2
$CH_3CHO + HO^\bullet \rightarrow CH_3CO(OO^\bullet) + H_2O - O_2$	R(291)	$3.6\ 10^9$		Schuchmann and Von Sonntag, 1988	16
$CH_3CHO + NO_3^\bullet \rightarrow CH_3C^\bullet O + NO_3^- + H^+$		$3.1\ 10^6$			
$CH_3C^\bullet O + O_2 \rightarrow CH_3CO(OO^\bullet)$		$2.0\ 10^9$			2
$CH_3CHO + NO_3^\bullet \rightarrow CH_3CO(OO^\bullet) + NO_3^- + H^+ - O_2$	R(292)	$3.1\ 10^6$		Rousse and George, 2004	3 - 26
$CH_3CHO + Cl_2^{\bullet-} \rightarrow CH_3C^\bullet O + 2\ Cl^- + H^+$		$4.0\ 10^4$			
$CH_3C^\bullet O + O_2 \rightarrow CH_3CO(OO^\bullet)$		$2.0\ 10^9$			2
$CH_3CHO + Cl_2^{\bullet-} \rightarrow CH_3CO(OO^\bullet) + 2\ Cl^- + H^+ - O_2$	R(293)	$4.0\ 10^4$		Jacobi et al., 1996	3 - 27
Pathway 1: $CH_3CH(OH)(OH) + HO^\bullet \rightarrow CH_3C^\bullet(OH)(OH) + H_2O$		$8.0\ 10^8$			BR: 67% - 28
$CH_3C^\bullet(OH)(OH) + O_2 \rightarrow CH_3C(OH)(OH)(OO^\bullet)$		$2.0\ 10^9$			2
Pathway 2. $CH_3CH(OH)(OH) + HO^\bullet \rightarrow CH_3CH(OH)(O^\bullet) + H_2O$		$4.0\ 10^8$			BR: 33% - 28
$CH_3CH(OH)(O^\bullet) \rightarrow CH_3C^\bullet(OH)(OH)$					10
$CH_3C^\bullet(OH)(OH) + O_2 \rightarrow CH_3C(OH)(OH)(OO^\bullet)$		$2.0\ 10^9$			2
$CH_3CH(OH)(OH) + HO^\bullet \rightarrow CH_3C(OH)(OH)(OO^\bullet) + H_2O - O_2$	R(294)	$1.2\ 10^9$		Schuchmann and Von Sonntag, 1988	16
Pathway 1: $CH_3CH(OH)(OH) + NO_3^\bullet \rightarrow CH_3C^\bullet(OH)(OH) + NO_3^- + H^+$		$7.4\ 10^5$			BR: 67%
$CH_3C^\bullet(OH)(OH) + O_2 \rightarrow CH_3C(OH)(OH)(OO^\bullet)$		$2.0\ 10^9$			2
Pathway 2. $CH_3CH(OH)(OH) + NO_3^\bullet \rightarrow CH_3CH(OH)(O^\bullet) + NO_3^- + H^+$		$3.6\ 10^5$			BR: 33%
$CH_3CH(OH)(O^\bullet) \rightarrow CH_3C^\bullet(OH)(OH)$					10
$CH_3C^\bullet(OH)(OH) + O_2 \rightarrow CH_3C(OH)(OH)(OO^\bullet)$		$2.0 \cdot 10^9$			2
$CH_3CH(OH)(OH) + NO_3^\bullet \rightarrow CH_3C(OH)(OH)(OO^\bullet) + NO_3^- + H^+ - O_2$	R(295)	$1.1\ 10^6$		Rousse and George, 2004	3 - 26
Pathway1: $CH_3CH(OH)(OH) + Cl_2^{\bullet-} \rightarrow CH_3C^\bullet(OH)(OH) + 2\ Cl^- + H^+$		$2.7\ 10^4$			BR: 67%
$CH_3C^\bullet(OH)(OH) + O_2 \rightarrow CH_3C(OH)(OH)(OO^\bullet)$		$2.0\ 10^9$			2
Pathway 2. $CH_3CH(OH)(OH) + Cl_2^{\bullet-} \rightarrow CH_3CH(OH)(O^\bullet) + 2\ Cl^- + H^+$		$1.3\ 10^4$			BR: 33%
$CH_3CH(OH)(O^\bullet) \rightarrow CH_3C^\bullet(OH)(OH)$					10
$CH_3C^\bullet(OH)(OH) + O_2 \rightarrow CH_3C(OH)(OH)(OO^\bullet)$		$2.0\ 10^9$			2
$CH_3CH(OH)(OH) + Cl_2^{\bullet-} \rightarrow CH_3C(OH)(OH)(OO^\bullet) + 2\ Cl^- + H^+ - O_2$	R(296)	$4.0\ 10^4$		Jacobi et al., 1996	3 - 27
$CH_3C(OH)(OH)(OO^\bullet) + OH^- \rightarrow CH_3C(OH)(O^-)(OO^\bullet) + H_2O$		$4.0\ 10^9$			
$CH_3C(OH)(O^-)(OO^\bullet) \rightarrow CH_3CO(OH) + O_2^{\bullet-}$					5
$CH_3C(OH)(OH)(OO^\bullet) + OH^- \rightarrow CH_3CO(OH) + O_2^{\bullet-} + H_2O$	R(297)	$4.0\ 10^9$			= $k(CH_3CH(OH)(OO^\bullet) + OH^-)$

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CH_3C(OH)(OH)(OO^•) \rightarrow CH_3CO(OH) + HO_2^•$	R(298)	$1.0\ 10^6$			17
$2\ CH_3CO(OO^•) \rightarrow 2\ C^•H_3 + 2\ CO_2 + O_2$		$1.6\ 10^8$			
$C^•H_3 + O_2 \rightarrow CH_3(OO^•)$		$2.0\ 10^9$			2
$2\ CH_3CO(OO^•) \rightarrow 2\ CH_3(OO^•) + 2\ CO_2 - O_2$	R(299)	$1.6\ 10^8$	-1600		= k(2 $CH_3CH_2(OO^•)$) - 29
$CH_3CO(OO^•) + O_2^{•-} \rightarrow CH_3CO(OO^-) + O_2$	R(300)	$1.0\ 10^9$		Schuchmann and Von Sonntag, 1988	30
Oxidation of Glycoladehyde					31
Pathway 1: $CH_2(OH)CHO + HO^• \rightarrow CH_2(OH)C^•O + H_2O$		$1.1\ 10^9$			BR: 77% - 32
$CH_2(OH)C^•O + O_2 \rightarrow CH_2(OH)CO(OO^•)$		$2.0\ 10^9$			2
Pathway 2: $CH_2(OH)CHO + HO^• \rightarrow CH^•(OH)CHO + H_2O$		$3.0\ 10^8$			BR: 23% - 32
$CH^•(OH)CHO + O_2 \rightarrow CH(OH)(OO^•)CHO$		$2.\ 0\ 10^9$			2
$CH_2(OH)CHO + HO^• \rightarrow 0.77\ CH_2(OH)CO(OO^•) + 0.23\ CH(OH)(OO^•)CHO + H_2O - O_2$	R(301)	$1.4\ 10^9$			33
Pathway 1: $CH_2(OH)CHO + NO_3^• \rightarrow CH_2(OH)C^•O + NO_3^- + H^+$		$2.4\ 10^6$			BR: 77%
$CH_2(OH)C^•O + O_2 \rightarrow CH_2(OH)CO(OO^•)$		$2.0\ 10^9$			2
Pathway 2: $CH_2(OH)CHO + NO_3^• \rightarrow CH^•(OH)CHO + NO_3^- + H^+$		$7.0\ 10^5$			BR: 23%
$CH^•(OH)CHO + O_2 \rightarrow CH(OH)(OO^•)CHO$		$2.0\ 10^9$			2
$CH_2(OH)CHO + NO_3^• \rightarrow 0.77\ CH_2(OH)CO(OO^•) + 0.23\ CH(OH)(OO^•)CHO + NO_3^- + H^+ - O_2$	R(302)	$3.1\ 10^6$			= k($CH_3CHO + NO_3^•$) - 3
Pathway 1: $CH_2(OH)CH(OH)(OH) + HO^• \rightarrow CH_2(OH)C^•(OH)(OH) + H_2O$		$3.6\ 10^8$			BR: 33% - 34
$CH_2(OH)C^•(OH)(OH) + O_2 \rightarrow CH_2(OH)C(OH)(OH)(OO^•)$		$2.0\ 10^9$			2
Pathway 2: $CH_2(OH)CH(OH)(OH) + HO^• \rightarrow CH^•(OH)CH(OH)(OH) + H_2O$		$3.1\ 10^8$			BR: 28% - 34
$CH^•(OH)CH(OH)(OH) + O_2 \rightarrow CH(OH)(OO^•)CH(OH)(OH)$		$2.0\ 10^9$			2
Pathway 3: $CH_2(OH)CH(OH)(OH) + HO^• \rightarrow CH_2(OH)CH(OH)(O^•) + H_2O$		$4.3\ 10^8$			BR: 39% - 34
$CH_2(OH)CH(OH)(O^•) \rightarrow C^•H_2(OH) + CHO(OH)$					21 - 22
$C^•H_2(OH) + O_2 \rightarrow CH_2(OH)(OO^•)$		$2.0\ 10^9$			2
$CH_2(OH)CH(OH)(OH) + HO^• \rightarrow 0.33\ CH_2(OH)C(OH)(OH)(OO^•) + 0.28\ CH(OH)(OO^•)CH(OH)(OH) + 0.39\ CHO(OH) + 0.39\ CH_2(OH)(OO^•) + H_2O - O_2$	R(303)	$1.1\ 10^9$			33
Pathway 1: $CH_2(OH)CH(OH)(OH) + NO_3^• \rightarrow CH_2(OH)C^•(OH)(OH) + NO_3^- + H^+$		$3.6\ 10^5$			BR: 33%
$CH_2(OH)C^•(OH)(OH) + O_2 \rightarrow CH_2(OH)C(OH)(OH)(OO^•)$		$2.0\ 10^9$			2
Pathway 2: $CH_2(OH)CH(OH)(OH) + NO_3^• \rightarrow CH^•(OH)CH(OH)(OH) + NO_3^- + H^+$		$3.1\ 10^5$			BR: 28%
$CH^•(OH)CH(OH)(OH) + O_2 \rightarrow CH(OH)(OO^•)CH(OH)(OH)$		$2.0\ 10^9$			2
Pathway 3: $CH_2(OH)CH(OH)(OH) + NO_3^• \rightarrow CH_2(OH)CH(OH)(O^•) + NO_3^- + H^+$		$4.3\ 10^5$			BR: 39%
$CH_2(OH)CH(OH)(O^•) \rightarrow C^•H_2(OH) + CHO(OH)$					21 - 22
$C^•H_2(OH) + O_2 \rightarrow CH_2(OH)(OO^•)$		$2.0\ 10^9$			2
$CH_2(OH)CH(OH)(OH) + NO_3^• \rightarrow 0.33\ CH_2(OH)C(OH)(OH)(OO^•) + 0.28\ CH(OH)(OO^•)CH(OH)(OH) + 0.39\ CHO(OH) + 0.39\ CH_2(OH)(OO^•) + NO_3^- + H^+ - O_2$	R(304)	$1.1\ 10^6$			= k($CH_3CH(OH)(OH) + NO_3^•$) - 3
$CH_2(OH)CO(OO^•) + O_2^{•-} \rightarrow CH_2(OH)CO(OO^-) + O_2$	R(305)	$1.0\ 10^9$			= k($CH_3CO(OO^•) + O_2^{•-}$)
$CH_2(OH)C(OH)(OH)(OO^•) + OH^- \rightarrow CH_2(OH)C(OH)(O-)(OO^•) + H_2O$		$4.0\ 10^9$			
$CH_2(OH)C(OH)(O^-)(OO^•) \rightarrow CH_2(OH)CO(OH) + O_2^{•-}$					5
$CH_2(OH)C(OH)(OH)(OO^•) + OH^- \rightarrow CH_2(OH)CO(OH) + O_2^{•-} + H_2O$	R(306)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^•) + OH^-$)
$CH_2(OH)C(OH)(OH)(OO^•) \rightarrow CH_2(OH)CO(OH) + HO_2^•$	R(307)	$1.0\ 10^6$			17
$CH(OH)(OO^•)CHO + OH^- \rightarrow CH(O^-)(OO^•)CHO + H_2O$		$4.0\ 10^9$			
$CH(O^-)(OO^•)CHO \rightarrow CHOCHO + O_2^{•-}$					5
$CH(OH)(OO^•)CHO + OH^- \rightarrow CHOCHO + O_2^{•-} + H_2O$	R(308)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^•) + OH^-$)
$CH(OH)(OO^•)CHO \rightarrow CHOCHO + HO_2^•$	R(309)	$1.9\ 10^2$			4

