

C1 compounds

Reactions		k ₂₉₈ (M ⁻ⁿ⁺¹ s ⁻¹)	Ea/R (K)	References	Notes
Oxidation of HMHP - HydroxyMethyl HydroPeroxide					
CH ₂ (OOH)(OH) + hν → CHO(OH) + HO• + HO ₂ • - O ₂	R(208)	Calculated			= J(H ₂ O ₂)
Pathway 1: CH ₂ (OOH)(OH) + HO• → CH ₂ (OH)(OO•) + H ₂ O		5.0 10 ⁸			BR: 80% - 1
Pathway 2: CH ₂ (OOH)(OH) + HO• → C•H(OOH)(OH) + H ₂ O		1.3 10 ⁸			BR: 20% - 1
C•H(OOH)(OH) + O ₂ → CH(OOH)(OH)(OO•)		2.0 10 ⁹			2
CH ₂ (OOH)(OH) + HO• → 0.80 CH ₂ (OH)(OO•) + 0.20 CH(OOH)(OH)(OO•) + H ₂ O - 0.20 O ₂	R(209)	6.3 10 ⁸			= k(CH ₃ (OOH) + HO•) - 1
Pathway 1: CH ₂ (OOH)(OH) + NO ₃ • → CH ₂ (OH)(OO•) + NO ₃ ⁻ + H ⁺					BR: 80%
Pathway 2: CH ₂ (OOH)(OH) + NO ₃ • → C•H(OOH)(OH) + NO ₃ ⁻ + H ⁺					BR: 20%
C•H(OOH)(OH) + O ₂ → CH(OOH)(OH)(OO•)		2.0 10 ⁹			2
CH ₂ (OOH)(OH) + NO ₃ • → 0.80 CH ₂ (OH)(OO•) + 0.20 CH(OOH)(OH)(OO•) + NO ₃ ⁻ + H ⁺	R(210)	4.9 10 ⁶	2000		= k(H ₂ O ₂ + NO ₃ •) - 3
Pathway 1: CH ₂ (OOH)(OH) + CO ₃ • ⁻ → CH ₂ (OH)(OO•) + HCO ₃ ⁻					BR: 80%
Pathway 2: CH ₂ (OOH)(OH) + CO ₃ • ⁻ → C•H(OOH)(OH) + HCO ₃ ⁻					BR: 20%
C•H(OOH)(OH) + O ₂ → CH(OOH)(OH)(OO•)		2.0 10 ⁹			2
CH ₂ (OOH)(OH) + CO ₃ • ⁻ → 0.80 CH ₂ (OH)(OO•) + 0.20 CH(OOH)(OH)(OO•) + HCO ₃ ⁻	R(211)	4.3 10 ⁵			= k(H ₂ O ₂ + CO ₃ • ⁻) - 3
Pathway 1: CH ₂ (OOH)(OH) + Cl ₂ • ⁻ → CH ₂ (OH)(OO•) + 2 Cl ⁻ + H ⁺					BR: 80%
Pathway 2: CH ₂ (OOH)(OH) + Cl ₂ • ⁻ → C•H(OOH)(OH) + 2 Cl ⁻ + H ⁺					BR: 20%
C•H(OOH)(OH) + O ₂ → CH(OOH)(OH)(OO•)		2.0 10 ⁹			2
CH ₂ (OOH)(OH) + Cl ₂ • ⁻ → 0.80 CH ₂ (OH)(OO•) + 0.20 CH(OOH)(OH)(OO•) + 2 Cl ⁻ + H ⁺	R(212)	6.2 10 ⁶			= k (H ₂ O ₂ + Cl ₂ • ⁻) - 3
Pathway 1: CH ₂ (OOH)(OH) + Cl• → CH ₂ (OH)(OO•) + Cl ⁻ + H ⁺					BR: 80%
Pathway 2: CH ₂ (OOH)(OH) + Cl• → C•H(OOH)(OH) + Cl ⁻ + H ⁺					BR: 20%
C•H(OOH)(OH) + O ₂ → CH(OOH)(OH)(OO•)		2.0 10 ⁹			2
CH ₂ (OOH)(OH) + Cl• → 0.80 CH ₂ (OH)(OO•) + 0.20 CH(OOH)(OH)(OO•) + Cl ⁻ + H ⁺	R(213)	2.0 10 ⁹			= k(H ₂ O ₂ + Cl•) - 3
Pathway 1: CH ₂ (OOH)(OH) + SO ₄ • ⁻ → CH ₂ (OH)(OO•) + SO ₄ ²⁻ + H ⁺					BR: 80%
Pathway 2: CH ₂ (OOH)(OH) + SO ₄ • ⁻ → C•H(OOH)(OH) + SO ₄ ²⁻ + H ⁺					BR: 20%
C•H(OOH)(OH) + O ₂ → CH(OOH)(OH)(OO•)		2.0 10 ⁹			2
CH ₂ (OOH)(OH) + SO ₄ • ⁻ → 0.80 CH ₂ (OH)(OO•) + 0.20 CH(OOH)(OH)(OO•) + SO ₄ ²⁻ + H ⁺	R(214)	1.2 10 ⁷			= k(H ₂ O ₂ + SO ₄ • ⁻) - 3
CH ₂ (OOH)(OH) + Fe ²⁺ → Fe ³⁺ + CHO(OH) + HO ₂ • + OH ⁻ - O ₂	R(215)	1.6 10 ¹			= k(CH ₃ (OOH) + Fe ²⁺)
CH ₂ (OH)(OO•) → CH ₂ O + HO ₂ •	R(216)	1.0 10 ¹			4
CH ₂ (OH)(OO•) + OH ⁻ → CH ₂ (O ⁻)(OO•) + H ₂ O		2.1 10 ¹⁰	7200	Neta et al., 1990	5
CH ₂ (O ⁻)(OO•) → CH ₂ O + O ₂ • ⁻					
CH ₂ (OH)(OO•) + OH ⁻ → CH ₂ O + O ₂ • ⁻ + H ₂ O	R(217)	2.1 10 ¹⁰	7200	Neta et al., 1990	
CH ₂ (OH)(OO•) + HO ₂ • → CH ₂ (OOH)(OH) + O ₂	R(218)	8.3 10 ⁵	2700		= k(HO ₂ • + HO ₂ •)
CH ₂ (OH)(OO•) + O ₂ • ⁻ → CH ₂ (OOH)(OH) + O ₂ + OH ⁻ - H ₂ O	R(219)	9.6 10 ⁷	910		= k(HO ₂ • + O ₂ • ⁻)
2 CH ₂ (OH)(OO•) → 2 CHO(OH) + H ₂ O ₂	R(220)	7.4 10 ⁸	1400	Huie and Clifton, 1993	
CH ₂ (OH)(OO•) + Fe ²⁺ → [FeOHCH ₂ O ₂] ²⁺	R(221)	5.9 10 ⁵		Khaikin et al., 1996	
[FeOHCH ₂ O ₂] ²⁺ → CH ₂ (OH)(OO•) + Fe ²⁺	R(222)	1.3 10 ³		Khaikin et al., 1996	
[FeOHCH ₂ O ₂] ²⁺ → Fe ³⁺ + CH ₂ (OOH)(OH) + OH ⁻ - H ₂ O	R(223)	1.0 10 ²		Khaikin et al., 1996	
[FeOHCH ₂ O ₂] ²⁺ + H ⁺ → Fe ³⁺ + CH ₂ (OOH)(OH)	R(224)	3.0 10 ⁴		Khaikin et al., 1996	
CH(OOH)(OH)(OO•) + OH ⁻ → CH(OOH)(O ⁻)(OO•) + H ₂ O		4.0 10 ⁹			
CH(O ⁻)(OOH)(OO•) → CHO(OOH) + O ₂ • ⁻					5
CH(OOH)(OH)(OO•) + OH ⁻ → CHO(OOH) + O ₂ • ⁻ + H ₂ O	R(225)	4.0 10 ⁹			= k(CH ₃ CH(OH)(OO•) + OH ⁻)
CH(OOH)(OH)(OO•) → CHO(OOH) + HO ₂ •	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 ₂ O ₂ + H ⁺ → CHO(OOH) + H ₂ O + H ⁺	R(227)	3.1 10 ⁻⁴	5235	De Filippis et al., 2009	7
CHO(OOH) + H ₂ O + H ⁺ → CHO(OH) + H ₂ O ₂ + H ⁺	R(228)	3.8 10 ⁻⁴	5235	De Filippis et al., 2009	7
CHO(OOH) + H ⁺ → CO ₂ + H ₂ O + H ⁺	R(229)	1.2 10 ⁻³	8735	De Filippis et al., 2009	7
Oxidation of MHP (Methyl HydroPeroxide)					
CH ₃ (OOH) + hν → CH ₂ O + HO• + HO ₂ • - O ₂	R(230)	Calculated			= J(H ₂ O ₂)
Pathway 1: CH ₃ (OOH) + HO• → CH ₃ (OO•) + H ₂ O		5.0 10 ⁸			BR: 80% - 8
Pathway 2: CH ₃ (OOH) + HO• → C•H ₂ (OOH) + H ₂ O		1.3 10 ⁸			BR: 20% - 8
C•H ₂ (OOH) + O ₂ → CH ₂ (OOH)(OO•)		2.0 10 ⁹			2
CH ₃ (OOH) + HO• → 0.80 CH ₃ (OO•) + 0.20 CH ₂ (OOH)(OO•) + H ₂ O - 0.20 O ₂	R(231)	6.3 10 ⁸		Monod et al., 2007	8
Pathway 1: CH ₃ (OOH) + NO ₃ • → CH ₃ (OO•) + NO ₃ ⁻ + H ⁺					BR: 80%
Pathway 2: CH ₃ (OOH) + NO ₃ • → C•H ₂ (OOH) + NO ₃ ⁻ + H ⁺					BR: 20%
C•H ₂ (OOH) + O ₂ → CH ₂ (OOH)(OO•)		2.0 10 ⁹			2
CH ₃ (OOH) + NO ₃ • → 0.80 CH ₃ (OO•) + 0.20 CH ₂ (OOH)(OO•) + NO ₃ ⁻ + H ⁺	R(232)	4.9 10 ⁶	2000		= k(H ₂ O ₂ + NO ₃ •) - 3
Pathway 1: CH ₃ (OOH) + CO ₃ • ⁻ → CH ₃ (OO•) + HCO ₃ ⁻					BR: 80%
Pathway 2: CH ₃ (OOH) + CO ₃ • ⁻ → C•H ₂ (OOH) + HCO ₃ ⁻					BR: 20%
C•H ₂ (OOH) + O ₂ → CH ₂ (OOH)(OO•)		2.0 10 ⁹			2
CH ₃ (OOH) + CO ₃ • ⁻ → 0.80 CH ₃ (OO•) + 0.20 CH ₂ (OOH)(OO•) + HCO ₃ ⁻	R(233)	4.3 10 ⁵			= k(H ₂ O ₂ + CO ₃ • ⁻) - 3
Pathway 1: CH ₃ (OOH) + Cl ₂ • ⁻ → CH ₃ (OO•) + 2 Cl ⁻ + H ⁺					BR: 80%
Pathway 2: CH ₃ (OOH) + Cl ₂ • ⁻ → C•H ₂ (OOH) + 2 Cl ⁻ + H ⁺					BR: 20%
C•H ₂ (OOH) + O ₂ → CH ₂ (OOH)(OO•)		2.0 10 ⁹			2
CH ₃ (OOH) + Cl ₂ • ⁻ → 0.80 CH ₃ (OO•) + 0.20 CH ₂ (OOH)(OO•) + 2 Cl ⁻ + H ⁺	R(234)	6.2 10 ⁶			= k(H ₂ O ₂ + Cl ₂ • ⁻) - 3
Pathway 1: CH ₃ (OOH) + Cl• → CH ₃ (OO•) + Cl ⁻ + H ⁺					BR: 80%
Pathway 2: CH ₃ (OOH) + Cl• → C•H ₂ (OOH) + Cl ⁻ + H ⁺					BR: 20%
C•H ₂ (OOH) + O ₂ → CH ₂ (OOH)(OO•)		2.0 10 ⁹			2
CH ₃ (OOH) + Cl• → 0.80 CH ₃ (OO•) + 0.20 CH ₂ (OOH)(OO•) + Cl ⁻ + H ⁺	R(235)	2.0 10 ⁹			= k(H ₂ O ₂ + Cl•) - 3
Pathway 1: CH ₃ (OOH) + SO ₄ • ⁻ → CH ₃ (OO•) + SO ₄ ²⁻ + H ⁺					BR: 80%
Pathway 2: CH ₃ (OOH) + SO ₄ • ⁻ → C•H ₂ (OOH) + SO ₄ ²⁻ + H ⁺					BR: 20%
C•H ₂ (OOH) + O ₂ → CH ₂ (OOH)(OO•)		2.0 10 ⁹			2
CH ₃ (OOH) + SO ₄ • ⁻ → 0.80 CH ₃ (OO•) + 0.20 CH ₂ (OOH)(OO•) + SO ₄ ²⁻ + H ⁺	R(236)	1.2 10 ⁷			= k(H ₂ O ₂ + SO ₄ • ⁻) - 3
CH ₃ (OOH) + HSO ₃ ⁻ → CH ₃ (OH) + SO ₄ ²⁻ + H ⁺	R(237)	1.8 10 ⁷	3800	Lind et al., 1987	
CH ₃ (OOH) + Fe ²⁺ → Fe ³⁺ + CH ₂ (OH)(OO•) + OH ⁻ - O ₂	R(238)	1.6 10 ¹		Chevallier et al., 2004	
CH ₃ (OO•) + HO ₂ • → CH ₃ (OOH) + O ₂	R(239)	4.2 10 ⁵	2700		= k(HO ₂ • + HO ₂ •)/2
CH ₃ (OO•) + O ₂ • ⁻ → CH ₃ (OOH) + O ₂ + OH ⁻ - H ₂ O	R(240)	4.8 10 ⁷	910		= k(HO ₂ • + O ₂ • ⁻)/2
Pathway 1: 2 CH ₃ (OO•) → 2 CH ₂ O + H ₂ O ₂		2.2 10 ⁷			BR: 20% - 9
Pathway 2: 2 CH ₃ (OO•) → 2 CH ₃ O• + O ₂		8.8 10 ⁷			BR: 80% - 9
CH ₃ O• → C•H ₂ OH					10
C•H ₂ OH + O ₂ → CH ₂ OH(OO•)		2.0 10 ⁹			2
2 CH ₃ (OO•) → 0.40 CH ₂ O + 1.60 CH ₂ OH(OO•) + 0.20 H ₂ O ₂ - 0.80 O ₂	R(241)	1.1 10 ⁸	2200	Herrmann et al., 1999	9
CH ₃ (OO•) + HSO ₃ ⁻ → CH ₃ (OOH) + SO ₃ • ⁻	R(242)	5.0 10 ⁵		Herrmann et al., 1999	
CH ₃ (OO•) + Fe ²⁺ → [FeCH ₃ O ₂] ²⁺	R(243)	8.6 10 ⁵		Khaikin et al., 1996	
[FeCH ₃ O ₂] ²⁺ → CH ₃ (OO•) + Fe ²⁺	R(244)	1.3 10 ³		Khaikin et al., 1996	
[FeCH ₃ O ₂] ²⁺ → Fe ³⁺ + CH ₃ (OOH) + OH ⁻ - H ₂ O	R(245)	1.0 10 ²		Khaikin et al., 1996	
[FeCH ₃ O ₂] ²⁺ + H ⁺ → Fe ³⁺ + CH ₃ (OOH)	R(246)	3.0 10 ⁴		Khaikin et al., 1996	

