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

C4 compounds

For C4 oxidation, considered chemical pathways represent at least 75% of the estimated reactivity.

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
Oxidation of Methacrolein (MACR)					1
Pathway 1: $CH_2=C(CH_3)CHO + HO^\bullet \rightarrow CH_2(OH)C^\bullet(CH_3)CHO$		$9.4\ 10^9$			BR: 100% - 2
$CH_2(OH)C^\bullet(CH_3)CHO + O_2 \rightarrow CH_2(OH)C(OO^\bullet)(CH_3)CHO$		$2.0\ 10^9$			3
$CH_2=C(CH_3)CHO + HO^\bullet \rightarrow CH_2(OH)C(OO^\bullet)(CH_3)CHO - O_2$	R(611)	$9.4 \cdot 10^9$	1203	Schöne et al., 2014	
$2\ CH_2(OH)C(OO^\bullet)(CH_3)CHO \rightarrow 2\ CH_2(OH)C(CH_3)(O^\bullet)CHO + O_2$		$4.0\ 10^8$			
$CH_2(OH)C(CH_3)(O^\bullet)CHO \rightarrow 0.50\ CH_3COCHO + 0.50\ C^\bullet H_2(OH) + 0.50\ CH_3COCH_2(OH) + 0.50\ C^\bullet HO$					4 - 5
$C^\bullet H_2(OH) + O_2 \rightarrow CH_2(OH)(OO^\bullet)$		$2.0\ 10^9$			3
$C^\bullet HO + O_2 \rightarrow CHO(OO^\bullet)$		$2.0\ 10^9$			3
$2\ CH_2(OH)C(OO^\bullet)(CH_3)CHO \rightarrow CH_3COCHO + CH_3COCH_2(OH) + CH_2(OH)(OO^\bullet) + CHO(OO^\bullet) - O_2$	R(612)	$4.0\ 10^8$			= k(2 $CH_3COCH_2(OO^\bullet)$) - 6
Oxidation of Hydroxymethacrolein (HMACR)					7
Pathway 1:$CH_2=C(CH_2(OH))CHO + HO^\bullet \rightarrow CH_2(OH)C^\bullet(CH_2(OH))CHO$		$9.4\ 10^9$			BR: 100% - 2
$CH_2(OH)C^\bullet(CH_2(OH))CHO + O_2 \rightarrow CH_2(OH)C(CH_2(OH))(OO^\bullet)CHO$		$2.0\ 10^9$			3
$CH_2=C(CH_2(OH))CHO + HO^\bullet \rightarrow CH_2(OH)C(CH_2(OH))(OO^\bullet)CHO - O_2$	R(613)	$9.4 \cdot 10^9$	1203		= k($CH_2=C(CH_3)CHO$ + $HO^\bullet$)
$2\ CH_2(OH)C(CH_2(OH))(OO^\bullet)CHO \rightarrow 2\ CH_2(OH)C(CH_2(OH))(O^\bullet)CHO + O_2$		$4.0\ 10^8$			
$CH_2(OH)C(CH_2(OH))(O^\bullet)CHO \rightarrow 0.50\ CH_2(OH)COCHO + 0.50\ C^\bullet H_2(OH) + 0.50\ CH_2(OH)COCH_2(OH) + 0.50\ C^\bullet HO$					4 - 5
$C^\bullet H_2(OH) + O_2 \rightarrow CH_2(OH)(OO^\bullet)$		$2.0\ 10^9$			3
$C^\bullet HO + O_2 \rightarrow CHO(OO^\bullet)$		$2.0\ 10^9$			3
$2\ CH_2(OH)C(CH_2(OH))(OO^\bullet)CHO \rightarrow CH_2(OH)COCHO + CH_2(OH)COCH_2(OH) + CH_2(OH)(OO^\bullet) + CHO(OO^\bullet) - O_2$	R(614)	$4.0\ 10^8$			= k(2 $CH_3COCH_2(OO^\bullet)$) - 6
Oxidation of Methylvinylketone (MVK)					8