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CH(OH)(OO^{\bullet})CH(OH)(OH) + OH^- \rightarrow CH(O^-)(OO^{\bullet})CH(OH)(OH) + H_2O$		$4.0\ 10^9$			
$CH(O^-)(OO^{\bullet})CH(OH)(OH) \rightarrow CHOCH(OH)(OH) + O_2^{\bullet-}$					5
$CH(OH)(OO^{\bullet})CH(OH)(OH) + OH^- \rightarrow CHOCH(OH)(OH) + O_2^{\bullet-} + H_2O$	R(310)	$4.0\ 10^9$			= $k(CH_3CH(OH)(OO^{\bullet}) + OH^-)$
$CH(OH)(OO^{\bullet})CH(OH)(OH) \rightarrow CHOCH(OH)(OH) + HO_2^{\bullet}$	R(311)	$1.9\ 10^2$			4
Oxidation of Glyoxal					35
Pathway 1: $CH(OH)(OH)CH(OH)(OH) + HO^{\bullet} \rightarrow CH(OH)(OH)C^{\bullet}(OH)(OH) + H_2O$		$3.0\ 10^8$			BR: 27% - 36
$CH(OH)(OH)C^{\bullet}(OH)(OH) + O_2 \rightarrow CH(OH)(OH)C(OH)(OH)(OO^{\bullet})$		$1.2\ 10^9$		Schaefer et al., 2014	
Pathway 2: $CH(OH)(OH)CH(OH)(OH) + HO^{\bullet} \rightarrow CH(OH)(OH)CH(OH)(O^{\bullet}) + H_2O$		$8.0\ 10^8$			BR: 73% - 36
$CH(OH)(OH)CH(OH)(O^{\bullet}) \rightarrow C^{\bullet}H(OH)(OH) + CHO(OH)$					21 - 22
$C^{\bullet}H(OH)(OH) + O_2 \rightarrow CH(OH)(OH)(OO^{\bullet})$		$2.0\ 10^9$			2
$CH(OH)(OH)CH(OH)(OH) + HO^{\bullet} \rightarrow 0.27\ CH(OH)(OH)C(OH)(OH)(OO^{\bullet}) + 0.73\ CHO(OH) + 0.73\ CH(OH)(OH)(OO^{\bullet}) + H_2O - O_2$	R(312)	$1.1\ 10^9$	1516	Buxton et al., 1997	
Pathway 1: $CH(OH)(OH)CH(OH)(OH) + NO_3^{\bullet} \rightarrow CH(OH)(OH)C^{\bullet}(OH)(OH) + NO_3^- + H^+$		$7.3\ 10^5$			BR: 27%
$CH(OH)(OH)C^{\bullet}(OH)(OH) + O_2 \rightarrow CH(OH)(OH)C(OH)(OH)(OO^{\bullet})$		$1.2\ 10^9$		Schaefer et al., 2014	
Pathway 2: $CH(OH)(OH)CH(OH)(OH) + NO_3^{\bullet} \rightarrow CH(OH)(OH)CH(OH)(O^{\bullet}) + NO_3^- + H^+$		$2.7\ 10^5$			BR: 73%
$CH(OH)(OH)CH(OH)(O^{\bullet}) \rightarrow C^{\bullet}H(OH)(OH) + CHO(OH)$					21 - 22
$C^{\bullet}H(OH)(OH) + O_2 \rightarrow CH(OH)(OH)(OO^{\bullet})$		$2.0\ 10^9$			2
$CH(OH)(OH)CH(OH)(OH) + NO_3^{\bullet} \rightarrow 0.27\ CH(OH)(OH)C(OH)(OH)(OO^{\bullet}) + 0.73\ CHO(OH) + 0.73\ CH(OH)(OH)(OO^{\bullet}) + NO_3^- + H^+ - O_2$	R(313)	$1.0\ 10^6$			3 - 37
Pathway 1: $CH(OH)(OH)CH(OH)(OH) + SO_4^{\bullet-} \rightarrow CH(OH)(OH)C^{\bullet}(OH)(OH) + SO_4^{2-} + H^+$		$1.8\ 10^7$			BR: 27%
$CH(OH)(OH)C^{\bullet}(OH)(OH) + O_2 \rightarrow CH(OH)(OH)C(OH)(OH)(OO^{\bullet})$		$1.2\ 10^9$		Schaefer et al., 2014	
Pathway 2: $CH(OH)(OH)CH(OH)(OH) + SO_4^{\bullet-} \rightarrow CH(OH)(OH)CH(OH)(O^{\bullet}) + SO_4^{2-} + H^+$		$6.0\ 10^6$			BR: 73%
$CH(OH)(OH)CH(OH)(O^{\bullet}) \rightarrow C^{\bullet}H(OH)(OH) + CHO(OH)$					21 - 22
$C^{\bullet}H(OH)(OH) + O_2 \rightarrow CH(OH)(OH)(OO^{\bullet})$		$2.0\ 10^9$			2
$CH(OH)(OH)CH(OH)(OH) + SO_4^{\bullet-} \rightarrow 0.27\ CH(OH)(OH)C(OH)(OH)(OO^{\bullet}) + 0.73\ CHO(OH) + 0.73\ CH(OH)(OH)(OO^{\bullet}) + SO_4^{2-} + H^+ - O_2$	R(314)	$2.4\ 10^7$		George et al., 2001	3
$CH(OH)(OH)C(OH)(OH)(OO^{\bullet}) + OH^- \rightarrow CH(OH)(OH)C(OH)(O^-)(OO^{\bullet}) + H_2O$		$4.0\ 10^9$			
$CH(OH)(OH)C(OH)(O^-)(OO^{\bullet}) \rightarrow CH(OH)(OH)CO(OH) + O_2^{\bullet-}$					5
$CH(OH)(OH)C(OH)(OH)(OO^{\bullet}) + OH^- \rightarrow CH(OH)(OH)CO(OH) + O_2^{\bullet-} + H_2O$	R(315)	$4.0\ 10^9$			= $k(CH_3CH(OH)(OO^{\bullet}) + OH^-)$
$CH(OH)(OH)C(OH)(OH)(OO^{\bullet}) \rightarrow CH(OH)(OH)CO(OH) + HO_2^{\bullet}$	R(316)	$1.0\ 10^6$			17
Acetic acid formation by Peracetic Acid oxidation					
$CH_3CO(OH) + H_2O_2 + H^+ \rightarrow CH_3CO(OOH) + H_2O + H^+$	R(317)	$3.1\ 10^{-4}$	5235		= $k(CHO(OH) + H_2O_2 + H^+)$ - 38
$CH_3CO(OOH) + H_2O + H^+ \rightarrow CH_3CO(OH) + H_2O_2 + H^+$	R(318)	$3.8\ 10^{-4}$			= $k(CHO(OOH) + H_2O + H^+)$ - 38
$CH_3CO(OOH) + HSO_3^- \rightarrow CH_3CO(OH) + H_2SO_4 - H^+$	R(319)	$4.8 \cdot 10^7$	3990	Lind et al., 1987	
Glycolic acid formation by Hydroxyperacetic Acid oxidation					
$CH_2(OH)CO(OH) + H_2O_2 + H^+ \rightarrow CH_2(OH)CO(OOH) + H_2O + H^+$	R(320)	$3.1\ 10^{-4}$	5235		= $k(CHO(OH) + H_2O_2 + H^+)$ - 39
$CH_2(OH)CO(OOH) + H_2O + H^+ \rightarrow CH_2(OH)CO(OH) + H_2O_2 + H^+$	R(321)	$3.8\ 10^{-4}$			= $k(CHO(OOH) + H_2O + H^+)$ - 39
Oxidation of Acetic Acid					
$CH_3CO(OH) + HO^{\bullet} \rightarrow C^{\bullet}H_2CO(OH) + H_2O$		$1.5\ 10^7$	1330		
$C^{\bullet}H_2CO(OH) + O_2 \rightarrow CH_2(OO^{\bullet})CO(OH)$		$2.0\ 10^9$			2
$CH_3CO(OH) + HO^{\bullet} \rightarrow CH_2(OO^{\bullet})CO(OH) + H_2O - O_2$	R(322)	$1.5\ 10^7$	1330	Chin and Wine, 1994	