Reactions		k_{298} ($M^{-n+1} s^{-1}$)	Ea/R (K)	References	Notes
$CH_2(OOH)(OO^{\bullet}) + OH^{\bullet} \rightarrow CH_2(OO^{\bullet})(OO^{\bullet}) + H_2O$		$4.0 \cdot 10^9$			
$CH_2(OO^{\bullet})(OO^{\bullet}) \rightarrow CHO(OH) + O_2^{\bullet-}$					11
$CH_2(OOH)(OO^{\bullet}) + OH^{\bullet} \rightarrow CHO(OH) + O_2^{\bullet-} + H_2O$	R(247)	$4.0 \cdot 10^9$			= $k(CH_3CH(OH)(OO^{\bullet}) + OH^{\bullet})$ - 12
$CH_2(OOH)(OO^{\bullet}) \rightarrow CHO(OH) + HO_2^{\bullet}$	R(248)	$1.0 \cdot 10^1$			= $k(CH_2(OH)(OO^{\bullet}) \rightarrow CH_2O + HO_2^{\bullet})$ - 13
Oxidation of Methanol					
$CH_3(OH) + HO^{\bullet} \rightarrow C^{\bullet}H_2(OH) + H_2O$		$1.0 \cdot 10^9$	600	Elliot and McCracken, 1989	
$C^{\bullet}H_2(OH) + O_2 \rightarrow CH_2(OH)(OO^{\bullet})$		$4.2 \cdot 10^9$		Schaefer et al., 2014	
$CH_3(OH) + HO^{\bullet} \rightarrow CH_2(OH)(OO^{\bullet}) + H_2O - O_2$	R(249)	$1.0 \cdot 10^9$	600	Elliot and McCracken, 1989	
$CH_3(OH) + NO_3^{\bullet} \rightarrow C^{\bullet}H_2(OH) + NO_3^- + H^+$					
$C^{\bullet}H_2(OH) + O_2 \rightarrow CH_2(OH)(OO^{\bullet})$		$4.2 \cdot 10^9$		Schaefer et al., 2014	
$CH_3(OH) + NO_3^{\bullet} \rightarrow CH_2(OH)(OO^{\bullet}) + NO_3^- + H^+ - O_2$	R(250)	$5.4 \cdot 10^5$	4300	Herrmann and Zellner, 1998	
$CH_3(OH) + CO_3^{\bullet-} \rightarrow C^{\bullet}H_2(OH) + HCO_3^-$					
$C^{\bullet}H_2(OH) + O_2 \rightarrow CH_2(OH)(OO^{\bullet})$		$4.2 \cdot 10^9$		Schaefer et al., 2014	
$CH_3(OH) + CO_3^{\bullet-} \rightarrow CH_2(OH)(OO^{\bullet}) + HCO_3^- - O_2$	R(251)	$5.7 \cdot 10^3$	3100	Clifton and Huie, 1993	
$CH_3(OH) + Cl_2^{\bullet-} \rightarrow C^{\bullet}H_2(OH) + 2 Cl^- + H^+$					
$C^{\bullet}H_2(OH) + O_2 \rightarrow CH_2(OH)(OO^{\bullet})$		$4.2 \cdot 10^9$		Schaefer et al., 2014	
$CH_3(OH) + Cl_2^{\bullet-} \rightarrow CH_2(OH)(OO^{\bullet}) + 2 Cl^- + H^+ - O_2$	R(252)	$5.0 \cdot 10^4$	5500	Jacobi et al., 1999	
$CH_3(OH) + Cl^{\bullet} \rightarrow C^{\bullet}H_2(OH) + Cl^- + H^+$					
$C^{\bullet}H_2(OH) + O_2 \rightarrow CH_2(OH)(OO^{\bullet})$		$4.2 \cdot 10^9$		Schaefer et al., 2014	
$CH_3(OH) + Cl^{\bullet} \rightarrow CH_2(OH)(OO^{\bullet}) + Cl^- + H^+ - O_2$	R(253)	$1.0 \cdot 10^9$	1450	Buxton et al., 2000	
$CH_3(OH) + SO_4^{\bullet-} \rightarrow C^{\bullet}H_2(OH) + SO_4^{2-} + H^+$					
$C^{\bullet}H_2(OH) + O_2 \rightarrow CH_2(OH)(OO^{\bullet})$		$4.2 \cdot 10^9$		Schaefer et al., 2014	
$CH_3(OH) + SO_4^{\bullet-} \rightarrow CH_2(OH)(OO^{\bullet}) + SO_4^{2-} + H^+ - O_2$	R(254)	$9.0 \cdot 10^6$	2200	Clifton and Huie, 1989	
Oxidation of Formaldehyde					14
Pathway 1: $CH_2(OH)(OH) + HO^{\bullet} \rightarrow CH^{\bullet}(OH)(OH) + H_2O$		$5.4 \cdot 10^8$			BR: 70% - 15
$CH^{\bullet}(OH)(OH) + O_2 \rightarrow CH(OH)(OH)(OO^{\bullet})$		$2.0 \cdot 10^9$			2
Pathway 2: $CH_2(OH)(OH) + HO^{\bullet} \rightarrow CH_2(OH)(O^{\bullet}) + H_2O$		$2.4 \cdot 10^8$			BR: 30% - 15
$CH_2(OH)(O^{\bullet}) \rightarrow C^{\bullet}H(OH)(OH)$					10
$CH^{\bullet}(OH)(OH) + O_2 \rightarrow CH(OH)(OH)(OO^{\bullet})$		$2.0 \cdot 10^9$			2
$CH_2(OH)(OH) + HO^{\bullet} \rightarrow CH(OH)(OH)(OO^{\bullet}) + H_2O - O_2$	R(255)	$7.8 \cdot 10^8$	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%
$CH^{\bullet}(OH)(OH) + O_2 \rightarrow CH(OH)(OH)(OO^{\bullet})$		$2.0 \cdot 10^9$			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
$CH^{\bullet}(OH)(OH) + O_2 \rightarrow CH(OH)(OH)(OO^{\bullet})$		$2.0 \cdot 10^9$			2
$CH_2(OH)(OH) + NO_3^{\bullet} \rightarrow CH(OH)(OH)(OO^{\bullet}) + NO_3^- + H^+ - O_2$	R(256)	$1.0 \cdot 10^6$	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%
$CH^{\bullet}(OH)(OH) + O_2 \rightarrow CH(OH)(OH)(OO^{\bullet})$		$2.0 \cdot 10^9$			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
$CH^{\bullet}(OH)(OH) + O_2 \rightarrow CH(OH)(OH)(OO^{\bullet})$		$2.0 \cdot 10^9$			2
$CH_2(OH)(OH) + CO_3^{\bullet-} \rightarrow CH(OH)(OH)(OO^{\bullet}) + HCO_3^- - O_2$	R(257)	$1.3 \cdot 10^4$		Zellner et al., 1996	3