Pathway 1: $CH_2=CHCOCH_3 + HO^\bullet \rightarrow CH_2(OH)C^\bullet HCOCH_3$		$7.0\ 10^9$			BR: 100% - 2
$CH_2(OH)C^\bullet HCOCH_3 + O_2 \rightarrow CH_2(OH)CH(OO^\bullet)COCH_3$		$2.0\ 10^9$			3
$CH_2=CHCOCH_3 + HO^\bullet \rightarrow CH_3COCH(OO^\bullet)CH_2(OH) - O_2$	R(615)	$7.3\ 10^9$	1443	Schöne et al., 2014	
Pathway 1: $2\ CH_3COCH(OO^\bullet)CH_2(OH) \rightarrow 2\ CH_3COCOCH_2(OH) + H_2O_2$		$1.8\ 10^8$			BR: 45%
Pathway 2: $2\ CH_3COCH(OO^\bullet)CH_2(OH) \rightarrow CH_2(OH)CH(OH)COCH_3 + CH_3COCOCH_2(OH) + O_2$		$8.0\ 10^7$			BR: 20%
Pathway 3: $2\ CH_3COCH(OO^\bullet)CH_2(OH) \rightarrow 2\ CH_3COCH(O^\bullet)CH_2(OH) + O_2$		$1.4\ 10^8$			BR: 35%
$CH_3COCH(O^\bullet)CH_2(OH) \rightarrow 0.50\ C^\bullet H_2(OH) + 0.50\ CH_3COCHO + 0.50\ CH_2(OH)CHO + 0.50\ CH_3C^\bullet O$					4 - 5
$C^\bullet H_2(OH) + O_2 \rightarrow CH_2(OH)(OO^\bullet)$		$2.0\ 10^9$			3
$CH_3C^\bullet O + O_2 \rightarrow CH_3CO(OO^\bullet)$		$2.0\ 10^9$			3
$2\ CH_3COCH(OO^\bullet)CH_2(OH) \rightarrow 1.10\ CH_3COCOCH_2(OH) + 0.20\ CH_2(OH)CH(OH)COCH_3 + 0.35\ CH_3COCHO + 0.35\ CH_2(OH)CHO + 0.35\ CH_2(OH)(OO^\bullet) + 0.35\ CH_3CO(OO^\bullet) + 0.45\ H_2O_2 - 0.15\ O_2$	R(616)	$4.0\ 10^8$			= k(2 $CH_3COCH_2(OO^\bullet)$) - 6
Oxidation of Hydroxymethylvinylketone (MVKOH)					9
Pathway 1: $CH_2=CHCOCH_2(OH) + HO^\bullet \rightarrow CH_2(OH)C^\bullet HCOCH_2(OH)$		$7.0\ 10^9$			BR: 100% - 2
$CH_2(OH)C^\bullet HCOCH_2(OH) + O_2 \rightarrow CH_2(OH)CH(OO^\bullet)COCH_2(OH)$		$2.0\ 10^9$			3
$CH_2=CHCOCH_2(OH) + HO^\bullet \rightarrow CH_2(OH)CH(OO^\bullet)COCH_2(OH) - O_2$	R(617)	$7.3\ 10^9$	1443		= k($CH_2=CHCOCH_3$ + $HO^\bullet$)
Pathway 1: $2\ CH_2(OH)COCH(OO^\bullet)CH_2(OH) \rightarrow 2\ CH_2(OH)COCOCH_2(OH) + H_2O_2$		$1.8\ 10^8$			BR: 45%
Pathway 2: $2\ CH_2(OH)COCH(OO^\bullet)CH_2(OH) \rightarrow CH_2(OH)COCH(OH)CH_2(OH) + CH_2(OH)COCOCH_2(OH) + O_2$		$8.0\ 10^7$			BR: 20%
Pathway 3: $2\ CH_2(OH)COCH(OO^\bullet)CH_2(OH) \rightarrow 2\ CH_2(OH)COCH(O^\bullet)CH_2(OH) + O_2$		$1.4\ 10^8$			BR: 35%
$CH_2(OH)COCH(O^\bullet)CH_2(OH) \rightarrow 0.50\ C^\bullet H_2(OH) + 0.50\ CH_2(OH)COCHO + 0.50\ CH_2(OH)CHO + 0.50\ CH_2(OH)C^\bullet O$					4 - 5
$C^\bullet H_2(OH) + O_2 \rightarrow CH_2(OH)(OO^\bullet)$		$2.0\ 10^9$			3