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CH_3CO(O^-) + HO^\bullet \rightarrow C^\bullet H_2CO(O^-) + H_2O$		$1.0\ 10^8$	1800		
$C^\bullet H_2CO(O^-) + O_2 \rightarrow CH_2(OO^\bullet)CO(O^-)$		$2.0\ 10^9$			2
$CH_3CO(O^-) + HO^\bullet \rightarrow CH_2(OO^\bullet)CO(O^-) + H_2O - O_2$	R(323)	$1.0\ 10^8$	1800	Fisher and Hamill, 1973	
$CH_3CO(OH) + NO_3^\bullet \rightarrow C^\bullet H_2CO(OH) + NO_3^- + H^+$		$1.3\ 10^4$	3800		
$C^\bullet H_2CO(OH) + O_2 \rightarrow CH_2(OO^\bullet)CO(OH)$		$2.0\ 10^9$			2
$CH_3CO(OH) + NO_3^\bullet \rightarrow CH_2(OO^\bullet)CO(OH) + NO_3^- + H^+ - O_2$	R(324)	$1.3\ 10^4$	3800	Exner et al., 1994	
$CH_3CO(O^-) + NO_3^\bullet \rightarrow C^\bullet H_2CO(O^-) + NO_3^- + H^+$		$2.3\ 10^6$	3800		
$C^\bullet H_2CO(O^-) + O_2 \rightarrow CH_2(OO^\bullet)CO(O^-)$					2
$CH_3CO(O^-) + NO_3^\bullet \rightarrow CH_2(OO^\bullet)CO(O^-) + NO_3^- + H^+ - O_2$	R(325)	$2.3\ 10^6$	3800	Exner et al., 1994	
$CH_3CO(O^-) + SO_4^{\bullet-} \rightarrow C^\bullet H_2CO(O^-) + SO_4^{2-} + H^+$		$5.1\ 10^6$			
$C^\bullet H_2CO(O^-) + O_2 \rightarrow CH_2(OO^\bullet)CO(O^-)$		$2.0\ 10^9$			2
$CH_3CO(O^-) + SO_4^{\bullet-} \rightarrow CH_2(OO^\bullet)CO(O^-) + SO_4^{2-} + H^+ - O_2$	R(326)	$5.1\ 10^6$		Huie and Clifton, 1990	
$CH_3CO(OH) + Cl_2^{\bullet-} \rightarrow C^\bullet H_2CO(OH) + 2\ Cl^- + H^+$		$1.5\ 10^3$	4930		
$C^\bullet H_2CO(OH) + O_2 \rightarrow CH_2(OO^\bullet)CO(OH)$		$2.0\ 10^9$			2
$CH_3CO(OH) + Cl_2^{\bullet-} \rightarrow CH_2(OO^\bullet)CO(OH) + 2\ Cl^- + H^+ - O_2$	R(327)	$1.5\ 10^3$	4930	Jacobi et al., 1999	
$CH_3CO(O^-) + Cl_2^{\bullet-} \rightarrow C^\bullet H_2CO(O^-) + 2\ Cl^- + H^+$		$2.6\ 10^6$	4800		
$C^\bullet H_2CO(O^-) + O_2 \rightarrow CH_2(OO^\bullet)CO(O^-)$		$2.0\ 10^9$			2
$CH_3CO(O^-) + Cl_2^{\bullet-} \rightarrow CH_2(OO^\bullet)CO(O^-) + 2\ Cl^- + H^+ - O_2$	R(328)	$2.6\ 10^6$	4800	Jacobi et al., 1996	
$CH_3CO(O^-) + CO_3^{\bullet-} \rightarrow C^\bullet H_2CO(O^-) + CO_3^{2-} + H^+$		$5.8\ 10^2$			
$C^\bullet H_2CO(O^-) + O_2 \rightarrow CH_2(OO^\bullet)CO(O^-)$		$2.0\ 10^9$			2
$CH_3CO(O^-) + CO_3^{\bullet-} \rightarrow CH_2(OO^\bullet)CO(O^-) + CO_3^{2-} + H^+ - O_2$	R(329)	$5.8\ 10^2$		Zellner et al., 1996	
Oxidation of Ethyl hydroperoxide (EHP)					
$CH_3CH_2(OOH) + Fe^{2+} \rightarrow CH_3CH_2(O^\bullet) + Fe^{3+} + OH^-$		$2.4\ 10^1$			
$CH_3CH_2(O^\bullet) \rightarrow CH_3C^\bullet H(OH)$		$5.0\ 10^5$			40 - 22
$CH_3C^\bullet H(OH) + O_2 \rightarrow CH_3CH(OH)(OO^\bullet)$		$4.6\ 10^9$		Adams and Willson, 1969	
$CH_3CH_2(OOH) + Fe^{2+} \rightarrow CH_3CH(OH)(OO^\bullet) + Fe^{3+} + OH^- - O_2$	R(330)	$2.4\ 10^1$		Chevallier et al., 2004	
Pathway 1: $CH_3CH_2(OOH) + HO^\bullet \rightarrow CH_3CH_2(OO^\bullet) + H_2O$		$4.6\ 10^8$		Monod et al., 2007	BR: 80%
Pathway 2: $CH_3CH_2(OOH) + HO^\bullet \rightarrow CH_3C^\bullet H(OOH) + H_2O$		$1.2\ 10^8$		Monod et al., 2007	BR: 20%
$CH_3C^\bullet H(OOH) + O_2 \rightarrow CH_3CH(OOH)(OO^\bullet)$		$2.0\ 10^9$			2
$CH_3CH_2(OOH) + HO^\bullet \rightarrow 0.80\ CH_3CH_2(OO^\bullet) + 0.20\ CH_3CH(OOH)(OO^\bullet) + H_2O - 0.20\ O_2$	R(331)	$5.8\ 10^8$		Monod et al., 2007	
$CH_3CH_2(OOH) + h\nu \rightarrow CH_3CH_2(O^\bullet) + HO^\bullet$		Calculated			
$CH_3CH_2(O^\bullet) + H_2O \rightarrow CH_3C^\bullet H(OH) + H_2O$		$5.0\ 10^5$			40
$CH_3C^\bullet H(OH) + O_2 \rightarrow CH_3CH(OH)(OO^\bullet)$		$4.6\ 10^9$		Adams and Willson, 1969	
$CH_3CH_2(OOH) + h\nu \rightarrow CH_3CH(OH)(OO^\bullet) + HO^\bullet - O_2$	R(332)	Calculated			= $J(H_2O_2)$
$CH_3CH(OOH)(OO^\bullet) + OH^- \rightarrow CH_3CH(OO^-)(OO^\bullet) + H_2O$		$4.0\ 10^9$			
$CH_3CH(OO^-)(OO^\bullet) \rightarrow CH_3CO(OH) + O_2^{\bullet-}$					11
$CH_3CH(OOH)(OO^\bullet) + OH^- \rightarrow CH_3CO(OH) + O_2^{\bullet-} + H_2O$	R(333)	$4.0\ 10^9$			= $k(CH_3CH(OH)(OO^\bullet) + OH^-)$ - 12
$CH_3CH(OOH)(OO^\bullet) \rightarrow CH_3CO(OH) + HO_2^\bullet$	R(334)	$1.9\ 10^2$			= $k(CH_3CH(OH)(OO^\bullet) \rightarrow CH_3CHO + HO_2^\bullet)$ - 41
Ethylperoxyl radical self-reaction					
Pathway 1: $2\ CH_3CH_2(OO^\bullet) \rightarrow 2\ CH_3CHO + H_2O_2$		$3.0\ 10^7$			BR: 20% - 42
Pathway 2: $2\ CH_3CH_2(OO^\bullet) \rightarrow 2\ CH_3CH_2(O^\bullet) + O_2$		$1.3\ 10^8$			BR: 80% - 42
$CH_3CH_2(O^\bullet) \rightarrow CH_3C^\bullet H(OH)$					10 - 22
$CH_3C^\bullet H(OH) + O_2 \rightarrow CH_3CH(OH)(OO^\bullet)$		$4.6\ 10^9$		Adams and Willson, 1969	

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
2 $CH_3CH_2(OO^\bullet)$ → 0.40 CH_3CHO + 1.60 $CH_3CH(OH)(OO^\bullet)$ + 0.20 H_2O_2 - 0.80 O_2	R(335)	1.6 10^8	-1600	Herrmann et al., 1999	
Oxidation of Acetic Acid Peroxyl radicals					
$CH_2(OO^\bullet)CO(OH)$ + $HO_2^\bullet$ → $CH_2(OOH)CO(OH)$ + O_2	R(336)	8.3 10^5	2700		= k($HO_2^\bullet$ + $HO_2^\bullet$)
$CH_2(OO^\bullet)CO(OH)$ + $O_2^{\bullet-}$ → $CH_2(OOH)CO(OH)$ + O_2 - H^+	R(337)	9.6 10^7	910		= k($HO_2^\bullet$ + $O_2^{\bullet-}$)
$CH_2(OO^\bullet)CO(OH)$ + HSO_3^- → $CH_2(OOH)CO(OH)$ + $SO_3^{\bullet-}$	R(338)	5.0 10^5			= k($CH_3(OO^\bullet)$ + HSO_3^-)
Pathway 1: 2 $CH_2(OO^\bullet)CO(OH)$ → 2 $CHOCO(OH)$ + H_2O_2		2.3 10^7			BR: 30% - 43
Pathway 2: 2 $CH_2(OO^\bullet)CO(OH)$ (+ *2 H_2O*) → 2 CH_2O + 2 CO_2 + H_2O_2 + 2 H_2O		2.3 10^7			BR: 30% - 43
Pathway 3: 2 $CH_2(OO^\bullet)CO(OH)$ → $CHOCO(OH)$ + $CH_2(OH)CO(OH)$ + O_2		2.3 10^7			BR: 30% - 43
Pathway 4: 2 $CH_2(OO^\bullet)CO(OH)$ → 2 $CH_2(O^\bullet)CO(OH)$ + O_2		6.0 10^6			BR: 10% - 43
$CH_2(O^\bullet)CO(OH)$ → $C^\bullet H(OH)CO(OH)$					10
$C^\bullet H(OH)CO(OH)$ + O_2 → $CH(OH)(OO^\bullet)CO(OH)$		2.0·10^9			2
2 $CH_2(OO^\bullet)CO(OH)$ → 0.90 $CHOCO(OH)$ + 0.30 $CH_2(OH)CO(OH)$ + 0.20 $CH(OH)(OO^\bullet)CO(OH)$ + 0.60 CH_2O + 0.60 CO_2 + 0.60 H_2O_2 + 0.20 O_2	R(339)	7.5 10^7			= k(2 $CH_2(OO^\bullet)CO(O^-)$) - 29
$CH_2(OO^\bullet)CO(O^-)$ + $HO_2^\bullet$ → $CH_2(OOH)CO(O^-)$ + O_2	R(340)	8.3 10^5	2700		= k($HO_2^\bullet$ + $HO_2^\bullet$)
$CH_2(OO^\bullet)CO(O^-)$ + $O_2^{\bullet-}$ → $CH_2(OOH)CO(O^-)$ + O_2 - H^+	R(341)	9.6 10^7	910		= k($HO_2^\bullet$ + $O_2^{\bullet-}$)
$CH_2(OO^\bullet)CO(O^-)$ + HSO_3^- → $CH_2(OOH)CO(O^-)$ + $SO_3^{\bullet-}$	R(342)	5.0 10^5			= k($CH_3(OO^\bullet)$ + HSO_3^-)
Pathway 1: 2 $CH_2(OO^\bullet)CO(O^-)$ → 2 $CHOCO(O^-)$ + H_2O_2		2.3 10^7		Schuchmann et al., 1985	BR: 30%
Pathway 2: 2 $CH_2(OO^\bullet)CO(O^-)$ (+ *2 H_2O*) → 2 CH_2O + 2 CO_2 + H_2O_2 + 2 OH^-		2.3 10^7		Schuchmann et al., 1985	BR: 30%
Pathway 3: 2 $CH_2(OO^\bullet)CO(O^-)$ → $CHOCO(O^-)$ + $CH_2(OH)CO(O^-)$ + O_2		2.3 10^7		Schuchmann et al., 1985	BR: 30%
Pathway 4: 2 $CH_2(OO^\bullet)CO(O^-)$ → 2 $CH_2(O^\bullet)CO(O^-)$ + O_2		6.0 10^6		Schuchmann et al., 1985	BR: 10%
$CH_2(O^\bullet)CO(O^-)$ → $C^\bullet H(OH)CO(O^-)$					10
$C^\bullet H(OH)CO(O^-)$ + O_2 → $CH(OH)(OO^\bullet)CO(O^-)$		2.0 10^9			2
2 $CH_2(OO^\bullet)CO(O^-)$ → 0.90 $CHOCO(O^-)$ + 0.30 $CH_2(OH)CO(O^-)$ + 0.20 $CH(OH)(OO^\bullet)CO(O^-)$ + 0.60 CH_2O + 0.60 CO_2 + 0.60 H_2O_2 + 0.60 OH^- + 0.20 O_2 - 0.60 H_2O	R(343)	7.5 10^7		Schuchmann et al., 1985	44
Oxidation of Oxalic acid					45
$CO(OH)CO(O^-)$ + $HO^\bullet$ → $C_2O_4^{\bullet-}$ + H_2O	R(344)	1.9 10^8	2800	Ervens et al., 2003	
$CO(O^-)CO(O^-)$ + $HO^\bullet$ → $C_2O_4^{\bullet-}$ + OH^-	R(345)	1.6 10^8	4300	Ervens et al., 2003	
$CO(OH)CO(O^-)$ + $SO_4^{\bullet-}$ → $C_2O_4^{\bullet-}$ + SO_4^{2-} + H^+	R(346)	1.7 10^6		Grgić et al., 2007	
$CO(O^-)CO(O^-)$ + $SO_4^{\bullet-}$ → $C_2O_4^{\bullet-}$ + SO_4^{2-}	R(347)	1.3 10^7		Grgić et al., 2007	
$C_2O_4^{\bullet-}$ + O_2 → $CO_2^{\bullet-}$ + CO_2		2.0 10^6		Mulazzani et al., 1986	
$CO_2^{\bullet-}$ + O_2 → CO_2 + $O_2^{\bullet-}$		2.4 10^9		Hislop and Bolton, 1999	
$C_2O_4^{\bullet-}$ + O_2 → 2 CO_2 + $O_2^{\bullet-}$	R(348)	2.4 10^9		Hislop and Bolton, 1999	
$CO(O^-)CO(O^-)$ + Fe^{3+} → $[Fe(C_2O_4)]^+$	R(349)	7.5 10^6			46
$[Fe(C_2O_4)]^+$ → $CO(O^-)CO(O^-)$ + Fe^{3+}	R(350)	3.0 10^{-3}		Moorhead and Sutin, 1966	47
$CO(O^-)CO(O^-)$ + $[Fe(C_2O_4)]^+$ → $[Fe(C_2O_4)_2]^-$	R(351)	1.9 10^4			46
$[Fe(C_2O_4)_2]^-$ → $CO(O^-)CO(O^-)$ + $[Fe(C_2O_4)]^+$	R(352)	3.0 10^{-3}			= k($[Fe(C_2O_4)]^+$ → $CO(O^-)CO(O^-)$ + Fe^{3+})
$CO(O^-)CO(O^-)$ + $[Fe(C_2O_4)_2]^-$ → $[Fe(C_2O_4)_3]^{3-}$	R(353)	4.8 10^1			46
$[Fe(C_2O_4)_3]^{3-}$ → $CO(O^-)CO(O^-)$ + $[Fe(C_2O_4)_2]^-$	R(354)	3.0 10^{-3}			= k($[Fe(C_2O_4)]^+$ → $CO(O^-)CO(O^-)$ + Fe^{3+})