Reactions		k_{298} ($M^{-n+1} s^{-1}$)	Ea/R (K)	References	Notes
Pathway 1: $CH_2(OH)(OH) + Cl_2^{\bullet-} \rightarrow CH^{\bullet}(OH)(OH) + 2 Cl^- + H^+ - O_2$		$2.0 \cdot 10^9$			BR: 70% 2
$CH^{\bullet}(OH)(OH) + O_2 \rightarrow CH(OH)(OH)(OO^{\bullet})$					BR: 30% 10
Pathway 2: $CH_2(OH)(OH) + Cl_2^{\bullet-} \rightarrow CH_2(OH)(O^{\bullet}) + 2 Cl^- + H^+ - O_2$		$2.0 \cdot 10^9$			2
$CH_2(OH)(O^{\bullet}) \rightarrow C^{\bullet}H(OH)(OH)$					
$CH^{\bullet}(OH)(OH) + O_2 \rightarrow CH(OH)(OH)(OO^{\bullet})$		$2.0 \cdot 10^9$			3
$CH_2(OH)(OH) + Cl_2^{\bullet-} \rightarrow CH(OH)(OH)(OO^{\bullet}) + 2 Cl^- + H^+ - O_2$	R(258)	$3.6 \cdot 10^4$	4400	Jacobi et al., 1999	
Pathway 1: $CH_2(OH)(OH) + Cl^{\bullet} \rightarrow CH^{\bullet}(OH)(OH) + Cl^- + H^+ - O_2$		$2.0 \cdot 10^9$			BR: 70% 2
$CH^{\bullet}(OH)(OH) + O_2 \rightarrow CH(OH)(OH)(OO^{\bullet})$					BR: 30% 10
Pathway 2: $CH_2(OH)(OH) + Cl^{\bullet} \rightarrow CH_2(OH)(O^{\bullet}) + Cl^- + H^+ - O_2$		$2.0 \cdot 10^9$			2
$CH_2(OH)(O^{\bullet}) \rightarrow C^{\bullet}H(OH)(OH)$					
$CH^{\bullet}(OH)(OH) + O_2 \rightarrow CH(OH)(OH)(OO^{\bullet})$		$2.0 \cdot 10^9$			3
$CH_2(OH)(OH) + Cl^{\bullet} \rightarrow CH(OH)(OH)(OO^{\bullet}) + Cl^- + H^+ - O_2$	R(259)	$1.4 \cdot 10^9$		Buxton et al., 2000	
Pathway 1: $CH_2(OH)(OH) + SO_4^{\bullet-} \rightarrow CH^{\bullet}(OH)(OH) + SO_4^{2-} + H^+ - O_2$		$2.0 \cdot 10^9$			BR: 70% 2
$CH^{\bullet}(OH)(OH) + O_2 \rightarrow CH(OH)(OH)(OO^{\bullet})$					BR: 30% 10
Pathway 2: $CH_2(OH)(OH) + SO_4^{\bullet-} \rightarrow CH_2(OH)(O^{\bullet}) + SO_4^{2-} + H^+ - O_2$		$2.0 \cdot 10^9$			2
$CH_2(OH)(O^{\bullet}) \rightarrow C^{\bullet}H(OH)(OH)$					
$CH^{\bullet}(OH)(OH) + O_2 \rightarrow CH(OH)(OH)(OO^{\bullet})$		$2.0 \cdot 10^9$			3
$CH_2(OH)(OH) + SO_4^{\bullet-} \rightarrow CH(OH)(OH)(OO^{\bullet}) + SO_4^{2-} + H^+ - O_2$	R(260)	$1.4 \cdot 10^7$	1300	Buxton et al., 1990	
$CH_2(OH)(OH) + FeO^{2+} \rightarrow CHO(OH) + Fe^{3+} + HO_2^{\bullet} + OH^- - O_2$	R(261)	$4.0 \cdot 10^2$	5350	Jacobsen et al., 1998	
$CH(OH)(OH)(OO^{\bullet}) + OH^- \rightarrow CH(OH)(O^{\bullet})(OO^{\bullet}) + H_2O$		$4.0 \cdot 10^9$			5
$CH(OH)(O^{\bullet})(OO^{\bullet}) \rightarrow CHO(OH) + O_2^{\bullet-}$					
$CH(OH)(OH)(OO^{\bullet}) + OH^- \rightarrow CHO(OH) + O_2^{\bullet-} + H_2O$	R(262)	$4.0 \cdot 10^9$			= $k(CH_3CH(OH)(OO^{\bullet}) + OH^-)$
$CH(OH)(OH)(OO^{\bullet}) \rightarrow CHO(OH) + HO_2^{\bullet}$	R(263)	$1.0 \cdot 10^6$			17
Oxidation of Formic acid					
$CHO(OH) + HO^{\bullet} \rightarrow CO(OH)(OO^{\bullet}) + H_2O - O_2$	R(264)	$1.0 \cdot 10^8$	1000	Chin and Wine, 1994	
$CHO(O^{\bullet}) + HO^{\bullet} \rightarrow CO(O^{\bullet})(OO^{\bullet}) + H_2O - O_2$	R(265)	$3.4 \cdot 10^9$	1200	Chin and Wine, 1994	
$CHO(OH) + NO_3^{\bullet} \rightarrow CO(OH)(OO^{\bullet}) + NO_3^- + H^+ - O_2$	R(266)	$3.8 \cdot 10^5$	3400	Exner et al., 1994	
$CHO(O^{\bullet}) + NO_3^{\bullet} \rightarrow CO(O^{\bullet})(OO^{\bullet}) + NO_3^- + H^+ - O_2$	R(267)	$5.1 \cdot 10^7$	2200	Exner et al., 1994	
$CHO(O^{\bullet}) + CO_3^{\bullet-} \rightarrow CO(O^{\bullet})(OO^{\bullet}) + HCO_3^- - O_2$	R(268)	$1.6 \cdot 10^5$		Zellner et al., 1996	
$CHO(OH) + Cl_2^{\bullet-} \rightarrow CO(OH)(OO^{\bullet}) + 2 Cl^- + H^+ - O_2$	R(269)	$8.0 \cdot 10^4$	4500	Jacobi et al., 1999	
$CHO(O^{\bullet}) + Cl_2^{\bullet-} \rightarrow CO(O^{\bullet})(OO^{\bullet}) + 2 Cl^- + H^+ - O_2$	R(270)	$1.3 \cdot 10^6$		Jacobi et al., 1996	
$CHO(OH) + Cl^{\bullet} \rightarrow CO(OH)(OO^{\bullet}) + Cl^- + H^+ - O_2$	R(271)	$1.3 \cdot 10^8$	1100	Buxton et al., 2000	
$CHO(O^{\bullet}) + Cl^{\bullet} \rightarrow CO(O^{\bullet})(OO^{\bullet}) + Cl^- + H^+ - O_2$	R(272)	$4.2 \cdot 10^9$	1900	Buxton et al., 2000	
$CHO(OH) + FeO^{2+} \rightarrow CO(OH)(OO^{\bullet}) + Fe^{3+} + H_2O - H^+ - O_2$	R(273)	$1.6 \cdot 10^2$	2680	Jacobsen et al., 1998	
$CHO(O^{\bullet}) + FeO^{2+} \rightarrow CO(O^{\bullet})(OO^{\bullet}) + Fe^{3+} + H_2O - H^+ - O_2$	R(274)	$3.0 \cdot 10^5$		Jacobsen et al., 1998	
$CO(OH)(OO^{\bullet}) + OH^- \rightarrow CO(O^{\bullet})(OO^{\bullet}) + H_2O$		$4.0 \cdot 10^9$			5
$CO(O^{\bullet})(OO^{\bullet}) \rightarrow CO_2 + O_2^{\bullet-}$					
$CO(OH)(OO^{\bullet}) + OH^- \rightarrow CO_2 + O_2^{\bullet-} + H_2O$	R(275)	$4.0 \cdot 10^9$			= $k(CH_3CH(OH)(OO^{\bullet}) + OH^-)$
$CO(OH)(OO^{\bullet}) \rightarrow CO_2 + HO_2^{\bullet}$	R(276)	$1.0 \cdot 10^6$			18
$CO(O^{\bullet})(OO^{\bullet}) \rightarrow CO_2 + O_2^{\bullet-}$	R(277)	$1.0 \cdot 10^6$			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: $CH_3CH_2(OH) + HO^{\bullet} \rightarrow CH_3C^{\bullet}H(OH) + H_2O$		$1.9 \cdot 10^9$			BR: 90% - 20