$CH_2(OH)C^\bullet O + O_2 \rightarrow CH_2(OH)CO(OO^\bullet)$		$2.0\ 10^9$			3

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
2 $CH_2(OH)CH(OO^•)COCH_2(OH)$ → 1.10 $CH_2(OH)COCOCH_2(OH)$ + 0.20 $CH_2(OH)COCH(OH)CH_2(OH)$ + 0.35 $CH_2(OH)COCHO$ + 0.35 $CH_2(OH)CHO$ + 0.35 $CH_2(OH)(OO^•)$ + 0.35 $CH_2(OH)CO(OO^•)$ + 0.45 H_2O_2 - 0.15 O_2	R(618)	4.0 10^8			= k(2 $CH_3COCH_2(OO^•)$) - 6
Oxidation of Hydroxybutanedione					10
Pathway 1: $CH_3C(OH)(OH)COCH_2(OH)$ + $HO^•$ → $CH_3C(OH)(O^•)COCH_2(OH)$ + H_2O		4.2 10^8			BR: 54% - 11
$CH_3C(OH)(O^•)COCH_2(OH)$ → $CH_3CO(OH)$ + $CH_2(OH)C^•O$					4 - 5
$CH_2(OH)C^•O$ + O_2 → $CH_2(OH)CO(OO^•)$		2.0 10^9			3
Pathway 2: $CH_3C(OH)(OH)COCH_2(OH)$ + $HO^•$ → $CH_3C(OH)(OH)COC^•H(OH)$ + H_2O		3.6 10^8			BR: 46% - 11
$CH_3C(OH)(OH)COC^•H(OH)$ + O_2 → $CH_3C(OH)(OH)COCH(OH)(OO^•)$		2.0 10^9			3
$CH_3C(OH)(OH)COCH_2(OH)$ + $HO^•$ → 0.54 $CH_3CO(OH)$ + 0.54 $CH_2(OH)CO(OO^•)$ + 0.46 $CH_3C(OH)(OH)COCH(OH)(OO^•)$ + H_2O - O_2	R(619)	7.8 10^8			12
Patway 1: $CH_3C(OH)(OH)COCH_2(OH)$ + $NO_3^•$ → $CH_3C(OH)(OH)COC^•H(OH)$ + NO_3^- + H^+		1.0 10^6			BR: 100%
$CH_3C(OH)(OH)COC^•H(OH)$ + O_2 → $CH_3C(OH)(OH)COCH(OH)(OO^•)$		2.0 10^9			3
$CH_3C(OH)(OH)COCH_2(OH)$ + $NO_3^•$ → $CH_3C(OH)(OH)COCH(OH)(OO^•)$ + NO_3^- + H^+ - O_2	R(620)	1.0 10^6			= k(CH(OH)(OH)CH(OH)(OH) + $NO_3^•$) - 13
Pathway 1: $CH_3COC(OH)(OH)CH_2(OH)$ + $HO^•$ → $CH_3COC(OH)(O^•)CH_2(OH)$ + H_2O		4.2·10^8			BR: 58% - 14
$CH_3COC(OH)(O^•)CH_2(OH)$ → $CH_3C^•O$ + $CH_2(OH)CO(OH)$					4 - 5
$CH_3C^•O$ + O_2 → $CH_3CO(OO^•)$		2.0·10^9			3
Pathway 2: $CH_3COC(OH)(OH)CH_2(OH)$ + $HO^•$ → $CH_3COC(OH)(OH)C^•H(OH)$ + H_2O		3.0 10^8			BR: 42% - 14
$CH_3COC(OH)(OH)C^•H(OH)$ + O_2 → $CH_3COC(OH)(OH)CH(OH)(OO^•)$		2.0 10^9			3
$CH_3COC(OH)(OH)CH_2(OH)$ + $HO^•$ → 0.58 $CH_2(OH)CO(OH)$ + 0.58 $CH_3CO(OO^•)$ + 0.42 $CH_3COC(OH)(OH)CH(OH)(OO^•)$ + H_2O - O_2	R(621)	7.2 10^8			12
Pathway 1: $CH_3COC(OH)(OH)CH_2(OH)$ + $NO_3^•$ → $CH_3COC(OH)(OH)C^•H(OH)$ + NO_3^- + H^+		1.0 10^6			BR: 100%
$CH_3COC(OH)(OH)C^•H(OH)$ + O_2 → $CH_3COC(OH)(OH)CH(OH)(OO^•)$		2.0 10^9			3
$CH_3COC(OH)(OH)CH_2(OH)$ + $NO_3^•$ → $CH_3COC(OH)(OH)CH(OH)(OO^•)$ + NO_3^- + H^+ - O_2	R(622)	1.0 10^6			= k(CH(OH)(OH)CH(OH)(OH) + $NO_3^•$) - 13