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$[Fe(C_2O_4)]^+ + hv \rightarrow Fe^{2+} + C_2O_4^{\bullet-}$	R(355)	Calculated		Long et al., 2013	
$[Fe(C_2O_4)_2]^- + hv \rightarrow Fe^{2+} + CO(O^-)CO(O^-) + C_2O_4^{\bullet-}$	R(356)	Calculated		Faust and Zepp, 1993	
$[Fe(C_2O_4)_3]^{3-} + hv \rightarrow Fe^{2+} + 2\ CO(O^-)CO(O^-) + C_2O_4^{\bullet-}$	R(357)	Calculated		Faust and Zepp, 1993	
Oxidation of 2-hydroperoxyacetic Acid					
Pathway 1: $CH_2(OOH)CO(OH) + HO^\bullet \rightarrow CH_2(OO^\bullet)CO(OH) + H_2O$		$4.6\ 10^8$			BR: 80% - 48
Pathway 2: $CH_2(OOH)CO(OH) + HO^\bullet \rightarrow C^\bullet H(OOH)CO(OH) + H_2O$		$1.2\ 10^8$			BR: 20% - 48
$C^\bullet H(OOH)CO(OH) + O_2 \rightarrow CH(OOH)(OO^\bullet)CO(OH)$		$2.0\ 10^9$			2
$CH_2(OOH)CO(OH) + HO^\bullet \rightarrow 0.80\ CH_2(OO^\bullet)CO(OH) + 0.20\ CH(OOH)(OO^\bullet)CO(OH) + H_2O - 0.20\ O_2$	R(358)	$5.8\ 10^8$			= $k(CH_3CH_2(OOH) + HO^\bullet)$
Pathway 1: $CH_2(OOH)CO(OH) + NO_3^\bullet \rightarrow CH_2(OO^\bullet)CO(OH) + NO_3^- + H^+$		$1.4\ 10^6$			BR: 80%
Pathway 2: $CH_2(OOH)CO(OH) + NO_3^\bullet \rightarrow C^\bullet H(OOH)CO(OH) + NO_3^- + H^+$		$3.0\ 10^5$			BR: 20%
$C^\bullet H(OOH)CO(OH) + O_2 \rightarrow CH(OOH)(OO^\bullet)CO(OH)$		$2.0\ 10^9$			2
$CH_2(OOH)CO(OH) + NO_3^\bullet \rightarrow 0.80\ CH_2(OO^\bullet)CO(OH) + 0.20\ CH(OOH)(OO^\bullet)CO(OH) + NO_3^- + H^+ - 0.20\ O_2$	R(359)	$1.7\ 10^6$		Herrmann and Zellner, 1998	3
$CH_2(OOH)CO(OH) + Fe^{2+} \rightarrow CH_2(O^\bullet)CO(OH) + Fe^{3+} + OH^-$		$2.4\ 10^1$			
$CH_2(O^\bullet)CO(OH) \rightarrow CH_2O + C^\bullet O(OH)$					21 - 22
$C^\bullet O(OH) + O_2 \rightarrow CO(OH)(OO^\bullet)$		$2.0\ 10^9$			2
$CH_2(OOH)CO(OH) + Fe^{2+} \rightarrow CH_2O + CO(OH)(OO^\bullet) + Fe^{3+} + OH^- - O_2$	R(360)	$2.4\ 10^1$			= $k(CH_3CH_2(OOH) + Fe^{2+})$
$CH_2(OOH)CO(OH) + hv \rightarrow CH_2(O^\bullet)CO(OH) + HO^\bullet$		Calculated			
$CH_2(O^\bullet)CO(OH) \rightarrow CH_2O + C^\bullet O(OH)$					21 - 22
$C^\bullet O(OH) + O_2 \rightarrow CO(OH)(OO^\bullet)$		$2.0\ 10^9$			2
$CH_2(OOH)CO(OH) + hv \rightarrow CH_2O + CO(OH)(OO^\bullet) + HO^\bullet - O_2$	R(361)	Calculated			= $J(CH_3CH_2(OOH) + hv)$
Pathway 1: $CH_2(OOH)CO(O^-) + HO^\bullet \rightarrow CH_2(OO^\bullet)CO(O^-) + H_2O$		$4.6\ 10^8$			BR: 80% - 48
Pathway 2: $CH_2(OOH)CO(O^-) + HO^\bullet \rightarrow C^\bullet H(OOH)CO(O^-) + H_2O$		$1.2\ 10^8$			BR: 20% - 48
$C^\bullet H(OOH)CO(O^-) + O_2 \rightarrow CH(OOH)(OO^\bullet)CO(O^-)$		$2.0\ 10^9$			2
$CH_2(OOH)CO(O^-) + HO^\bullet \rightarrow 0.80\ CH_2(OO^\bullet)CO(O^-) + 0.20\ CH(OOH)(OO^\bullet)CO(O^-) + H_2O - 0.20\ O_2$	R(362)	$5.8\ 10^8$			= $k(CH_3CH_2(OOH) + HO^\bullet)$
Pathway 1: $CH_2(OOH)CO(O^-) + NO_3^\bullet \rightarrow CH_2(OO^\bullet)CO(O^-) + NO_3^- + H^+$		$5.7\ 10^6$			BR: 80%
Pathway 2: $CH_2(OOH)CO(O^-) + NO_3^\bullet \rightarrow C^\bullet H(OOH)CO(O^-) + NO_3^- + H^+$		$1.4\ 10^6$			BR: 20%
$C^\bullet H(OOH)CO(O^-) + O_2 \rightarrow CH(OOH)(OO^\bullet)CO(O^-)$		$2.0\ 10^9$			2
$CH_2(OOH)CO(O^-) + NO_3^\bullet \rightarrow 0.80\ CH_2(OO^\bullet)CO(O^-) + 0.20\ CH(OOH)(OO^\bullet)CO(O^-) + NO_3^- + H^+ - 0.20\ O_2$	R(363)	$7.1\ 10^6$		Herrmann and Zellner, 1998	3
$CH_2(OOH)CO(O^-) + Fe^{2+} \rightarrow CH_2(O^\bullet)CO(O^-) + Fe^{3+} + OH^-$		$2.4\ 10^1$			
$CH_2(O^\bullet)CO(O^-) \rightarrow CH_2O + C^\bullet O(O^-)$					21 - 22
$C^\bullet O(O^-) + O_2 \rightarrow CO(O^-)(OO^\bullet)$		$2.0\ 10^9$			2
$CO(O^-)(OO^\bullet) \rightarrow CO_2 + O_2^{\bullet-}$					5
$CH_2(OOH)CO(O^-) + Fe^{2+} \rightarrow CH_2O + CO_2 + Fe^{3+} + OH^- + O_2^{\bullet-} - O_2$	R(364)	$2.4\ 10^1$			= $k(CH_3CH_2(OOH) + Fe^{2+})$
$CH_2(OOH)CO(O^-) + hv \rightarrow CH_2(O^\bullet)CO(O^-) + HO^\bullet$		Calculated			
$CH_2(O^\bullet)CO(O^-) + H_2O \rightarrow C^\bullet H(OH)CO(O^-) + H_2O$		$8.0\ 10^6$			10
$C^\bullet H(OH)CO(O^-) + O_2 \rightarrow CH(OH)(OO^\bullet)CO(O^-)$		$2.0\ 10^9$			2
$CH_2(OOH)CO(O^-) + hv \rightarrow CH(OH)(OO^\bullet)CO(O^-) + HO^\bullet - O_2$	R(365)	Calculated			= $J(CH_3CH_2(OOH) + hv)$
$CH(OOH)(OO^\bullet)CO(OH) + OH^- \rightarrow CH(OO^-)(OO^\bullet)CO(OH) + H_2O$		$4.0\ 10^9$			
$CH(OO^-)(OO^\bullet)CO(OH) \rightarrow CO(OH)CO(OH) + O_2^{\bullet-}$					11
$CH(OOH)(OO^\bullet)CO(OH) + OH^- \rightarrow CO(OH)CO(OH) + O_2^{\bullet-} + H_2O$	R(366)	$4.0\ 10^9$			= $k(CH_3CH(OH)(OO^\bullet) + OH^-)$ - 12
$CH(OOH)(OO^\bullet)CO(OH) \rightarrow CO(OH)CO(OH) + HO_2^\bullet$	R(367)	$1.9\ 10^2$			= $k(CH(OH)(OO^\bullet)CO(OH) \rightarrow CHOCO(OH) + HO_2^\bullet)$ - 49