$CH_3C^{\bullet}H(OH) + O_2 \rightarrow CH_3CH(OH)(OO^{\bullet})$		$4.6 \cdot 10^9$		Adams and Willson, 1969	
Pathway 2: $CH_3CH_2(OH) + HO^{\bullet} \rightarrow CH_2^{\bullet}CH_2(OH) + H_2O$		$2.0 \cdot 10^8$			BR: 10% - 20
$CH_2^{\bullet}CH_2(OH) + O_2 \rightarrow CH_2(OH)CH_2(OO^{\bullet})$		$4.6 \cdot 10^9$		Adams and Willson, 1969	
$CH_3CH_2(OH) + HO^{\bullet} \rightarrow 0.90 CH_3CH(OH)(OO^{\bullet}) + 0.10 CH_2(OH)CH_2(OO^{\bullet}) + H_2O - O_2$	R(278)	$2.1 \cdot 10^9$	830	Monod et al., 2005	
Pathway 1: $CH_3CH_2(OH) + NO_3^{\bullet} \rightarrow CH_3C^{\bullet}H(OH) + NO_3^- + H^+$		$2.0 \cdot 10^6$			BR: 90%
$CH_3C^{\bullet}H(OH) + O_2 \rightarrow CH_3CH(OH)(OO^{\bullet})$		$4.6 \cdot 10^9$		Adams and Willson, 1969	
Pathway 2: $CH_3CH_2(OH) + NO_3^{\bullet} \rightarrow CH_2^{\bullet}CH_2(OH) + NO_3^- + H^+$		$2.0 \cdot 10^5$			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	
$CH_3CH_2(OH) + NO_3^{\bullet} \rightarrow 0.90 CH_3CH(OH)(OO^{\bullet}) + 0.10 CH_2(OH)CH_2(OO^{\bullet}) + NO_3^- + H^+ - O_2$	R(279)	$2.2 \cdot 10^6$	3300	Herrmann and Zellner, 1998	3
Pathway 1: $CH_3CH_2(OH) + FeO^{2+} \rightarrow CH_3C^{\bullet}H(OH) + Fe^{3+} + OH^-$		$2.2 \cdot 10^3$			BR: 90%
$CH_3C^{\bullet}H(OH) + O_2 \rightarrow CH_3CH(OH)(OO^{\bullet})$		$4.6 \cdot 10^9$		Adams and Willson, 1969	
Pathway 2: $CH_3CH_2(OH) + FeO^{2+} \rightarrow CH_2^{\bullet}CH_2(OH) + Fe^{3+} + OH^-$		$3.0 \cdot 10^2$			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: $CH_3CH_2(OH) + SO_4^{\bullet-} \rightarrow CH_3C^{\bullet}H(OH) + SO_4^{2-} + H^+$		$3.7 \cdot 10^7$			BR: 90%
$CH_3C^{\bullet}H(OH) + O_2 \rightarrow CH_3CH(OH)(OO^{\bullet})$		$4.6 \cdot 10^9$		Adams and Willson, 1969	
Pathway 2: $CH_3CH_2(OH) + SO_4^{\bullet-} \rightarrow CH_2^{\bullet}CH_2(OH) + SO_4^{2-} + H^+$		$4.0 \cdot 10^6$			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	
$CH_3CH_2(OH) + SO_4^{\bullet-} \rightarrow 0.90 CH_3CH(OH)(OO^{\bullet}) + 0.10 CH_2(OH)CH_2(OO^{\bullet}) + SO_4^{2-} + H^+ - O_2$	R(281)	$4.1 \cdot 10^7$	1760	Clifton and Huie, 1989	3
Patway 1: $CH_3CH_2(OH) + Cl_2^{\bullet-} \rightarrow CH_3C^{\bullet}H(OH) + 2 Cl^- + H^+$		$1.1 \cdot 10^5$			BR: 90%
$CH_3C^{\bullet}H(OH) + O_2 \rightarrow CH_3CH(OH)(OO^{\bullet})$		$4.6 \cdot 10^9$		Adams and Willson, 1969	
Pathway 2: $CH_3CH_2(OH) + Cl_2^{\bullet-} \rightarrow CH_2^{\bullet}CH_2(OH) + 2 Cl^- + H^+$		$1.0 \cdot 10^4$			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	
$CH_3CH_2(OH) + Cl_2^{\bullet-} \rightarrow 0.90 CH_3CH(OH)(OO^{\bullet}) + 0.10 CH_2(OH)CH_2(OO^{\bullet}) + 2 Cl^- + H^+ - O_2$	R(282)	$1.2 \cdot 10^5$		Zellner et al., 1996	3
Pathway 1: $CH_3CH_2(OH) + CO_3^{\bullet-} \rightarrow CH_3C^{\bullet}H(OH) + CO_3^{2-} + H^+$		$1.3 \cdot 10^4$			BR: 90%
$CH_3C^{\bullet}H(OH) + O_2 \rightarrow CH_3CH(OH)(OO^{\bullet})$		$4.6 \cdot 10^9$		Adams and Willson, 1969	
Pathway 2: $CH_3CH_2(OH) + CO_3^{\bullet-} \rightarrow CH_2^{\bullet}CH_2(OH) + CO_3^{2-} + H^+$		$2.0 \cdot 10^3$			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	
$CH_3CH_2(OH) + CO_3^{\bullet-} \rightarrow 0.90 CH_3CH(OH)(OO^{\bullet}) + 0.10 CH_2(OH)CH_2(OO^{\bullet}) + CO_3^{2-} + H^+ - O_2$	R(283)	$1.5 \cdot 10^4$		Kuz'min, 1972	3
$CH_3CH(OH)(OO^{\bullet}) + OH^- \rightarrow CH_3CH(O)(OO^{\bullet}) + H_2O$		$4.0 \cdot 10^9$			
$CH_3CH(O^{\bullet})(OO^{\bullet}) \rightarrow CH_3CHO + O_2^{\bullet-}$					5
$CH_3CH(OH)(OO^{\bullet}) + OH^- \rightarrow CH_3CHO + O_2^{\bullet-} + H_2O$	R(284)	$4.0 \cdot 10^9$		Neta et al., 1990	
$CH_3CH(OH)(OO^{\bullet}) \rightarrow CH_3CHO + HO_2^{\bullet}$	R(285)	$5.2 \cdot 10^1$	7217	Von Sonntag, 1987	
Pathway 1: $2 CH_2(OH)CH_2(OO^{\bullet}) \rightarrow 2 CH_2(OH)CHO + H_2O_2$		$5.0 \cdot 10^7$			BR: 50%
Pathway 2: $2 CH_2(OH)CH_2(OO^{\bullet}) \rightarrow CH_2(OH)CH_2(OH) + CH_2(OH)CHO + O_2$		$3.3 \cdot 10^7$			BR: 33%
Pathway 3: $2 CH_2(OH)CH_2(OO^{\bullet}) \rightarrow 2 CH_2(O^{\bullet})CH_2(OH) + O_2$		$1.7 \cdot 10^7$			BR: 17%
$CH_2(O^{\bullet})CH_2(OH) \rightarrow C^{\bullet}H_2(OH) + CH_2O$					21 - 22
$C^{\bullet}H_2(OH) + O_2 \rightarrow CH_2(OH)(OO^{\bullet})$		$2.0 \cdot 10^9$			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)	$1.0 \cdot 10^8$		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 ₃ CH(OH)(OO [•]) + 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					
$CH_3CHO + HO^\bullet \rightarrow CH_3C^\bullet O + H_2O$		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
$CH_3CHO + Cl_2^- \rightarrow CH_3C^\bullet O + 2 Cl^- + H^+$		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 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: $CH_3CH(OH)(OH) + Cl_2^- \rightarrow CH_3C^\bullet(OH)(OH) + 2 Cl^- + H^+$		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 ₃ CH(OH)(OO [•]) + OH ⁻)