Pathway 1: $CH_3C(OH)(OH)C(OH)(OH)CH_2(OH)$ + $HO^•$ → $CH_3C(OH)(O^•)C(OH)(OH)CH_2(OH)$ + H_2O		4.6 10^8			BR: 38% - 15
$CH_3C(OH)(O^•)C(OH)(OH)CH_2(OH)$ → $CH_3CO(OH)$ + $CH_2(OH)C^•(OH)(OH)$					4 - 5
$CH_2(OH)C^•(OH)(OH)$ + O_2 → $CH_2(OH)C(OH)(OH)(OO^•)$		2.0 10^9			3
Pathway 2: $CH_3C(OH)(OH)C(OH)(OH)CH_2(OH)$ + $HO^•$ → $CH_3C(OH)(OH)C(OH)(O^•)CH_2(OH)$ + H_2O		4.3 10^8			BR: 36% - 15
$CH_3C(OH)(OH)C(OH)(O^•)CH_2(OH)$ → $CH_3C(OH)(OH)CO(OH)$ + $C^•H_2(OH)$					4 - 5
$C^•H_2(OH)$ + O_2 → $CH_2(OH)(OO^•)$		2.0 10^9			3
Pathway 3: $CH_3C(OH)(OH)C(OH)(OH)CH_2(OH)$ + $HO^•$ → $CH_3C(OH)(OH)C(OH)(OH)C^•H(OH)$ + H_2O		3.1 10^8			BR: 26% - 15
$CH_3C(OH)(OH)C(OH)(OH)C^•H(OH)$ + O_2 → $CH_3C(OH)(OH)C(OH)(OH)CH(OH)(OO^•)$		2.0 10^9			3
$CH_3C(OH)(OH)C(OH)(OH)CH_2(OH)$ + $HO^•$ → 0.38 $CH_3CO(OH)$ + 0.38 $CH_2(OH)C(OH)(OH)(OO^•)$ + 0.36 $CH_3C(OH)(OH)CO(OH)$ + 0.36 $CH_2(OH)(OO^•)$ + 0.26 $CH_3C(OH)(OH)C(OH)(OH)CH(OH)(OO^•)$ + H_2O - O_2	R(623)	1.2 10^9			12
Pathway 1: $CH_3C(OH)(OH)C(OH)(OH)CH_2(OH)$ + $NO_3^•$ → $CH_3C(OH)(OH)C(OH)(OH)C^•H(OH)$ + NO_3^- + H^+		1.0 10^6			BR: 100%
$CH_3C(OH)(OH)C(OH)(OH)C^•H(OH)$ + O_2 → $CH_3C(OH)(OH)C(OH)(OH)CH(OH)(OO^•)$		2.0 10^9			3
$CH_3C(OH)(OH)C(OH)(OH)CH_2(OH)$ + $NO_3^•$ → $CH_3C(OH)(OH)C(OH)(OH)CH(OH)(OO^•)$ + NO_3^- + H^+ - O_2	R(624)	1.0 10^6			= k(CH(OH)(OH)CH(OH)(OH) + $NO_3^•$) - 13
$CH_3C(OH)(OH)COCH(OH)(OO^•)$ + OH^- → $CH_3C(OH)(OH)COCH(O^-)(OO^•)$ + H_2O		4.0 10^9			
$CH_3C(OH)(OH)COCH(O^-)(OO^•)$ → $CH_3C(OH)(OH)COCHO$ + $O_2^{•-}$					16
$CH_3C(OH)(OH)COCH(OH)(OO^•)$ + OH^- → $CH_3C(OH)(OH)COCHO$ + $O_2^{•-}$ + H_2O	R(625)	4.0 10^9			= k($CH_3CH(OH)(OO^•)$ + OH^-)
$CH_3C(OH)(OH)COCH(OH)(OO^•)$ → $CH_3C(OH)(OH)COCHO$ + $HO_2^•$	R(626)	1.9 10^2			17
$CH_3COC(OH)(OH)CH(OH)(OO^•)$ + OH^- → $CH_3COC(OH)(OH)CH(O^-)(OO^•)$ + H_2O		4.0 10^9			
$CH_3COC(OH)(OH)CH(O^-)(OO^•)$ → $CH_3COC(OH)(OH)$ CHO + $O_2^{•-}$					16
$CH_3COC(OH)(OH)CH(OH)(OO^•)$ + OH^- → $CH_3COC(OH)(OH)CHO$ + $O_2^{•-}$ + H_2O	R(627)	4.0 10^9			= k($CH_3CH(OH)(OO^•)$ + OH^-)

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CH_3COC(OH)(OH)CH(OH)(OO^•) \rightarrow CH_3COC(OH)(OH)CHO + HO_2^•$	R(628)	$1.9\ 10^2$			17
$CH_3C(OH)(OH)C(OH)(OH)CH(OH)(OO^•) + OH^- \rightarrow CH_3C(OH)(OH)C(OH)(OH)CH(O^-)(OO^•) + H_2O$		$4.0\ 10^9$			