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CH(OOH)(OO^{\bullet})CO(O^{-}) + OH^{-} \rightarrow CH(OO^{-})(OO^{\bullet})CO(O^{-}) + H_2O$		$4.0\ 10^{9}$			
$CH(OO^{-})(OO^{\bullet})CO(O^{-}) \rightarrow CO(OH)CO(O^{-}) + O_2^{\bullet-}$					11
$CH(OOH)(OO^{\bullet})CO(O^{-}) + OH^{-} \rightarrow CO(OH)CO(O^{-}) + O_2^{\bullet-} + H_2O$	R(368)	$4.0\ 10^{9}$			= $k(CH_3CH(OH)(OO^{\bullet}) + OH^{-})$ - 12
$CH(OOH)(OO^{\bullet})CO(O^{-}) \rightarrow CO(OH)CO(O^{-}) + HO_2^{\bullet}$	R(369)	$1.9\ 10^{2}$			= $k(CH(OH)(OO^{\bullet})CO(O^{-}) \rightarrow CHOCO(O^{-}) + HO_2^{\bullet})$ - 50
Oxidation of Glycolic acid					
Pathway 1: $CH_2(OH)CO(OH) + HO^{\bullet} \rightarrow C^{\bullet}H(OH)CO(OH) + H_2O$		$3.7\ 10^{8}$			BR: 62% - 15
$C^{\bullet}H(OH)CO(OH) + O_2 \rightarrow CH(OH)(OO^{\bullet})CO(OH)$		$2.0\ 10^{9}$			2
Pathway 2: $CH_2(OH)CO(OH) + HO^{\bullet} \rightarrow CH_2(O^{\bullet})CO(OH) + H_2O$		$2.3\ 10^{8}$			BR: 38% - 15
$CH_2(O^{\bullet})CO(OH) \rightarrow CH_2O + C^{\bullet}O(OH)$					21 - 22
$C^{\bullet}O(OH) + O_2 \rightarrow CO(OH)(OO^{\bullet})$		$2.0\ 10^{9}$			2
$CH_2(OH)CO(OH) + HO^{\bullet} \rightarrow 0.62\ CH(OH)(OO^{\bullet})CO(OH) + 0.38\ CH_2O + 0.38\ CO(OH)(OO^{\bullet}) + H_2O - O_2$	R(370)	$6.0\ 10^{8}$		Buxton et al., 1988	
Pathway 1: $CH_2(OH)CO(OH) + NO_3^{\bullet} \rightarrow C^{\bullet}H(OH)CO(OH) + NO_3^{-} + H^{+}$		$5.6\ 10^{5}$			BR: 62%
$C^{\bullet}H(OH)CO(OH) + O_2 \rightarrow CH(OH)(OO^{\bullet})CO(OH)$		$2.0\ 10^{9}$			2
Pathway 2: $CH_2(OH)CO(OH) + NO_3^{\bullet} \rightarrow CH_2(O^{\bullet})CO(OH) + NO_3^{-} + H^{+}$		$3.5\ 10^{5}$			BR: 38%
$CH_2(O^{\bullet})CO(OH) \rightarrow CH_2O + C^{\bullet}O(OH)$					21 - 22
$C^{\bullet}O(OH) + O_2 \rightarrow CO(OH)(OO^{\bullet})$		$2.0\ 10^{9}$			2
$CH_2(OH)CO(OH) + NO_3^{\bullet} \rightarrow 0.62\ CH(OH)(OO^{\bullet})CO(OH) + 0.38\ CH_2O + 0.38\ CO(OH)(OO^{\bullet}) + NO_3^{-} + H^{+} - O_2$	R(371)	$9.1\ 10^{5}$	3971	De Semainville et al., 2007	3
$CH(OH)(OO^{\bullet})CO(OH) + OH^{-} \rightarrow CH(O^{-})(OO^{\bullet})CO(OH) + H_2O$		$4.0\ 10^{9}$			
$CH(O^{-})(OO^{\bullet})CO(OH) \rightarrow CHOCO(OH) + O_2^{\bullet-}$					5
$CH(OH)(OO^{\bullet})CO(OH) + OH^{-} \rightarrow CHOCO(OH) + O_2^{\bullet-} + H_2O$	R(372)	$4.0\ 10^{9}$			= $k(CH_3CH(OH)(OO^{\bullet}) + OH^{-})$
$CH(OH)(OO^{\bullet})CO(OH) \rightarrow CHOCO(OH) + HO_2^{\bullet}$	R(373)	$1.9\ 10^{2}$			4
Pathway 1: $CH_2(OH)CO(O^{-}) + HO^{\bullet} \rightarrow C^{\bullet}H(OH)CO(O^{-}) + H_2O$		$5.2\ 10^{8}$			BR: 60% - 15
$C^{\bullet}H(OH)CO(O^{-}) + O_2 \rightarrow CH(OH)(OO^{\bullet})CO(O^{-})$		$2.0\ 10^{9}$			2
Pathway 2: $CH_2(OH)CO(O^{-}) + HO^{\bullet} \rightarrow CH_2(O^{\bullet})CO(O^{-}) + H_2O$		$1.6\ 10^{8}$			BR: 19% - 15
$CH_2(O^{\bullet})CO(O^{-}) \rightarrow CH_2O + C^{\bullet}O(O^{-})$					21 - 22
$C^{\bullet}O(O^{-}) + O_2 \rightarrow CO(O^{-})(OO^{\bullet})$		$2.0\ 10^{9}$			2
$CO(O^{-})(OO^{\bullet}) \rightarrow CO_2 + O_2^{\bullet-}$					5
Pathway 3: $CH_2(OH)CO(O^{-}) + HO^{\bullet} \rightarrow CH_2(OH)CO(O^{\bullet}) + OH^{-}$		$1.8\ 10^{8}$			BR: 21% - 15
$CH_2(OH)CO(O^{\bullet}) \rightarrow C^{\bullet}H_2(OH) + CO_2$					21 - 22
$C^{\bullet}H_2(OH) + O_2 \rightarrow CH_2(OH)(OO^{\bullet})$		$2.0\ 10^{9}$			2
$CH_2(OH)CO(O^{-}) + HO^{\bullet} \rightarrow 0.60\ CH(OH)(OO^{\bullet})CO(O^{-}) + 0.21\ CH_2(OH)(OO^{\bullet}) + 0.19\ CH_2O + 0.40\ CO_2 + 0.19\ O_2^{\bullet-} + 0.21\ OH^{-} + 0.79\ H_2O - O_2$	R(374)	$8.6\ 10^{8}$		Buxton et al., 1988	
Pathway 1: $CH_2(OH)CO(O^{-}) + NO_3^{\bullet} \rightarrow C^{\bullet}H(OH)CO(O^{-}) + NO_3^{-} + H^{+}$		$7.6\ 10^{6}$			BR: 76%
$C^{\bullet}H(OH)CO(O^{-}) + O_2 \rightarrow CH(OH)(OO^{\bullet})CO(O^{-})$		$2.0\ 10^{9}$			2
Pathway 2: $CH_2(OH)CO(O^{-}) + NO_3^{\bullet} \rightarrow CH_2(O^{\bullet})CO(O^{-}) + NO_3^{-} + H^{+}$		$2.4\ 10^{6}$			BR: 24%
$CH_2(O^{\bullet})CO(O^{-}) \rightarrow CH_2O + C^{\bullet}O(O^{-})$					21 - 22
$C^{\bullet}O(O^{-}) + O_2 \rightarrow CO(O^{-})(OO^{\bullet})$		$2.0\ 10^{9}$			2
$CO(O^{-})(OO^{\bullet}) \rightarrow CO_2 + O_2^{\bullet-}$					5
$CH_2(OH)CO(O^{-}) + NO_3^{\bullet} \rightarrow 0.76\ CH(OH)(OO^{\bullet})CO(O^{-}) + 0.24\ CH_2O + 0.24\ CO_2 + 0.24\ O_2^{\bullet-} + NO_3^{-} + H^{+} - O_2$	R(375)	$1.0\ 10^{7}$	3008	De Semainville et al., 2007	3
$CH(OH)(OO^{\bullet})CO(O^{-}) + OH^{-} \rightarrow CH(O^{-})(OO^{\bullet})CO(O^{-}) + H_2O$		$4.0\ 10^{9}$			
$CH(O^{-})(OO^{\bullet})CO(O^{-}) \rightarrow CHOCO(O^{-}) + O_2^{\bullet-}$					5
$CH(OH)(OO^{\bullet})CO(O^{-}) + OH^{-} \rightarrow CHOCO(O^{-}) + O_2^{\bullet-} + H_2O$	R(376)	$4.0\ 10^{9}$			= $k(CH_3CH(OH)(OO^{\bullet}) + OH^{-})$

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CH(OH)(OO^{\bullet})CO(O^{-}) \rightarrow CHOCO(O^{-}) + HO_2^{\bullet}$	R(377)	$1.9\ 10^{2}$			4
Oxidation of Glyoxylic acid					51
Pathway 1: $CH(OH)(OH)CO(OH) + HO^{\bullet} \rightarrow C^{\bullet}(OH)(OH)CO(OH) + H_2O$		$5.0\ 10^{7}$			BR: 15% - 15
$C^{\bullet}(OH)(OH)CO(OH) + O_2 \rightarrow CO(OH)C(OH)(OH)(OO^{\bullet})$		$2.0\ 10^{9}$			2
Pathway 2: $CH(OH)(OH)CO(OH) + HO^{\bullet} \rightarrow CH(O^{\bullet})(OH)CO(OH) + H_2O$		$2.8\ 10^{8}$			BR: 85% - 15
$CH(O^{\bullet})(OH)CO(OH) \rightarrow CHO(OH) + C^{\bullet}O(OH)$					21 - 22
$C^{\bullet}O(OH) + O_2 \rightarrow CO(OH)(OO^{\bullet})$		$2.0\ 10^{9}$			2
$CH(OH)(OH)CO(OH) + HO^{\bullet} \rightarrow 0.15\ CO(OH)C(OH)(OH)(OO^{\bullet}) + 0.85\ CHO(OH) + 0.85\ CO(OH)(OO^{\bullet}) + H_2O - O_2$	R(378)	$3.3\ 10^{8}$	1000	Ervens et al., 2003 - corrected by Schaefer, 2012	52
Pathway 1: $CH(OH)(OH)CO(OH) + NO_3^{\bullet} \rightarrow C^{\bullet}(OH)(OH)CO(OH) + H^{+} + NO_3^{-}$		$2.0\ 10^{5}$			BR: 15%
$C^{\bullet}(OH)(OH)CO(OH) + O_2 \rightarrow CO(OH)C(OH)(OH)(OO^{\bullet})$		$2.0\ 10^{9}$			2
Pathway 2: $CH(OH)(OH)CO(OH) + NO_3^{\bullet} \rightarrow CH(O^{\bullet})(OH)CO(OH) + H^{+} + NO_3^{-}$		$9.0\ 10^{5}$			BR: 85%
$CH(O^{\bullet})(OH)CO(OH) \rightarrow CHO(OH) + C^{\bullet}O(OH)$					21 - 22
$C^{\bullet}O(OH) + O_2 \rightarrow CO(OH)(OO^{\bullet})$		$2.0\ 10^{9}$			2
$CH(OH)(OH)CO(OH) + NO_3^{\bullet} \rightarrow 0.15\ CO(OH)C(OH)(OH)(OO^{\bullet}) + 0.85\ CHO(OH) + 0.85\ CO(OH)(OO^{\bullet}) + H^{+} + NO_3^{-} - O_2$	R(379)	$1.0\ 10^{6}$			= k(CH(OH)(OH)CH(OH)(OH) + $NO_3^{\bullet}$) - 3
Pathway 1: $CH(OH)(OH)CO(O^{-}) + HO^{\bullet} \rightarrow C^{\bullet}(OH)(OH)CO(O^{-}) + H_2O$		$6.0\ 10^{8}$			BR: 26% - 53
$C^{\bullet}(OH)(OH)CO(O^{-}) + O_2 \rightarrow CO(O^{-})C(OH)(OH)(OO^{\bullet})$		$2.0\ 10^{9}$			2
Pathway 2: $CH(OH)(OH)CO(O^{-}) + HO^{\bullet} \rightarrow CH(O^{\bullet})(OH)CO(O^{-}) + H_2O$		$1.9\ 10^{9}$			BR: 74% - 53
$CH(O^{\bullet})(OH)CO(O^{-}) \rightarrow CHO(OH) + C^{\bullet}O(O^{-})$					21 - 22
$C^{\bullet}O(O^{-}) + O_2 \rightarrow CO(O^{-})(OO^{\bullet})$		$2.0\ 10^{9}$			2
$CO(O^{-})(OO^{\bullet}) \rightarrow CO_2 + O_2^{\bullet-}$					5
$CH(OH)(OH)CO(O^{-}) + HO^{\bullet} \rightarrow 0.26\ CO(O^{-})C(OH)(OH)(OO^{\bullet}) + 0.74\ CHO(OH) + 0.74\ CO_2 + 0.74\ O_2^{\bullet-} + H_2O - O_2$	R(380)	$2.5\ 10^{9}$	4300	Ervens et al., 2003 corrected by Schaefer, 2012	52
Pathway 1: $CH(OH)(OH)CO(O^{-}) + NO_3^{\bullet} \rightarrow C^{\bullet}(OH)(OH)CO(O^{-}) + H^{+} + NO_3^{-}$		$5.0\ 10^{4}$			BR: 26%
$C^{\bullet}(OH)(OH)CO(O^{-}) + O_2 \rightarrow CO(O^{-})C(OH)(OH)(OO^{\bullet})$		$2.0\ 10^{9}$			2
Pathway 2: $CH(OH)(OH)CO(O^{-}) + NO_3^{\bullet} \rightarrow CH(O^{\bullet})(OH)CO(O^{-}) + H^{+} + NO_3^{-}$		$1.3\ 10^{5}$			BR: 74%
$CH(O^{\bullet})(OH)CO(O^{-}) \rightarrow CHO(OH) + C^{\bullet}O(O^{-})$					21 - 22
$C^{\bullet}O(O^{-}) + O_2 \rightarrow CO(O^{-})(OO^{\bullet})$		$2.0\ 10^{9}$			2
$CO(O^{-})(OO^{\bullet}) \rightarrow CO_2 + O_2^{\bullet-}$					5
$CH(OH)(OH)CO(O^{-}) + NO_3^{\bullet} \rightarrow 0.26\ CO(O^{-})C(OH)(OH)(OO^{\bullet}) + 0.74\ CHO(OH) + 0.74\ CO_2 + 0.74\ O_2^{\bullet-} + NO_3^{-} + H^{+} - O_2$	R(381)	$1.8\ 10^{5}$		Herrmann and Zellner, 1998	3
$CH(OH)(OH)CO(O^{-}) + H_2O_2 \rightarrow CHO(O^{-}) + CO_2 + 2\ H_2O$	R(382)	$1.1\ 10^{-1}$		Schöne and Herrmann, 2014	
$CO(OH)C(OH)(OH)(OO^{\bullet}) + OH^{-} \rightarrow CO(OH)C(OH)(O^{-})(OO^{\bullet}) + H_2O$		$4.0\ 10^{9}$			
$CO(OH)C(OH)(O^{-})(OO^{\bullet}) \rightarrow CO(OH)CO(OH) + O_2^{\bullet-}$					5
$CO(OH)C(OH)(OH)(OO^{\bullet}) + OH^{-} \rightarrow CO(OH)CO(OH) + O_2^{\bullet-} + H_2O$	R(383)	$4.0\ 10^{9}$			= k($CH_3CH(OH)(OO^{\bullet}) + OH^{-}$)
$CO(OH)C(OH)(OH)(OO^{\bullet}) \rightarrow CO(OH)CO(OH) + HO_2^{\bullet}$	R(384)	$1.0\ 10^{6}$			17
$CO(O^{-})C(OH)(OH)(OO^{\bullet}) + OH^{-} \rightarrow CO(O^{-})C(OH)(O^{-})(OO^{\bullet}) + H_2O$		$4.0\ 10^{9}$			
$CO(O^{-})C(OH)(O^{-})(OO^{\bullet}) \rightarrow CO(O^{-})CO(OH) + O_2^{\bullet-}$					5
$CO(O^{-})C(OH)(OH)(OO^{\bullet}) + OH^{-} \rightarrow CO(O^{-})CO(OH) + O_2^{\bullet-} + H_2O$	R(385)	$4.0\ 10^{9}$			= k($CH_3CH(OH)(OO^{\bullet}) + OH^{-}$)
$CO(O^{-})C(OH)(OH)(OO^{\bullet}) \rightarrow CO(O^{-})CO(OH) + HO_2^{\bullet}$	R(386)	$1.0\ 10^{6}$			17