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

Reactions		k ₂₉₈ (M ⁻ⁿ⁺¹ s ⁻¹)	Ea/R (K)	References	Notes
CH(OH)(OO•)CH(OH)(OH) + OH ⁻ → CH(O ⁻)(OO•)CH(OH)(OH) + H ₂ O		4.0 10 ⁹			
CH(O ⁻)(OO•)CH(OH)(OH) → CHOCH(OH)(OH) + O ₂ • ⁻					5
CH(OH)(OO•)CH(OH)(OH) + OH ⁻ → CHOCH(OH)(OH) + O ₂ • ⁻ + H ₂ O	R(310)	4.0 10 ⁹			= k(CH ₃ CH(OH)(OO•) + OH ⁻)
CH(OH)(OO•)CH(OH)(OH) → CHOCH(OH)(OH) + HO ₂ •	R(311)	1.9 10 ²			4
Oxidation of Glyoxal					35
Pathway 1: CH(OH)(OH)CH(OH)(OH) + HO• → CH(OH)(OH)C•(OH)(OH) + H ₂ O		3.0 10 ⁸			BR: 27% - 36
CH(OH)(OH)C•(OH)(OH) + O ₂ → CH(OH)(OH)C(OH)(OH)(OO•)		1.2 10 ⁹		Schaefer et al., 2014	
Pathway 2: CH(OH)(OH)CH(OH)(OH) + HO• → CH(OH)(OH)CH(OH)(O•) + H ₂ O		8.0 10 ⁸			BR: 73% - 36
CH(OH)(OH)CH(OH)(O•) → C•H(OH)(OH) + CHO(OH)					21 - 22
C•H(OH)(OH) + O ₂ → CH(OH)(OH)(OO•)		2.0 10 ⁹			2
CH(OH)(OH)CH(OH)(OH) + HO• → 0.27 CH(OH)(OH)C(OH)(OH)(OO•) + 0.73 CHO(OH) + 0.73 CH(OH)(OH)(OO•) + H ₂ O - O ₂	R(312)	1.1 10 ⁹	1516	Buxton et al., 1997	
Pathway 1: CH(OH)(OH)CH(OH)(OH) + NO ₃ • → CH(OH)(OH)C•(OH)(OH) + NO ₃ ⁻ + H ⁺		7.3 10 ⁵			BR: 27%
CH(OH)(OH)C•(OH)(OH) + O ₂ → CH(OH)(OH)C(OH)(OH)(OO•)		1.2 10 ⁹		Schaefer et al., 2014	
Pathway 2: CH(OH)(OH)CH(OH)(OH) + NO ₃ • → CH(OH)(OH)CH(OH)(O•) + NO ₃ ⁻ + H ⁺		2.7 10 ⁵			BR: 73%
CH(OH)(OH)CH(OH)(O•) → C•H(OH)(OH) + CHO(OH)					21 - 22
C•H(OH)(OH) + O ₂ → CH(OH)(OH)(OO•)		2.0 10 ⁹			2
CH(OH)(OH)CH(OH)(OH) + NO ₃ • → 0.27 CH(OH)(OH)C(OH)(OH)(OO•) + 0.73 CHO(OH) + 0.73 CH(OH)(OH)(OO•) + NO ₃ ⁻ + H ⁺ - O ₂	R(313)	1.0 10 ⁶			3 - 37
Pathway 1: CH(OH)(OH)CH(OH)(OH) + SO ₄ • ⁻ → CH(OH)(OH)C•(OH)(OH) + SO ₄ ²⁻ + H ⁺		1.8 10 ⁷			BR: 27%
CH(OH)(OH)C•(OH)(OH) + O ₂ → CH(OH)(OH)C(OH)(OH)(OO•)		1.2 10 ⁹		Schaefer et al., 2014	
Pathway 2: CH(OH)(OH)CH(OH)(OH) + SO ₄ • ⁻ → CH(OH)(OH)CH(OH)(O•) + SO ₄ ²⁻ + H ⁺		6.0 10 ⁶			BR: 73%
CH(OH)(OH)CH(OH)(O•) → C•H(OH)(OH) + CHO(OH)					21 - 22
C•H(OH)(OH) + O ₂ → CH(OH)(OH)(OO•)		2.0 10 ⁹			2
CH(OH)(OH)CH(OH)(OH) + SO ₄ • ⁻ → 0.27 CH(OH)(OH)C(OH)(OH)(OO•) + 0.73 CHO(OH) + 0.73 CH(OH)(OH)(OO•) + SO ₄ ²⁻ + H ⁺ - O ₂	R(314)	2.4 10 ⁷		George et al., 2001	3
CH(OH)(OH)C(OH)(OH)(OO•) + OH ⁻ → CH(OH)(OH)C(OH)(O ⁻)(OO•) + H ₂ O		4.0 10 ⁹			5
CH(OH)(OH)C(OH)(O ⁻)(OO•) → CH(OH)(OH)CO(OH) + O ₂ • ⁻					
CH(OH)(OH)C(OH)(OH)(OO•) + OH ⁻ → CH(OH)(OH)CO(OH) + O ₂ • ⁻ + H ₂ O	R(315)	4.0 10 ⁹			= k(CH ₃ CH(OH)(OO•) + OH ⁻)
CH(OH)(OH)C(OH)(OH)(OO•) → CH(OH)(OH)CO(OH) + HO ₂ •	R(316)	1.0 10 ⁶			17
Acetic acid formation by Peracetic Acid oxidation					
CH ₃ CO(OH) + H ₂ O ₂ + H ⁺ → CH ₃ CO(OOH) + H ₂ O + H ⁺	R(317)	3.1 10 ⁻⁴	5235		= k(CHO(OH) + H ₂ O ₂ + H ⁺) - 38
CH ₃ CO(OOH) + H ₂ O + H ⁺ → CH ₃ CO(OH) + H ₂ O ₂ + H ⁺	R(318)	3.8 10 ⁻⁴			= k(CHO(OOH) + H ₂ O + H ⁺) - 38
CH ₃ CO(OOH) + HSO ₃ ⁻ → CH ₃ CO(OH) + H ₂ SO ₄ - H ⁺	R(319)	4.8·10 ⁷	3990	Lind et al., 1987	
Glycolic acid formation by Hydroxyperacetic Acid oxidation					
CH ₂ (OH)CO(OH) + H ₂ O ₂ + H ⁺ → CH ₂ (OH)CO(OOH) + H ₂ O + H ⁺	R(320)	3.1 10 ⁻⁴	5235		= k(CHO(OH) + H ₂ O ₂ + H ⁺) - 39
CH ₂ (OH)CO(OOH) + H ₂ O + H ⁺ → CH ₂ (OH)CO(OH) + H ₂ O ₂ + H ⁺	R(321)	3.8 10 ⁻⁴			= k(CHO(OOH) + H ₂ O + H ⁺) - 39
Oxidation of Acetic Acid					
CH ₃ CO(OH) + HO• → C•H ₂ CO(OH) + H ₂ O		1.5 10 ⁷	1330		
C•H ₂ CO(OH) + O ₂ → CH ₂ (OO•)CO(OH)		2.0 10 ⁹			2
CH ₃ CO(OH) + HO• → CH ₂ (OO•)CO(OH) + H ₂ O - 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
$CH_3CO(O^\cdot) + HO^\cdot \rightarrow C^*H_2CO(O^\cdot) + H_2O$ $C^*H_2CO(O^\cdot) + O_2 \rightarrow CH_2(OO^\cdot)CO(O^\cdot)$ $CH_3CO(O^\cdot) + HO^\cdot \rightarrow CH_2(OO^\cdot)CO(O^\cdot) + H_2O - O_2$	R(323)	$1.0 \cdot 10^8$ $2.0 \cdot 10^9$ $1.0 \cdot 10^8$	1800	Fisher and Hamill, 1973	2
$CH_3CO(OH) + NO_3^\cdot \rightarrow C^*H_2CO(OH) + NO_3^- + H^+$ $C^*H_2CO(OH) + O_2 \rightarrow CH_2(OO^\cdot)CO(OH)$ $CH_3CO(OH) + NO_3^\cdot \rightarrow CH_2(OO^\cdot)CO(OH) + NO_3^- + H^+ - O_2$ $CH_3CO(O^\cdot) + NO_3^\cdot \rightarrow C^*H_2CO(O^\cdot) + NO_3^- + H^+$ $C^*H_2CO(O^\cdot) + O_2 \rightarrow CH_2(OO^\cdot)CO(O^\cdot)$ $CH_3CO(O^\cdot) + NO_3^\cdot \rightarrow CH_2(OO^\cdot)CO(O^\cdot) + NO_3^- + H^+ - O_2$	R(324)	$1.3 \cdot 10^4$ $2.0 \cdot 10^9$ $1.3 \cdot 10^4$ $2.3 \cdot 10^6$	3800	Exner et al., 1994	2
$CH_3CO(O^\cdot) + SO_4^{\cdot-} \rightarrow C^*H_2CO(O^\cdot) + SO_4^{2-} + H^+$ $C^*H_2CO(O^\cdot) + O_2 \rightarrow CH_2(OO^\cdot)CO(O^\cdot)$ $CH_3CO(O^\cdot) + SO_4^{\cdot-} \rightarrow CH_2(OO^\cdot)CO(O^\cdot) + SO_4^{2-} + H^+ - O_2$	R(325)	$5.1 \cdot 10^6$ $2.0 \cdot 10^9$	3800	Exner et al., 1994	2
$CH_3CO(OH) + Cl_2^{\cdot-} \rightarrow C^*H_2CO(OH) + 2 Cl^- + H^+$ $C^*H_2CO(OH) + O_2 \rightarrow CH_2(OO^\cdot)CO(OH)$ $CH_3CO(OH) + Cl_2^{\cdot-} \rightarrow CH_2(OO^\cdot)CO(OH) + 2 Cl^- + H^+ - O_2$	R(326)	$1.5 \cdot 10^3$ $2.0 \cdot 10^9$ $1.5 \cdot 10^3$	4930	Huie and Clifton, 1990	2
$CH_3CO(O^\cdot) + Cl_2^{\cdot-} \rightarrow C^*H_2CO(O^\cdot) + 2 Cl^- + H^+$ $C^*H_2CO(O^\cdot) + O_2 \rightarrow CH_2(OO^\cdot)CO(O^\cdot)$ $CH_3CO(O^\cdot) + Cl_2^{\cdot-} \rightarrow CH_2(OO^\cdot)CO(O^\cdot) + 2 Cl^- + H^+ - O_2$	R(327)	$2.6 \cdot 10^6$ $2.0 \cdot 10^9$	4800	Jacobi et al., 1999	2
$CH_3CO(O^\cdot) + CO_3^{\cdot-} \rightarrow C^*H_2CO(O^\cdot) + CO_3^{2-} + H^+$ $C^*H_2CO(O^\cdot) + O_2 \rightarrow CH_2(OO^\cdot)CO(O^\cdot)$ $CH_3CO(O^\cdot) + CO_3^{\cdot-} \rightarrow CH_2(OO^\cdot)CO(O^\cdot) + CO_3^{2-} + H^+ - O_2$	R(328)	$5.8 \cdot 10^2$ $2.0 \cdot 10^9$	4800	Jacobi et al., 1996	2
$CH_3CO(O^\cdot) + CO_3^{\cdot-} \rightarrow CH_2(OO^\cdot)CO(O^\cdot) + CO_3^{2-} + H^+ - O_2$	R(329)	$5.8 \cdot 10^2$		Zellner et al., 1996	
Oxidation of Ethyl hydroperoxide (EHP)					
$CH_3CH_2(OOH) + Fe^{2+} \rightarrow CH_3CH_2(O^\cdot) + Fe^{3+} + OH^-$ $CH_3CH_2(O^\cdot) \rightarrow CH_3C^*H(OH)$ $CH_3C^*H(OH) + O_2 \rightarrow CH_3CH(OH)(OO^\cdot)$ $CH_3CH_2(OOH) + Fe^{2+} \rightarrow CH_3CH(OH)(OO^\cdot) + Fe^{3+} + OH^- - O_2$ Pathway 1: $CH_3CH_2(OOH) + HO^\cdot \rightarrow CH_3CH_2(OO^\cdot) + H_2O$ Pathway 2: $CH_3CH_2(OOH) + HO^\cdot \rightarrow CH_3C^*H(OOH) + H_2O$ $CH_3C^*H(OOH) + O_2 \rightarrow CH_3CH(OOH)(OO^\cdot)$ $CH_3CH_2(OOH) + HO^\cdot \rightarrow 0.80 CH_3CH_2(OO^\cdot) + 0.20 CH_3CH(OOH)(OO^\cdot) + H_2O - 0.20 O_2$	R(330)	$2.4 \cdot 10^1$ $5.0 \cdot 10^5$ $4.6 \cdot 10^9$ $2.4 \cdot 10^1$ $4.6 \cdot 10^8$ $1.2 \cdot 10^8$ $2.0 \cdot 10^9$		Adams and Willson, 1969 Chevallier et al., 2004 Monod et al., 2007 Monod et al., 2007	40 - 22 BR: 80% BR: 20% 2
$CH_3CH_2(OOH) + hv \rightarrow CH_3CH_2(O^\cdot) + HO^\cdot$ $CH_3CH_2(O^\cdot) + H_2O \rightarrow CH_3C^*H(OH) + H_2O$ $CH_3C^*H(OH) + O_2 \rightarrow CH_3CH(OH)(OO^\cdot)$ $CH_3CH_2(OOH) + hv \rightarrow CH_3CH(OH)(OO^\cdot) + HO^\cdot - O_2$ $CH_3CH(OOH)(OO^\cdot) + OH^- \rightarrow CH_3CH(OO^-)(OO^\cdot) + H_2O$ $CH_3CH(OO^-)(OO^\cdot) \rightarrow CH_3CO(OH) + O_2^{\cdot-}$	R(331)	$5.8 \cdot 10^8$ Calculated $5.0 \cdot 10^5$ $4.6 \cdot 10^9$		Monod et al., 2007	
$CH_3CH(OOH)(OO^\cdot) + OH^- \rightarrow CH_3CO(OH) + O_2^{\cdot-} + H_2O$	R(332)	Calculated $4.0 \cdot 10^9$		Adams and Willson, 1969	40 = J(H ₂ O ₂)
$CH_3CH(OOH)(OO^\cdot) + OH^- \rightarrow CH_3CO(OH) + O_2^{\cdot-} + H_2O$	R(333)	$4.0 \cdot 10^9$			11 = k(CH ₃ CH(OH)(OO [•]) + OH ⁻) - 12
$CH_3CH(OOH)(OO^\cdot) \rightarrow CH_3CO(OH) + HO_2^\cdot$	R(334)	$1.9 \cdot 10^2$			= k(CH ₃ CH(OH)(OO [•]) → CH ₃ CHO + HO ₂ [•]) - 41
Ethylperoxyl radical self-reaction					
Pathway 1: $2 CH_3CH_2(OO^\cdot) \rightarrow 2 CH_3CHO + H_2O_2$ Pathway 2: $2 CH_3CH_2(OO^\cdot) \rightarrow 2 CH_3CH_2(O^\cdot) + O_2$ $CH_3CH_2(O^\cdot) \rightarrow CH_3C^*H(OH)$ $CH_3C^*H(OH) + O_2 \rightarrow CH_3CH(OH)(OO^\cdot)$		$3.0 \cdot 10^7$ $1.3 \cdot 10^8$ $4.6 \cdot 10^9$		Adams and Willson, 1969	BR: 20% - 42 BR: 80% - 42 10 - 22