$CH_3C(OH)(OH)C(OH)(OH)CH(O^-)(OO^•) \rightarrow CH_3C(OH)(OH)C(OH)(OH)CHO + O_2^{•-}$					16
$CH_3C(OH)(OH)C(OH)(OH)CH(OH)(OO^•) + OH^- \rightarrow CH_3C(OH)(OH)C(OH)(OH)CHO + O_2^{•-} + H_2O$	R(629)	$4.0\ 10^9$			= $k(CH_3CH(OH)(OO^•) + OH^-)$
$CH_3C(OH)(OH)C(OH)(OH)CH(OH)(OO^•) \rightarrow CH_3C(OH)(OH)C(OH)(OH)CHO + HO_2^•$	R(630)	$1.9\ 10^2$			17
Oxidation of 3,4-dihydroxybutan-2-one					18
Pathway 1: $CH_2(OH)CH(OH)COCH_3 + HO^• \rightarrow C^•H(OH)CH(OH)COCH_3 + H_2O$		$7.9\ 10^8$			BR: 81% - 19
$C^•H(OH)CH(OH)COCH_3 + O_2 \rightarrow CH(OH)(OO^•)CH(OH)COCH_3$		$2.0\ 10^9$			3
Pathway 2: $CH_2(OH)CH(OH)COCH_3 + HO^• \rightarrow CH_2(OH)C^•(OH)COCH_3 + H_2O$		$1.9\ 10^8$			BR: 19% - 19
$CH_2(OH)C^•(OH)COCH_3 + O_2 \rightarrow CH_2(OH)C(OH)(OO^•)COCH_3$		$2.0\ 10^9$			3
$CH_2(OH)CH(OH)COCH_3 + HO^• \rightarrow 0.81\ CH(OH)(OO^•)CH(OH)COCH_3 + 0.19\ CH_2(OH)C(OH)(OO^•)COCH_3 + H_2O - O_2$	R(631)	$9.8\ 10^8$			12
Pathway 1: $CH_2(OH)CH(OH)COCH_3 + NO_3^• \rightarrow C^•H(OH)CH(OH)COCH_3 + NO_3^- + H^+$		$8.1\ 10^5$			BR: 81%
$C^•H(OH)CH(OH)COCH_3 + O_2 \rightarrow CH(OH)(OO^•)CH(OH)COCH_3$		$2.0\ 10^9$			3
Pathway 2: $CH_2(OH)CH(OH)COCH_3 + NO_3^• \rightarrow CH_2(OH)C^•(OH)COCH_3 + NO_3^- + H^+$		$1.9\ 10^5$			BR: 19%
$CH_2(OH)C^•(OH)COCH_3 + O_2 \rightarrow CH_2(OH)C(OH)(OO^•)COCH_3$		$2.0\ 10^9$			3
$CH_2(OH)CH(OH)COCH_3 + NO_3^• \rightarrow 0.81\ CH(OH)(OO^•)CH(OH)COCH_3 + 0.19\ CH_2(OH)C(OH)(OO^•)COCH_3 + NO_3^- + H^+ - O_2$	R(632)	$1.0\ 10^6$			= $k(CH(OH)(OH)CH(OH)(OH) + NO_3^•)$ -13
$CH(OH)(OO^•)CH(OH)COCH_3 + OH^- \rightarrow CH(O^-)(OO^•)CH(OH)COCH_3 + H_2O$		$4.0\ 10^9$			
$CH(O^-)(OO^•)CH(OH)COCH_3 \rightarrow CH_3COCH(OH)CHO + O_2^{•-}$					16
$CH(OH)(OO^•)CH(OH)COCH_3 + OH^- \rightarrow CH_3COCH(OH)CHO + O_2^{•-} + H_2O$	R(633)	$4.0\ 10^9$			= $k(CH_3CH(OH)(OO^•) + OH^-)$
$CH(OH)(OO^•)CH(OH)COCH_3 \rightarrow CH_3COCH(OH)CHO + HO_2^•$	R(634)	$1.9\ 10^2$			17
$CH_2(OH)C(OH)(OO^•)COCH_3 + OH^- \rightarrow CH_2(OH)C(O^-)(OO^•)COCH_3 + H_2O$		$4.0\ 10^9$			
$CH_2(OH)C(O^-)(OO^•)COCH_3 \rightarrow CH_3COCOCH_2(OH) + O_2^{•-}$					16
$CH_2(OH)C(OH)(OO^•)COCH_3 + OH^- \rightarrow CH_3COCOCH_2(OH) + O_2^{•-} + H_2O$	R(635)	$4.0\ 10^9$			= $k(CH_3CH(OH)(OO^•) + OH^-)$