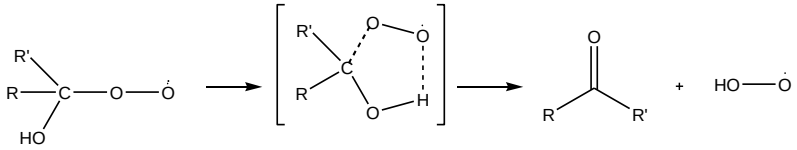
Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
R(OO•) produced by C3 oxidation					54
Pathway 1: 2 $CHOCH_2(OO^•)$ → 2 CHOCHO + H_2O_2		1.8 10^8			BR: 45%
Pathway 2: 2 $CHOCH_2(OO^•)$ → CHOCHO + $CH_2(OH)CHO$ + O_2		8.0 10^7			BR: 20%
Pathway 3: 2 $CHOCH_2(OO^•)$ →2 $CHOCH_2(O^•)$ + O_2		1.4 10^8			BR: 35%
$CHOCH_2(O^•)$ → $C^•HO$ + CH_2O					21 - 22
$C^•HO$ + O_2 → $CHO(OO^•)$		2.0 10^9			2
2 $CHOCH_2(OO^•)$ → 1.10 CHOCHO + 0.20 $CH_2(OH)CHO$ + 0.70 CH_2O + 0.70 $CHO(OO^•)$ + 0.45 H_2O_2 - 0.15 O_2	R(387)	4.0 10^8			= k(2 $CH_3COCH_2(OO^•)$) - 29
Pathway 1: 2 $CH(OH)(OH)CH_2(OO^•)$+ *2 H_2O* → 2 $CH(OH)(OH)CH(OH)(OH)$ + H_2O_2		1.8 10^8			BR: 45%
Pathway 2: 2 $CH(OH)(OH)CH_2(OO^•)$ + *H_2O* → $CH(OH)(OH)CH(OH)(OH)$ + $CH_2(OH)CH(OH)(OH)$ + O_2		8.0 10^7			BR: 20%
Pathway 3: 2 $CH(OH)(OH)CH_2(OO^•)$ → 2 $CH(OH)(OH)CH_2(O^•)$ + O_2		1.4 10^8			BR: 35%
$CH(OH)(OH)CH_2(O^•)$ → $C^•H(OH)(OH)$ + CH_2O					21 - 22
$C^•H(OH)(OH)$ + O_2 → $CH(OH)(OH)(OO^•)$		2.0 10^9			2
2 $CH(OH)(OH)CH_2(OO^•)$ → 1.10 $CH(OH)(OH)CH(OH)(OH)$ + 0.20 $CH_2(OH)CH(OH)(OH)$ + 0.70 CH_2O + 0.70 $CH(OH)(OH)(OO^•)$ + 0.45 H_2O_2 - 0.15 O_2	R(388)	4.0 10^8			= k(2 $CH_3COCH_2(OO^•)$) - 29

1 - The reactivity of HMHP with $HO^•$ is supposed similar to the reactivity of MHP with $HO^•$. $k(CH_2(OOH)(OH) + HO^•) = k(CH_3(OOH) + HO^•)$ and the branching ratio are identical to those measured by Monod et al. (2007) for MHP.

2 - We assumed a fast rate constant equal to 2.0 10^9 M^{-1} s^{-1} based on values compiled in Neta et al. (1990). This reaction is not a rate-determining step.

3 - The oxidation by the radicals ($NO_3^•$, $SO_4^{•-}$, $Cl^•$, $Cl_2^{•-}$, $CO_3^{•-}$) is supposed to produce the same $R(OO^•)$ as the oxidation by $HO^•$ with the same branching ratios. The electron transfer pathways are not considered for these radicals.

4 - The $HO_2^•$ elimination rate constant depends on the substituent attached to the carbon atom bearing the peroxyl function.



Von Sonntag (1987) compiled the following rate constants for :

R	R'	k (s^{-1})
H	H	<10
H	CH_3	52
H	$CH_2(OH)$	190
CH_3	CH_3	665

For secondary carbon atom bearing the peroxyl function, we assumed a rate of 665 s^{-1}.

For primary carbon atom, we assumed a value of 52 s^{-1}. If the neighboring carbon atom is bearing an oxygenated function, we assumed a value of 190 s^{-1}.

5 - Non-limiting reaction following Bothe et al. (1978).

6 - We suppose that the $HO_2^•$ elimination for $CH(OH)(OOH)(OO^•)$ is similar to the one for $RC(OH)(OH)(OO^•)$ with the same rate constant equal to 1.0 10^6 s^{-1}.

7 - We followed the work from De Filippis et al. (2009); rate constants have been recalculated at 25°C; we supposed a slow production of CO_2.

The equilibrium is explicitly considered because the formation of performic acid is slow.

8 - Following Monod et al., (2007), the branching ratio is assumed to be 80/20.

9 - The branching ratio is estimated to be 20% by Schuchmann and von Sonntag (1984) for the CH_2O formation. Monod et al. (2007) estimated that the alkoxyl radical formation pathway ($CH_3O^\bullet$) is the main pathway. We therefore assumed a branching ratio of 80% for this pathway.

10 - DeCosta and Pincock (1989) showed that electron transfer proceeds with a rate constant around 1.0 10^{10} s^{-1}. We assumed that the electron transfer is non limiting.

11 - We suppose that this step is a non-limiting reaction.

12 - We suppose that the H-abstraction on the (OOH)($OO^\bullet$) group by OH^- proceeds as fast as the H-abstraction for the (OH)($OO^\bullet$) group (k = 4.0 10^9 M^{-1} s^{-1}).

13 - We suppose that the $HO_2^\bullet$ elimination from CH_2(OOH)($OO^\bullet$) is as fast as the one of CH_2(OH)($OO^\bullet$).

14 - We consider only the reactivity of the hydrated form that represent 99% of the total formaldehyde.

15 - Branching ratios are calculated by the SAR from Doussin and Monod (2013).

16 - The rate constant comes from the literature; the branching ratio are estimated by the SAR from Doussin and Monod (2013).

17 - Von Sonntag (1987) et Schuchmann and Von Sonntag (1988) have shown that the $HO_2^\bullet$ elimination for RC(OH)(OH)($OO^\bullet$) species is fast. This is confirmed by Mc Elroy and Waygood (1991) for hydrated formaldehyde. We supposed a kinetic constant equal to 1.0 10^6 s^{-1}.

18 - We suppose that the $HO_2^\bullet$ elimination for CO(OH)($OO^\bullet$) is similar to the one for RC(OH)(OH)($OO^\bullet$) with the same rate constant equal to 1.0 10^6 s^{-1}.

19 - This reaction is non-limiting following Bothe et al. (1978). We consider a rate constant of 1.0 10^6 s^{-1}.

20 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 87% for CH_2, 9% for CH_3 and 4% for (OH). The 2 first pathways are considered corresponding to 96% of the total reactivity. They have been scaled to 90/10%.

21 - Hilborn and Pincock (1991) showed that acyl alkoxyl radical RCO($O^\bullet$) are fragmented with a rate constant around 1.0 10^9 s^{-1}. We assumed that the alkoxy fragmentation is non limiting.

22 - For alkoxyl radical, we assume an electron transfer reaction. When an oxygenated functional group is in β-position, we assume a fragmentation of the corresponding c-c bond. When there are two oxygenated function in β-position, we assume that the fragmentation occurs in priority on the C-CO(OH) bond.

23 - 3 pathways are considered corresponding to 90% of the total reactivity. Branching ratio in Piesiak et al. (1984) are 45/30/15%. They have been scaled to 50/33/17%.

24 - K_h = 1.2; we consider the reactivity of the hydrated and non-hydrated forms.

25 - Branching ratios are calculated by the SAR from Doussin and Monod (2013). The major pathway is the H-abstraction from CHO (97%) and is the only considered way. It has been scaled to 100%.

26 - Rousse and George (2004) measured global rate constant for acetaldehyde. We decompose it into the sum of k($CH_3CHO + NO_3^\bullet$) and k($CH_3CH(OH)(OH) + NO_3^\bullet$) weighted by the proportion of the hydrated and the non-hydrated form : $k_{global} = k(CH_3CHO+NO_3\cdot)\times\frac{1}{1+K_h} + k(CH_3CH(OH)(OH)+NO_3\cdot)\times\frac{K_h}{1+K_h}$ To determine k($CH_3CHO + NO_3^\bullet$) and k($CH_3CH(OH)(OH) + NO_3^\bullet$), we assumed that their ratio is equal to the ratio $\frac{k(CH_3CHO+HO\cdot)}{k(CH_3CH(OH)(OH)+HO\cdot)}$. k_{global} = 2.0 10^6 M^{-1} s^{-1} and k($CH_3CHO + NO_3^\bullet$) = 3.1 10^6 M^{-1} s^{-1} and k($CH_3CH(OH)(OH) + NO_3^\bullet$) = 1.1 10^6 M^{-1} s^{-1}.