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

Reactions		k_{298} ($M^{-n+1} s^{-1}$)	Ea/R (K)	References	Notes
$[Fe(C_2O_4)]^+ + h\nu \rightarrow Fe^{2+} + C_2O_4^{\bullet-}$	R(355)	Calculated		Long et al., 2013	
$[Fe(C_2O_4)_2]^- + h\nu \rightarrow Fe^{2+} + CO(O^-)CO(O^-) + C_2O_4^{\bullet-}$	R(356)	Calculated		Faust and Zepp, 1993	
$[Fe(C_2O_4)_3]^{3-} + h\nu \rightarrow Fe^{2+} + 2 CO(O^-)CO(O^-) + C_2O_4^{\bullet-}$	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: $CH_2(OOH)CO(OH) + HO^\bullet \rightarrow C^*H(OOH)CO(OH) + H_2O$		1.2 10 ⁸			BR: 20% - 48
$C^*H(OOH)CO(OH) + O_2 \rightarrow CH(OOH)(OO^\bullet)CO(OH)$		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 ₃ CH ₂ (OOH) + HO [•])
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: $CH_2(OOH)CO(OH) + NO_3^\bullet \rightarrow C^*H(OOH)CO(OH) + NO_3^- + H^+$		3.0 10 ⁵			BR: 20%
$C^*H(OOH)CO(OH) + O_2 \rightarrow CH(OOH)(OO^\bullet)CO(OH)$		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			
$CH_2(O^\bullet)CO(OH) \rightarrow CH_2O + C^*O(OH)$					21 - 22
$C^*O(OH) + O_2 \rightarrow CO(OH)(OO^\bullet)$		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 ₃ CH ₂ (OOH) + Fe ²⁺)
$CH_2(OOH)CO(OH) + h\nu \rightarrow CH_2(O^\bullet)CO(OH) + HO^\bullet$		Calculated			
$CH_2(O^\bullet)CO(OH) \rightarrow CH_2O + C^*O(OH)$					21 - 22
$C^*O(OH) + O_2 \rightarrow CO(OH)(OO^\bullet)$		2.0 10 ⁹			2
$CH_2(OOH)CO(OH) + h\nu \rightarrow CH_2O + CO(OH)(OO^\bullet) + HO^\bullet - O_2$	R(361)	Calculated			= J(CH ₃ CH ₂ (OOH) + hν)
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: $CH_2(OOH)CO(O^-) + HO^\bullet \rightarrow C^*H(OOH)CO(O^-) + H_2O$		1.2 10 ⁸			BR: 20% - 48
$C^*H(OOH)CO(O^-) + O_2 \rightarrow CH(OOH)(OO^\bullet)CO(O^-)$		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 ₃ CH ₂ (OOH) + HO [•])
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: $CH_2(OOH)CO(O^-) + NO_3^\bullet \rightarrow C^*H(OOH)CO(O^-) + NO_3^- + H^+$		1.4 10 ⁶			BR: 20%
$C^*H(OOH)CO(O^-) + O_2 \rightarrow CH(OOH)(OO^\bullet)CO(O^-)$		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			
$CH_2(O^\bullet)CO(O^-) \rightarrow CH_2O + C^*O(O^-)$					21 - 22
$C^*O(O^-) + O_2 \rightarrow CO(O^-)(OO^\bullet)$		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 ₃ CH ₂ (OOH) + Fe ²⁺)
$CH_2(OOH)CO(O^-) + h\nu \rightarrow CH_2(O^\bullet)CO(O^-) + HO^\bullet$		Calculated			
$CH_2(O^\bullet)CO(O^-) + H_2O \rightarrow C^*H(OH)CO(O^-) + H_2O$		8.0 10 ⁶			10
$C^*H(OH)CO(O^-) + O_2 \rightarrow CH(OH)(OO^\bullet)CO(O^-)$		2.0 10 ⁹			2
$CH_2(OOH)CO(O^-) + h\nu \rightarrow CH(OH)(OO^\bullet)CO(O^-) + HO^\bullet - O_2$	R(365)	Calculated			= J(CH ₃ CH ₂ (OOH) + hν)
$CH(OOH)(OO^\bullet)CO(OH) + OH^- \rightarrow CH(OO^-)(OO^\bullet)CO(OH) + H_2O$		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 ₃ CH(OH)(OO [•]) + 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 [•])CO(OH) → CHOCO(OH) + HO ₂ [•]) - 49

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

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

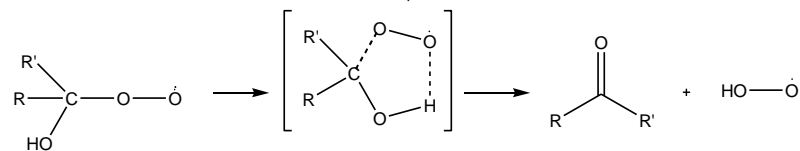
Reactions		k_{298} ($M^{-n+1} s^{-1}$)	Ea/R (K)	References	Notes
R(OO•) produced by C3 oxidation					54
Pathway 1: $2 \text{ CHOCH}_2(\text{OO}^\bullet) \rightarrow 2 \text{ CHOCHO} + \text{H}_2\text{O}_2$		$1.8 \cdot 10^8$			BR: 45%
Pathway 2: $2 \text{ CHOCH}_2(\text{OO}^\bullet) \rightarrow \text{CHOCHO} + \text{CH}_2(\text{OH})\text{CHO} + \text{O}_2$		$8.0 \cdot 10^7$			BR: 20%
Pathway 3: $2 \text{ CHOCH}_2(\text{OO}^\bullet) \rightarrow 2 \text{ CHOCH}_2(\text{O}^\bullet) + \text{O}_2$		$1.4 \cdot 10^8$			BR: 35%
$\text{CHOCH}_2(\text{O}^\bullet) \rightarrow \text{C}^\bullet\text{HO} + \text{CH}_2\text{O}$					21 - 22
$\text{C}^\bullet\text{HO} + \text{O}_2 \rightarrow \text{CHO}(\text{OO}^\bullet)$		$2.0 \cdot 10^9$			2
$2 \text{ CHOCH}_2(\text{OO}^\bullet) \rightarrow 1.10 \text{ CHOCHO} + 0.20 \text{ CH}_2(\text{OH})\text{CHO} + 0.70 \text{ CH}_2\text{O} + 0.70 \text{ CHO}(\text{OO}^\bullet) + 0.45 \text{ H}_2\text{O}_2 - 0.15 \text{ O}_2$	R(387)	$4.0 \cdot 10^8$			= $k(2 \text{ CH}_3\text{COCH}_2(\text{OO}^\bullet)) - 29$
Pathway 1: $2 \text{ CH}(\text{OH})(\text{OH})\text{CH}_2(\text{OO}^\bullet) + 2 \text{ H}_2\text{O} \rightarrow 2 \text{ CH}(\text{OH})(\text{OH})\text{CH}(\text{OH})(\text{OH}) + \text{H}_2\text{O}_2$		$1.8 \cdot 10^8$			BR: 45%
Pathway 2: $2 \text{ CH}(\text{OH})(\text{OH})\text{CH}_2(\text{OO}^\bullet) + \text{H}_2\text{O} \rightarrow \text{CH}(\text{OH})(\text{OH})\text{CH}(\text{OH})(\text{OH}) + \text{CH}_2(\text{OH})\text{CH}(\text{OH})(\text{OH}) + \text{O}_2$		$8.0 \cdot 10^7$			BR: 20%
Pathway 3: $2 \text{ CH}(\text{OH})(\text{OH})\text{CH}_2(\text{OO}^\bullet) \rightarrow 2 \text{ CH}(\text{OH})(\text{OH})\text{CH}_2(\text{O}^\bullet) + \text{O}_2$		$1.4 \cdot 10^8$			BR: 35%
$\text{CH}(\text{OH})(\text{OH})\text{CH}_2(\text{O}^\bullet) \rightarrow \text{C}^\bullet\text{H}(\text{OH})(\text{OH}) + \text{CH}_2\text{O}$					21 - 22
$\text{C}^\bullet\text{H}(\text{OH})(\text{OH}) + \text{O}_2 \rightarrow \text{CH}(\text{OH})(\text{OH})(\text{OO}^\bullet)$		$2.0 \cdot 10^9$			2
$2 \text{ CH}(\text{OH})(\text{OH})\text{CH}_2(\text{OO}^\bullet) \rightarrow 1.10 \text{ CH}(\text{OH})(\text{OH})\text{CH}(\text{OH})(\text{OH}) + 0.20 \text{ CH}_2(\text{OH})\text{CH}(\text{OH})(\text{OH}) + 0.70 \text{ CH}_2\text{O} + 0.70$	R(388)	$4.0 \cdot 10^8$			= $k(2 \text{ CH}_3\text{COCH}_2(\text{OO}^\bullet)) - 29$
$\text{CH}(\text{OH})(\text{OH})(\text{OO}^\bullet) + 0.45 \text{ H}_2\text{O}_2 - 0.15 \text{ O}_2$					