27 - Jacobi et al. (1996) measured global rate constant for acetaldehyde. We decompose it into the sum of k($CH_3CHO + Cl_2^{\bullet-}$) and k($CH_3CH(OH)(OH) + Cl_2^{\bullet-}$) weighted by the proportion of the hydrated and the non-hydrated form : $k_{global} = k\left(CH_3CHO + Cl_2^{\bullet-}\right)\times\frac{1}{1+K_h} + k\left(CH_3CH(OH)(OH) + Cl_2^{\bullet-}\right)\times\frac{K_h}{1+K_h}$ To determine k($CH_3CHO + Cl_2^{\bullet-}$) and k($CH_3CH(OH)(OH) + Cl_2^{\bullet-}$), we assumed that their ratio is equal to the ratio $\frac{k(CH_3CHO+HO\cdot)}{k(CH_3CH(OH)(OH)+HO\cdot)}$. k_{global} = 4.0 10^4 M^{-1} s^{-1} and k($CH_3CHO + Cl_2^{\bullet-}$) = 6.3 10^4 M^{-1} s^{-1} and k($CH_3CH(OH)(OH) + Cl_2^{\bullet-}$) = 2.1 10^4 M^{-1} s^{-1}.

28 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 63% for CH, 31% for OH and 6% for CH_3. The 2 first pathways are considered corresponding to 94% of the total reactivity. They have been scaled to 67/33%.

29 - For self-reaction of peroxy radicals, we follow these similarity criteria:

Peroxyl categories	Model compounds	References
>C($OO^\bullet$)CO(OH)/>C($OO^\bullet$)CO(O^-)	$CH_2(OO^\bullet)CO(O^-)$	Schuchmann et al. (1985)
>C(OH)C($OO^\bullet$)<	$CH_2(OH)CH_2(OO^\bullet)$	Piesiak et al. (1984)
>COC($OO^\bullet$)<	$CH_3COCH_2(OO^\bullet)$	Zegota et al. (1986b)
Others	$CH_3CH_2(OO^\bullet)$	Monod et al. (2007)

30 - Reaction of $CH_3CO(OO^\bullet)$ with $HO_2^\bullet$ is not considered because we assumed that this reaction is much slower than the reaction with $O_2^{\bullet-}$ that proceeds by electron transfer.

31 - K_h = 10; we consider the reactivity of the hydrated and non-hydrated forms.

32 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 70% for CHO, 25% for CH_2 and 5% for OH. The 2 first pathways are considered corresponding to 95% of the total reactivity. They have been scaled to 77/23%.

33 - Rate constant calculated from Doussin and Monod (2013).
34 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 30% for CH on CH(OH)(OH), 26% for CH_2, 36% for (OH) on CH(OH)(OH), and 8% for (OH) on CH_2(OH). The 3 first pathways are considered corresponding to 92% of the total reactivity. They have been scaled to 33/28/39%.
35 - The hydration constants for the di-hydrated and mono-hydrated forms are respectively equal to 173 and 0.85 ; we only consider the reactivity of the di-hydrated form.
36 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 73% for (OH), 27% for CH. The 2 pathways are considered corresponding to 100% of the total reactivity.
37 - We suppose a rate constant of $1.0\ 10^6\ M^{-1}\ s^{-1}$ typical of values measured in Neta and Huie (1986).
38 - We consider the slow equilibrium leading to the formation of peracetic acid ($CH_3CO(OOH)$) through the oxidation of acetic acid by H_2O_2 in the same way than for performic acid (CHO(OOH)).
39 - We consider the slow equilibrium leading to the formation of hydroxyperacetic acid ($CH_3CO(OOH)$) through the oxidation of glycolic acid by H_2O_2 in the same way than for performic acid (CHO(OOH)).
40 - Following Chevallier et al. (2004), we suppose the electron transfer rate constant for $CH_3CH_2(O^\bullet)$ to be equal to the one for $CH_3O^\bullet$ estimated in Schuchmann and von Sonntag (1984).
41 - We suppose that the $HO_2^\bullet$ elimination from $CH_3CH(OOH)(OO^\bullet)$ is as fast as the one of $CH_3CH(OH)(OO^\bullet)$.
42 - Schuchmann and von Sonntag (1984) estimated that branching ratio for pathway 1 is 20%. Following Monod et al. (2007), the "alkoxy" pathway (pathway 2) is more likely to occur. We considered a 80% branching ratio for pathway 2.
43 - Tetroxides form by the self reaction of the peroxyl radical are not stable and further decompose following different pathways. These pathways are supposed to be similar to the self reaction of $CH_2(OO^\bullet)CO(O^-)$ described by Schuchmann et al. (1985) with the same branching ratio.
44 - Schuchmann et al. (1985) measured a global rate constant for the $CH_2(OO^\bullet)CO(O^-)$ of $2k = 1.5\ 10^8\ M^{-1}\ s^{-1}$. The reaction with $O_2^{\bullet-}$ accounts for 13% of the total degradation and is neglected. The self-reaction therefore represents 87% of the total degradation. Branching ratio for pathways 1 to 4 measured by Schuchmann et al. (1985) (27/25/25/10) are scaled to 100% (30/30/30/10) with the global reaction rate $7.5\ 10^7\ M^{-1}\ s^{-1}$.
45 - The reactivity of the diacid form is neglected due to the very low pKa (~ 1.2).
46 - The equilibrium constants are from Martell and Smith (1977). $\log K(CO(O^-)CO(O^-) + Fe^{3+} \leftrightarrow [Fe(C_2O_4)]^+) = 9.4$; $\log K(2\ CO(O^-)CO(O^-) + Fe^{3+} \leftrightarrow [Fe(C_2O_4)_2]^-) = 16.2$; $\log K(3\ CO(O^-)CO(O^-) + Fe^{3+} \leftrightarrow [Fe(C_2O_4)_3]^{3-}) = 20.4$). We calculate the equilibrium constants : $\log K(CO(O^-)CO(O^-) + [Fe(C_2O_4)]^+ \leftrightarrow [Fe(C_2O_4)_2]^-) = 6.8$; $\log K(CO(O^-)CO(O^-) + [Fe(C_2O_4)_2]^- \leftrightarrow [Fe(C_2O_4)_3]^{3-} = 4.2$. With these equilibrium constants and the backward rate constant, we calculate the forward rate constants.
47 - Moorhead and Sutin (1966) measured rate constants for the equilibrium $Fe(OH)^{2+} + CO(OH)CO(O^-) \leftrightarrow Fe(C_2O_4)^+$: $k_{backward} = 3.0\ 10^{-3}\ s^{-1}$ and $k_{forward} = 2.0\ 10^4\ M^{-1}\ s^{-1}$. The equilibrium constant is similar to Martell and Smith (1977). We suppose that the rate constant of the reaction $[Fe(C_2O_4)]^+ \rightarrow CO(O^-)CO(O^-) + Fe^{3+}$ is equal to $3.0\ 10^{-3}\ s^{-1}$.
48 - The reactivity of $CH_2(OOH)CO(OH)/CH_2(OOH)CO(O^-)$ with $HO^\bullet$ is supposed similar to the reactivity of EHP (Ethyl hydroperoxide) with $HO^\bullet$. Therefore, we applied the same branching ratio 80/20%.
49 - We suppose that the $HO_2^\bullet$ elimination from $CO(OH)CH(OOH)(OO^\bullet)$ is as fast as the one of $CH(OH)(OO^\bullet)CO(OH)$.
50 - We suppose that the $HO_2^\bullet$ elimination from $CO(O^-)CH(OOH)(OO^\bullet)$ is as fast as the one of $CH(OH)(OO^\bullet)CO(O^-)$.
51 - The hydration constants are $1.1\ 10^3$ for glyoxylic acid and $1.65\ 10^1$ for glyoxylate. We therefore consider only the reactivity of the hydrated forms.
52 - The values from Ervens et al. (2003) was corrected following Shaeffer (2012).
53 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 69% for (OH), 24% for CH on CH(OH)(OH) and 7% for the electron-transfer. The 2 first pathways are considered corresponding to 93% of the total reactivity. They have been recalculated to 74/26%.
54 - This radical is produced in the oxidation of 3-oxopropionic acid (C3).

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Equilibria

Species		K_a or K_h	-ΔH/R (K)	References	Notes
C1 compounds					
Formaldehyde					
$CH_2O + H_2O \leftrightarrow CH_2(OH)(OH)$	T(18)	$1.3\ 10^3$	3777	Winkelman et al., 2002	
$CHO(OO^\bullet) + H_2O \leftrightarrow CH(OH)(OH)(OO^\bullet)$	T(19)	$1.3\ 10^3$	3777		1 = $K_h(CH_2O/CH_2(OH)(OH))$
Formic acid					
$CHO(OH) \leftrightarrow CHO(O^-) + H^+$	T(20)	$1.8\ 10^{-4}$	150	Prue and Read, 1966	
$CO(OH)(OO^\bullet) \leftrightarrow CO(O^-)(OO^\bullet) + H^+$	T(21)	$1.8\ 10^{-4}$	150		2 = $K_a(CHO(O^-)/CHO(OH))$
C2 compounds					
Acetaldehyde					
$CH_3CHO + H_2O \leftrightarrow CH_3CH(OH)(OH)$	T(22)	1.2		Buschmann et al., 1980	
$CH_3CO(OO^\bullet) + H_2O \leftrightarrow CH_3C(OH)(OH)(OO^\bullet)$	T(23)	1.2			1 = $K_h(CH_3CHO/CH_3CH(OH)(OH))$
Glycolaldehyde					
$CH_2(OH)CHO + H_2O \leftrightarrow CH_2(OH)CH(OH)(OH)$	T(24)	$1.0\ 10^1$		Sørensen, 1972	
$CH_2(OH)CO(OO^\bullet) + H_2O \leftrightarrow CH_2(OH)C(OH)(OH)(OO^\bullet)$	T(25)	$1.0\ 10^1$			1 = $K_h(CH_2(OH)CHO/CH_2(OH)CH(OH)(OH))$
$CH(OH)(OO^\bullet)CHO + H_2O \leftrightarrow CH(OH)(OO^\bullet)CH(OH)(OH)$	T(26)	$1.0\ 10^1$			1 = $K_h(CH_2(OH)CHO/CH_2(OH)CH(OH)(OH))$
Glyoxal					
$CHOCHO + H_2O \leftrightarrow CHOCH(OH)(OH)$	T(27)	$8.5\ 10^{-1}$		Ruiz-Montoya and Rodriguez-Mellado, 1994	
$CHOCHO + 2\ H_2O \leftrightarrow CH(OH)(OH)CH(OH)(OH)$	T(28)	$1.7\ 10^2$		Ruiz-Montoya and Rodriguez-Mellado, 1994	
$CHOCO(OO^\bullet) + H_2O \leftrightarrow CHOC(OH)(OH)(OO^\bullet)$	T(29)	$8.5\ 10^{-1}$			1 = $K_h(CHOCHO/CHOCH(OH)(OH))$
$CHOCO(OO^\bullet) + 2\ H_2O \leftrightarrow CH(OH)(OH)C(OH)(OH)(OO^\bullet)$	T(30)	$1.7\ 10^2$			1 =$K_h(CHOCHO/CH(OH)(OH)CH(OH)(OH))$
Hydroxyperacetic acid					
$CH_2(OH)CO(OOH) \leftrightarrow CH_2(OH)CO(OO^-) + H^+$	T(31)	$6.3\ 10^{-9}$			2 = $K_a(CH_3CO(OO^-)/CH_3CO(OOH))$
Peracetic acid					
$CH_3CO(OOH) \leftrightarrow CH_3CO(OO^-) + H^+$	T(32)	$6.3\ 10^{-9}$		Schuchmann and Von Sonntag, 1988	