1 - The reactivity of HMHP with HO• is supposed similar to the reactivity of MHP with HO•. $k(\text{CH}_2(\text{OOH})(\text{OH}) + \text{HO}^\bullet) = k(\text{CH}_3(\text{OOH}) + \text{HO}^\bullet)$ 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 $2.0 \cdot 10^9 \text{ M}^{-1} \text{ s}^{-1}$ 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^\bullet , $\text{SO}_4^{\bullet-}$, Cl^\bullet , $\text{Cl}_2^{\bullet-}$, $\text{CO}_3^{\bullet-}$) 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^\bullet elimination rate constant depends on the substituent attached to the carbon atom bearing the peroxy 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 peroxy 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^\bullet elimination for $\text{CH}(\text{OH})(\text{OOH})(\text{OO}^\bullet)$ is similar to the one for $\text{RC}(\text{OH})(\text{OH})(\text{OO}^\bullet)$ with the same rate constant equal to $1.0 \cdot 10^6 \text{ s}^{-1}$.

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 CH₂O formation. Monod et al. (2007) estimated that the alkoxy radical formation pathway (CH₃O•) 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 10¹⁰ 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•) group by OH• proceeds as fast as the H-abstraction for the (OH)(OO•) group (k = 4.0 10⁹ M⁻¹ s⁻¹).

13 - We suppose that the HO₂• elimination from CH₂(OOH)(OO•) is as fast as the one of CH₂(OH)(OO•).

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 HO₂• elimination for RC(OH)(OH)(OO•) species is fast. This is confirmed by Mc Elroy and Waygood (1991) for hydrated formaldehyde. We supposed a kinetic constant equal to 1.0 10⁶ s⁻¹.

18 - We suppose that the HO₂• elimination for CO(OH)(OO•) is similar to the one for RC(OH)(OH)(OO•) with the same rate constant equal to 1.0 10⁶ s⁻¹.

19 - This reaction is non-limiting following Bothe et al. (1978). We consider a rate constant of 1.0 10⁶ s⁻¹.

20 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 87% for CH₂, 9% for CH₃ 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 alkoxy radical RCO(O•) are fragmented with a rate constant around 1.0 10⁹ s⁻¹. We assumed that the alkoxy fragmentation is non limiting.

22 - For alkoxy 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(CH₃CHO + NO₃•) and k(CH₃CH(OH)(OH) + NO₃•) weighted by the proportion of the hydrated and the non-hydrated form : $k_{\text{global}} = k(\text{CH}_3\text{CHO} + \text{NO}_3\cdot) \times \frac{1}{1+K_h} + k(\text{CH}_3\text{CH(OH)(OH)} + \text{NO}_3\cdot) \times \frac{K_h}{1+K_h}$ To determine k(CH₃CHO + NO₃•) and k(CH₃CH(OH)(OH) + NO₃•), we assumed that their ratio is equal to the ratio $\frac{k(\text{CH}_3\text{CHO} + \text{HO}\cdot)}{k(\text{CH}_3\text{CH(OH)(OH)} + \text{HO}\cdot)}$. $k_{\text{global}} = 2.0 \text{ } 10^6 \text{ M}^{-1} \text{ s}^{-1}$ and $k(\text{CH}_3\text{CHO} + \text{NO}_3\cdot) = 3.1 \text{ } 10^6 \text{ M}^{-1} \text{ s}^{-1}$ and $k(\text{CH}_3\text{CH(OH)(OH)} + \text{NO}_3\cdot) = 1.1 \text{ } 10^6 \text{ M}^{-1} \text{ s}^{-1}$.

27 - Jacobi et al. (1996) measured global rate constant for acetaldehyde. We decompose it into the sum of k(CH₃CHO + Cl₂•) and k(CH₃CH(OH)(OH) + Cl₂•) weighted by the proportion of the hydrated and the non-hydrated form : $k_{\text{global}} = k(\text{CH}_3\text{CHO} + \text{Cl}_2\cdot) \times \frac{1}{1+K_h} + k(\text{CH}_3\text{CH(OH)(OH)} + \text{Cl}_2\cdot) \times \frac{K_h}{1+K_h}$ To determine k(CH₃CHO + Cl₂•) and k(CH₃CH(OH)(OH) + Cl₂•), we assumed that their ratio is equal to the ratio $\frac{k(\text{CH}_3\text{CHO} + \text{HO}\cdot)}{k(\text{CH}_3\text{CH(OH)(OH)} + \text{HO}\cdot)}$. $k_{\text{global}} = 4.0 \text{ } 10^4 \text{ M}^{-1} \text{ s}^{-1}$ and $k(\text{CH}_3\text{CHO} + \text{Cl}_2\cdot) = 6.3 \text{ } 10^4 \text{ M}^{-1} \text{ s}^{-1}$ and $k(\text{CH}_3\text{CH(OH)(OH)} + \text{Cl}_2\cdot) = 2.1 \text{ } 10^4 \text{ M}^{-1} \text{ s}^{-1}$.

28 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 63% for CH, 31% for OH and 6% for CH₃. 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:

Peroxy categories	Model compounds	References
>C(OO•)CO(OH)/>C(OO•)CO(O•)	CH ₂ (OO•)CO(O•)	Schuchmann et al. (1985)
>C(OH)C(OO•)<	CH ₂ (OH)CH ₂ (OO•)	Piesiak et al. (1984)
>COC(OO•)<	CH ₃ COCH ₂ (OO•)	Zegota et al. (1986b)
Others	CH ₃ CH ₂ (OO•)	Monod et al. (2007)

30 - Reaction of CH₃CO(OO•) with HO₂• is not considered because we assumed that this reaction is much slower than the reaction with O₂• 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 CH₂ and 5% for OH. The 2 first pathways are considered corresponding to 95% of the total reactivity. They have been scaled to 77/23%.

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- 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 CH₂, 36% for (OH) on CH(OH)(OH), and 8% for (OH) on CH₂(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 $1.0 \cdot 10^6 \text{ M}^{-1} \text{ s}^{-1}$ typical of values measured in Neta and Huie (1986).
- 38 - We consider the slow equilibrium leading to the formation of peracetic acid (CH₃CO(OOH)) through the oxidation of acetic acid by H₂O₂ in the same way than for performic acid (CHO(OOH)).
- 39 - We consider the slow equilibrium leading to the formation of hydroxyperacetic acid (CH₃CO(OOH)) through the oxidation of glycolic acid by H₂O₂ in the same way than for performic acid (CHO(OOH)).
- 40 - Following Chevallier et al. (2004), we suppose the electron transfer rate constant for CH₃CH₂(O•) to be equal to the one for CH₃O• estimated in Schuchmann and von Sonntag (1984).
- 41 - We suppose that the HO₂• elimination from CH₃CH(OOH)(OO•) is as fast as the one of CH₃CH(OH)(OO•).
- 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 peroxy radical are not stable and further decompose following different pathways. These pathways are supposed to be similar to the self reaction of CH₂(OO•)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 CH₂(OO•)CO(O•) of $2k = 1.5 \cdot 10^8 \text{ M}^{-1} \text{ s}^{-1}$. The reaction with O₂• 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 $7.5 \cdot 10^7 \text{ M}^{-1} \text{ s}^{-1}$.
- 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). $\log K(\text{CO}(\text{O}^-)\text{CO}(\text{O}^-) + \text{Fe}^{3+} \leftrightarrow [\text{Fe}(\text{C}_2\text{O}_4)]^+)$ = 9.4 ; $\log K(2 \text{ CO}(\text{O}^-)\text{CO}(\text{O}^-) + \text{Fe}^{3+} \leftrightarrow [\text{Fe}(\text{C}_2\text{O}_4)_2]^-)$ = 16.2 ; $\log K(3 \text{ CO}(\text{O}^-)\text{CO}(\text{O}^-) + \text{Fe}^{3+} \leftrightarrow [\text{Fe}(\text{C}_2\text{O}_4)_3]^{3-})$ = 20.4). We calculate the equilibrium constants : $\log K(\text{CO}(\text{O}^-)\text{CO}(\text{O}^-) + [\text{Fe}(\text{C}_2\text{O}_4)]^+ \leftrightarrow [\text{Fe}(\text{C}_2\text{O}_4)_2]^-)$ = 6.8 ; $\log K(\text{CO}(\text{O}^-)\text{CO}(\text{O}^-) + [\text{Fe}(\text{C}_2\text{O}_4)_2]^- \leftrightarrow [\text{Fe}(\text{C}_2\text{O}_4)_3]^{3-})$ = 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 $\text{Fe}(\text{OH})^{2+} + \text{CO}(\text{OH})\text{CO}(\text{O}^-) \leftrightarrow \text{Fe}(\text{C}_2\text{O}_4)^+$: $k_{\text{backward}} = 3.0 \cdot 10^{-3} \text{ s}^{-1}$ and $k_{\text{forward}} = 2.0 \cdot 10^4 \text{ M}^{-1} \text{ s}^{-1}$. The equilibrium constant is similar to Martell and Smith (1977). We suppose that the rate constant of the reaction $[\text{Fe}(\text{C}_2\text{O}_4)]^+ \rightarrow \text{CO}(\text{O}^-)\text{CO}(\text{O}^-) + \text{Fe}^{3+}$ is equal to $3.0 \cdot 10^{-3} \text{ s}^{-1}$.
- 48 - The reactivity of CH₂(OOH)CO(OH)/CH₂(OOH)CO(O•) with HO• is supposed similar to the reactivity of EHP (Ethyl hydroperoxide) with HO•. Therefore, we applied the same branching ratio 80/20%.
- 49 - We suppose that the HO₂• elimination from CO(OH)CH(OOH)(OO•) is as fast as the one of CH(OH)(OO•)CO(OH).
- 50 - We suppose that the HO₂• elimination from CO(O•)CH(OOH)(OO•) is as fast as the one of CH(OH)(OO•)CO(O•).
- 51 - The hydration constants are $1.1 \cdot 10^3$ for glyoxylic acid and $1.65 \cdot 10^1$ 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 ₂ O + H ₂ O ↔ CH ₂ (OH)(OH)	T(18)	1.3 10 ³	3777	Winkelman et al., 2002	
CHO(OO [•]) + H ₂ O ↔ CH(OH)(OH)(OO [•])	T(19)	1.3 10 ³	3777		1 = K _h (CH ₂ O/CH ₂ (OH)(OH))
Formic acid					
CHO(OH) ↔ CHO(O ⁻) + H ⁺	T(20)	1.8 10 ⁻⁴	150	Prue and Read, 1966	
CO(OH)(OO [•]) ↔ CO(O ⁻)(OO [•]) + H ⁺	T(21)	1.8 10 ⁻⁴	150		2 = K _a (CHO(O ⁻)/CHO(OH))
C2 compounds					
Acetaldehyde					
CH ₃ CHO + H ₂ O ↔ CH ₃ CH(OH)(OH)	T(22)	1.2		Buschmann et al., 1980	
CH ₃ CO(OO [•]) + H ₂ O ↔ CH ₃ C(OH)(OH)(OO [•])	T(23)	1.2			1 = K _h (CH ₃ CHO/CH ₃ CH(OH)(OH))
Glycolaldehyde					
CH ₂ (OH)CHO + H ₂ O ↔ CH ₂ (OH)CH(OH)(OH)	T(24)	1.0 10 ¹		Sørensen, 1972	
CH ₂ (OH)CO(OO [•]) + H ₂ O ↔ CH ₂ (OH)C(OH)(OH)(OO [•])	T(25)	1.0 10 ¹			1 = K _h (CH ₂ (OH)CHO/CH ₂ (OH)CH(OH)(OH))
CH(OH)(OO [•])CHO + H ₂ O ↔ CH(OH)(OO [•])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 ₂ O ↔ CHOCH(OH)(OH)	T(27)	8.5 10 ⁻¹		Ruiz-Montoya and Rodriguez-Mellado, 1994	
CHOCHO + 2 H ₂ O ↔ CH(OH)(OH)CH(OH)(OH)	T(28)	1.7 10 ²			Ruiz-Montoya and Rodriguez-Mellado, 1994
CHOCO(OO [•]) + H ₂ O ↔ CHOC(OH)(OH)(OO [•])	T(29)	8.5 10 ⁻¹			1 = K _h (CHOCHO/CHOCH(OH)(OH))
CHOCO(OO [•]) + 2 H ₂ O ↔ CH(OH)(OH)C(OH)(OH)(OO [•])	T(30)	1.7 10 ²			1 =K _h (CHOCHO/CH(OH)(OH)CH(OH)(OH))
Hydroxyperacetic acid					
CH ₂ (OH)CO(OOH) ↔ CH ₂ (OH)CO(OO ⁻) + H ⁺	T(31)	6.3 10 ⁻⁹			2 = K _a (CH ₃ CO(OO ⁻)/CH ₃ CO(OOH))
Peracetic acid					
CH ₃ CO(OOH) ↔ CH ₃ CO(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 ₃ CO(OH) ↔ CH ₃ CO(O ⁻) + H ⁺	T(33)	1.7 10 ⁻⁵		Lide and Frederikse, 1995	
Oxalic acid					
CO(OH)CO(OH) ↔ CO(OH)CO(O ⁻) + H ⁺	T(34)	5.6 10 ⁻²		Martell and Smith, 1977	
CO(OH)CO(O ⁻) ↔ CO(O ⁻)CO(O ⁻) + H ⁺	T(35)	5.4 10 ⁻⁵		Martell and Smith, 1977	
2-hydroperoxyacetic acid					
CH ₂ (OOH)CO(OH) ↔ CH ₂ (OOH)CO(O ⁻) + H ⁺	T(36)	1.7 10 ⁻⁵			2 = K _a (CH ₃ CO(O ⁻)/CH ₃ CO(OH))
CH ₂ (OO [•])CO(OH) ↔ CH ₂ (OO [•])CO(O ⁻) + H ⁺	T(37)	1.7 10 ⁻⁵			2 = K _a (CH ₃ CO(O ⁻)/CH ₃ CO(OH))
CH(OOH)(OO [•])CO(OH) ↔ CH(OOH)(OO [•])CO(OH) + H ⁺	T(38)	1.7 10 ⁻⁵			2 = K _a (CH ₃ CO(O ⁻)/CH ₃ CO(OH))
Glycolic acid					
CH ₂ (OH)CO(OH) ↔ CH ₂ (OH)CO(O ⁻) + H ⁺	T(39)	1.5 10 ⁻⁴		Lide and Frederikse, 1995	
CH(OH)(OO [•])CO(OH) ↔ CH(OH)(OO [•])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) ↔ CHOCO(O ⁻) + H ⁺	T(41)	6.6 10 ⁻⁴		Buxton et al., 1997	
CHOCO(OH) + H ₂ O ↔ CH(OH)(OH)CO(OH)	T(42)	1.1 10 ³		Tur'yan, 1998	
CHOCO(O ⁻) + H ₂ O ↔ CH(OH)(OH)CO(O ⁻)	T(43)	1.7 10 ¹		Tur'yan, 1998	
CO(OH)CO(OO [•]) ↔ CO(O ⁻)CO(OO [•]) + H ⁺	T(44)	6.6 10 ⁻⁴			2 = K _a (CHOCO(O ⁻)/CHOCO(OH))
CO(OH)CO(OO [•]) + H ₂ O ↔ CO(OH)C(OH)(OH)(OO [•])	T(45)	1.1 10 ³			2 = K _h (CHOCO(OH)/CH(OH)(OH)CO(OH)) = K _h (CHOCO(O ⁻)/CH(OH)(OH)CO(O ⁻))
CO(O ⁻)CO(OO [•]) + H ₂ O ↔ CO(O ⁻)C(OH)(OH)(OO [•])	T(46)	1.7 10 ¹			3
R(OO[•]) from C3 oxidation					
CHOCH ₂ (OO [•]) + H ₂ O ↔ CH(OH)(OH)CH ₂ (OO [•])	T(47)	1.0 10 ¹			= 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 ₂ O	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 ₃ CH 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 ₃ CHO	T(27)	1.3 10 ¹	5890	Sander, 2015	3
CH ₃ CO(OO•)	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 ₃ CO(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 ₃ CO(OH)	T(33)	4.1 10 ³	6200	Sander, 2015	

Species		H (298K) (M atm ⁻¹)	-ΔH/R (K)	References	Notes
Ethyl hydroperoxide CH ₃ CH 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 ₃ CO(OONO ₂)	T(39)	2.8	5730	Sander, 2015	
Ethyl nitrate CH ₃ CH 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)	$-\Delta H$ (J/mol)	$-\Delta S$ (J/mol/K)	References	Notes
C1 compounds		1				
HMHP (Hydro Methyl Hydro Peroxide) <chem>CH2(OOH)(OH)</chem>	T(18)	$5.0 \cdot 10^{-2}$			Estimated	2
Performic acid <chem>CHO(OOH)</chem>	T(19)	$5.0 \cdot 10^{-2}$			Estimated	2
MHP (Methyl Hydroperoxide) <chem>CH3(OOH)</chem>	T(20)	$5.0 \cdot 10^{-3}$	$2.7 \cdot 10^4$	$1.4 \cdot 10^2$	Davidovits et al., 2011	
Methanol <chem>CH3(OH)</chem>	T(21)	$1.7 \cdot 10^{-2}$	$3.3 \cdot 10^4$	$1.5 \cdot 10^2$	Davidovits et al., 2011	
Formaldehyde <chem>CH2O</chem>	T(22)	$4.0 \cdot 10^{-2}$			Sander, 2015	Mean value between 260- 270K
Formic acid <chem>CHO(OH)</chem>	T(23)	$1.5 \cdot 10^{-2}$	$3.3 \cdot 10^4$	$1.5 \cdot 10^2$	Davidovits et al., 2011	
Methyl nitrate <chem>CH3(ONO2)</chem>	T(24)	$5.0 \cdot 10^{-2}$			Estimated	2
C2 compounds						
Ethanol <chem>CH3CH2(OH)</chem>	T(25)	$9.0 \cdot 10^{-3}$	$4.6 \cdot 10^4$	$1.9 \cdot 10^2$	Davidovits et al., 2011	
Ethylene glycol <chem>CH2(OH)CH2(OH)</chem>	T(26)	$3.3 \cdot 10^{-2}$	$2.2 \cdot 10^4$	$1.0 \cdot 10^2$	Davidovits et al., 2011	
Acetaldehyde <chem>CH3CHO</chem>	T(27)	$3.0 \cdot 10^{-2}$			Sander, 2015	Measured at 267K
<chem>CH3CO(OO*)</chem>	T(28)	$5.0 \cdot 10^{-2}$			Estimated	2
Glycolaldehyde <chem>CH2(OH)CHO</chem>	T(29)	$5.0 \cdot 10^{-2}$			Estimated	2
Glyoxal <chem>CHOCHO</chem>	T(30)	$1.0 \cdot 10^{-2}$			Sander, 2015	Mean value between 260- 285K
Peracetic acid <chem>CH3CO(OOH)</chem>	T(31)	$5.0 \cdot 10^{-2}$			Estimated	2
Hydroxyperacetic acid <chem>CH2(OH)CO(OOH)</chem>	T(32)	$5.0 \cdot 10^{-2}$			Estimated	2

Species		α (298K)	$-\Delta H$ (J/mol)	$-\Delta S$ (J/mol/K)	References	Notes
Acetic acid CH ₃ CO(OH)	T(33)	2.0 10 ⁻²	3.4 10 ⁴	1.5 10 ²	Davidovits et al., 2011	
Ethyl hydroperoxide CH ₃ CH 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 ₃ CO(OONO ₂)	T(39)	1.0 10 ⁻³			Kirchner et al., 1990	Measured at 282K
Ethyl nitrate CH ₃ CH 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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