Species		K_a or K_h	-ΔH/R (K)	References	Notes
Acetic acid					
$CH_3CO(OH) \leftrightarrow CH_3CO(O^-) + H^+$	T(33)	$1.7\ 10^{-5}$		Lide and Frederikse, 1995	
Oxalic acid					
$CO(OH)CO(OH) \leftrightarrow CO(OH)CO(O^-) + H^+$	T(34)	$5.6\ 10^{-2}$		Martell and Smith, 1977	
$CO(OH)CO(O^-) \leftrightarrow CO(O^-)CO(O^-) + H^+$	T(35)	$5.4\ 10^{-5}$		Martell and Smith, 1977	
2-hydroperoxyacetic acid					
$CH_2(OOH)CO(OH) \leftrightarrow CH_2(OOH)CO(O^-) + H^+$	T(36)	$1.7\ 10^{-5}$			2 = $K_a(CH_3CO(O^-)/CH_3CO(OH))$
$CH_2(OO^\bullet)CO(OH) \leftrightarrow CH_2(OO^\bullet)CO(O^-) + H^+$	T(37)	$1.7\ 10^{-5}$			2 = $K_a(CH_3CO(O^-)/CH_3CO(OH))$
$CH(OOH)(OO^\bullet)CO(OH) \leftrightarrow CH(OOH)(OO^\bullet)CO(OH) + H^+$	T(38)	$1.7\ 10^{-5}$			2 = $K_a(CH_3CO(O^-)/CH_3CO(OH))$
Glycolic acid					
$CH_2(OH)CO(OH) \leftrightarrow CH_2(OH)CO(O^-) + H^+$	T(39)	$1.5\ 10^{-4}$		Lide and Frederikse, 1995	
$CH(OH)(OO^\bullet)CO(OH) \leftrightarrow CH(OH)(OO^\bullet)CO(O^-) + H^+$	T(40)	$1.5\ 10^{-4}$			2 = $K_a(CH_2(OH)CO(O^-)/CH_2(OH)CO(OH))$
Glyoxylic acid					
$CHOCO(OH) \leftrightarrow CHOCO(O^-) + H^+$	T(41)	$6.6\ 10^{-4}$		Buxton et al., 1997	
$CHOCO(OH) + H_2O \leftrightarrow CH(OH)(OH)CO(OH)$	T(42)	$1.1\ 10^{3}$		Tur'yan, 1998	
$CHOCO(O^-) + H_2O \leftrightarrow CH(OH)(OH)CO(O^-)$	T(43)	$1.7\ 10^{1}$		Tur'yan, 1998	
$CO(OH)CO(OO^\bullet) \leftrightarrow CO(O^-)CO(OO^\bullet) + H^+$	T(44)	$6.6\ 10^{-4}$			2 = $K_a(CHOCO(O^-)/CHOCO(OH))$
$CO(OH)CO(OO^\bullet) + H_2O \leftrightarrow CO(OH)C(OH)(OH)(OO^\bullet)$	T(45)	$1.1\ 10^{3}$			2 = $K_h(CHOCO(OH)/CH(OH)(OH)CO(OH))$
$CO(O^-)CO(OO^\bullet) + H_2O \leftrightarrow CO(O^-)C(OH)(OH)(OO^\bullet)$	T(46)	$1.7\ 10^{1}$			= $K_h(CHOCO(O^-)/CH(OH)(OH)CO(O^-))$
R(OO•) from C3 oxidation					
$CHOCH_2(OO^\bullet) + H_2O \leftrightarrow CH(OH)(OH)CH_2(OO^\bullet)$	T(47)	$1.0\ 10^{1}$			3 = $K_h(CH_2(OH)CHO/CH_2(OH)CH(OH)(OH))$

1 - For peroxy radicals, we assumed that the hydration constant is similar to the parent species.
2 - For peroxy radicals, we assumed that the acidity constant is similar to the parent species.
3 - This radical is produced in the oxidation of 3-oxopropionic acid (C3).

Henry's law constants

Species		H (298K) ($M\ atm^{-1}$)	-ΔH/R (K)	References	Notes
C1 compounds					
HMHP (Hydro Methyl Hydro Peroxide)					
$CH_2(OOH)(OH)$	T(18)	$1.7\ 10^6$	9870	Sander, 2015	
Performic acid					
CHO(OOH)	T(19)	$4.7\ 10^5$	6014	Estimated	1 - 2
MHP (Methyl Hydro Peroxide)					
$CH_3(OOH)$	T(20)	$3.1\ 10^2$	5240	O'Sullivan et al., 1996	
Methanol					
$CH_3(OH)$	T(21)	$2.2\ 10^2$	5210	Snider and Dawson, 1985	
Formaldehyde					
CH_2O	T(22)	$3.2\ 10^3$	7100	Sander, 2015	3
Formic acid					
CHO(OH)	T(23)	$8.9\ 10^3$	6100	Johnson et al., 1996	
Methyl nitrate					
$CH_3(ONO_2)$	T(24)	2.0	4740	Sander, 2015	
C2 compounds					
Ethanol					
$CH_3CH_2(OH)$	T(25)	$2.0\ 10^2$	6630	Snider and Dawson, 1985	
Ethylene glycol					
$CH_2(OH)CH_2(OH)$	T(26)	$4.0\ 10^6$		Bone et al., 1983	
Acetaldehyde					
CH_3CHO	T(27)	$1.3\ 10^1$	5890	Sander, 2015	3
$CH_3CO(OO^{\bullet})$	T(28)	$1.0\ 10^{-1}$		Sander, 2015	
Glycolaldehyde					
$CH_2(OH)CHO$	T(29)	$4.1\ 10^4$	3850	Betterton and Hoffmann, 1988	3
Glyoxal					
CHOCHO	T(30)	$4.2\ 10^5$	7480	Ip et al., 2009	3
Peracetic acid					
$CH_3CO(OOH)$	T(31)	$8.4\ 10^2$	5300	O'Sullivan et al., 1996	
Hydroxyperacetic acid					
$CH_2(OH)CO(OOH)$	T(32)	$4.8\ 10^4$	6014	Estimated	1 - 2
Acetic acid					
$CH_3CO(OH)$	T(33)	$4.1\ 10^3$	6200	Sander, 2015	

Species		H (298K) ($M\ atm^{-1}$)	-ΔH/R (K)	References	Notes
Ethyl hydroperoxide					
$CH_3CH_2(OOH)$	T(34)	$3.4\ 10^2$		O'Sullivan et al., 1996	
Oxalic acid					
CO(OH)CO(OH)	T(35)	$5.0\ 10^8$		Saxena and Hildemann, 1996	
2-hydroperoxy acetic acid					
$CH_2(OOH)CO(OH)$	T(36)	$1.5\ 10^6$	6014	Estimated	1 - 2
Glycolic acid					
$CH_2(OH)CO(OH)$	T(37)	$2.4\ 10^4$	4030	Ip et al., 2009	
Glyoxylic acid					
CHOCO(OH)	T(38)	$9.0\ 10^9$		Saxena and Hildemann, 1996	3
PAN					
$CH_3CO(OONO_2)$	T(39)	2.8	5730	Sander, 2015	
Ethyl nitrate					
$CH_3CH_2(ONO_2)$	T(40)	1.6	5360	Sander, 2015	
2-hydroxyethyl nitrate					
$CH_2(OH)CH_2(ONO_2)$	T(41)	$4.0\ 10^4$		Sander, 2015	

1 - Estimated by the SAR GROMHE (Raventos-Duran et al., 2010).

2 - When unavailable, the temperature dependence (enthalpy of dissolution) is set at 50 kJ mol^{-1}; -ΔH/R = 6014 K.

3 - Effective Henry's law constant.

Accommodation coefficients

Species		α (298K)	-ΔH (J/mol)	-ΔS (J/mol/K)	References	Notes
C1 compounds		1				
HMHP (Hydro Methyl Hydro Peroxide)						
$CH_2(OOH)(OH)$	T(18)	$5.0\ 10^{-2}$			Estimated	2
Performic acid						
$CHO(OOH)$	T(19)	$5.0\ 10^{-2}$			Estimated	2
MHP (Methyl Hydroperoxide)						
$CH_3(OOH)$	T(20)	$5.0\ 10^{-3}$	$2.7\ 10^{4}$	$1.4\ 10^{2}$	Davidovits et al., 2011	
Methanol						
$CH_3(OH)$	T(21)	$1.7\ 10^{-2}$	$3.3\ 10^{4}$	$1.5\ 10^{2}$	Davidovits et al., 2011	
Formaldehyde						
CH_2O	T(22)	$4.0\ 10^{-2}$			Sander, 2015	Mean value between 260-270K
Formic acid						
$CHO(OH)$	T(23)	$1.5\ 10^{-2}$	$3.3\ 10^{4}$	$1.5\ 10^{2}$	Davidovits et al., 2011	
Methyl nitrate						
$CH_3(ONO_2)$	T(24)	$5.0\ 10^{-2}$			Estimated	2
C2 compounds						
Ethanol						
$CH_3CH_2(OH)$	T(25)	$9.0\ 10^{-3}$	$4.6\ 10^{4}$	$1.9\ 10^{2}$	Davidovits et al., 2011	
Ethylene glycol						
$CH_2(OH)CH_2(OH)$	T(26)	$3.3\ 10^{-2}$	$2.2\ 10^{4}$	$1.0\ 10^{2}$	Davidovits et al., 2011	
Acetaldehyde						
CH_3CHO	T(27)	$3.0\ 10^{-2}$			Sander, 2015	Measured at 267K
$CH_3CO(OO^{\bullet})$	T(28)	$5.0\ 10^{-2}$			Estimated	2
Glycolaldehyde						
$CH_2(OH)CHO$	T(29)	$5.0\ 10^{-2}$			Estimated	2
Glyoxal						
$CHOCHO$	T(30)	$1.0\ 10^{-2}$			Sander, 2015	Mean value between 260-285K
Peracetic acid						
$CH_3CO(OOH)$	T(31)	$5.0\ 10^{-2}$			Estimated	2
Hydroxyperacetic acid						
$CH_2(OH)CO(OOH)$	T(32)	$5.0\ 10^{-2}$			Estimated	2

Species		α (298K)	-ΔH (J/mol)	-ΔS (J/mol/K)	References	Notes
Acetic acid						
$CH_3CO(OH)$	T(33)	$2.0\ 10^{-2}$	$3.4\ 10^{4}$	$1.5\ 10^{2}$	Davidovits et al., 2011	
Ethyl hydroperoxide						
$CH_3CH_2(OOH)$	T(34)	$5.0\ 10^{-2}$			Estimated	2
Oxalic acid						
$CO(OH)CO(OH)$	T(35)	$5.0\ 10^{-2}$			Estimated	2
2-hydroperoxy acetic acid						
$CH_2(OOH)CO(OH)$	T(36)	$5.0\ 10^{-2}$			Estimated	2
Glycolic acid						
$CH_2(OH)CO(OH)$	T(37)	$5.0\ 10^{-2}$			Estimated	2
Glyoxylic acid						
$CHOCO(OH)$	T(38)	$5.0\ 10^{-2}$			Estimated	2
PAN						
$CH_3CO(OONO_2)$	T(39)	$1.0\ 10^{-3}$			Kirchner et al., 1990	Measured at 282K
Ethyl nitrate						
$CH_3CH_2(ONO_2)$	T(40)	$5.0\ 10^{-2}$			Estimated	2
2-hydroxyethyl nitrate						
$CH_2(OH)CH_2(ONO_2)$	T(41)	$5.0\ 10^{-2}$			Estimated	2

1 - α can be calculated with ΔH and ΔS; this allows considering the temperature dependency of α following Jayne et al. (1997) : $\frac{\alpha}{1-\alpha} = \exp\left(\frac{-\Delta G}{RT}\right)$; $\Delta G = \Delta H - T\Delta S$

2 - Estimated equal $5.0\ 10^{-2}$ following Lelieveld and Crutzen (1991) and Davidovits et al. (2011).

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