$CH_2(OH)C(OH)(OO^•)COCH_3 \rightarrow CH_3COCOCH_2(OH) + HO_2^•$	R(636)	$1.9\ 10^2$			17
Oxidation of 1,4-dihydroxybutanedione					20
Pathway 1: $CH_2(OH)C(OH)(OH)C(OH)(OH)CH_2(OH) + HO^• \rightarrow CH_2(OH)C(OH)(OH)C(OH)(O^•)CH_2(OH) + H_2O$		$8.1\ 10^8$			BR: 58% - 21
$CH_2(OH)C(OH)(OH)C(OH)(O^•)CH_2(OH) \rightarrow CH_2(OH)C^•(OH)(OH) + CH_2(OH)CO(OH)$					4 - 5
$CH_2(OH)C^•(OH)(OH) + O_2 \rightarrow CH_2(OH)C(OH)(OH)(OO^•)$		$2.0\ 10^9$			3
Pathway 2: $CH_2(OH)C(OH)(OH)C(OH)(OH)CH_2(OH) + HO^• \rightarrow CH_2(OH)C(OH)(OH)C(OH)(OH)C^•H(OH) + H_2O$		$5.9\ 10^8$			BR: 42% - 21
$CH_2(OH)C(OH)(OH)C(OH)(OH)C^•H(OH) + O_2 \rightarrow CH_2(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OO^•)$		$2.0\ 10^9$			3
$CH_2(OH)C(OH)(OH)C(OH)(OH)CH_2(OH) + HO^• \rightarrow 0.58\ CH_2(OH)CO(OH) + 0.58\ CH_2(OH)C(OH)(OH)(OO^•) + 0.42\ CH_2(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OO^•) + H_2O - O_2$	R(637)	$1.4\ 10^9$			12
Pathway 1: $CH_2(OH)C(OH)(OH)C(OH)(OH)CH_2(OH) + NO_3^• \rightarrow CH_2(OH)C(OH)(OH)C(OH)(OH)C^•H(OH) + NO_3^- + H^+$		$1.0\ 10^6$			BR: 100%
$CH_2(OH)C(OH)(OH)C(OH)(OH)C^•H(OH) + O_2 \rightarrow CH_2(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OO^•)$		$2.0\ 10^9$			3
$CH_2(OH)C(OH)(OH)C(OH)(OH)CH_2(OH) + NO_3^• \rightarrow CH_2(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OO^•) + NO_3^- + H^+ - O_2$	R(638)	$1.0\ 10^6$			= $k(CH(OH)(OH)CH(OH)(OH) + NO_3^•)$- 13
$CH_2(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OO^•) + OH^- \rightarrow CH_2(OH)C(OH)(OH)C(OH)(OH)CH(O^-)(OO^•) + H_2O$		$4.0\ 10^9$			
$CH_2(OH)C(OH)(OH)C(OH)(OH)CH(O^-)(OO^•) \rightarrow CH_2(OH)C(OH)(OH)C(OH)(OH)CHO + O_2^{•-}$					16
$CH_2(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OO^•) + OH^- \rightarrow CH_2(OH)C(OH)(OH)C(OH)(OH)CHO + O_2^{•-} + H_2O$	R(639)	$4.0\ 10^9$			= $k(CH_3CH(OH)(OO^•) + OH^-)$
$CH_2(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OO^•) \rightarrow CH_2(OH)C(OH)(OH)C(OH)(OH)CHO + HO_2^•$	R(640)	$1.9\ 10^2$			17
Oxidation of 1,3,4-trihydroxybutanone					22
Pathway 1: $CH_2(OH)COCH(OH)CH_2(OH) + HO^• \rightarrow CH_2(OH)COCH(OH)C^•H(OH) + H_2O$		$7.5\ 10^8$			BR: 58% - 23
$CH_2(OH)COCH(OH)C^•H(OH) + O_2 \rightarrow CH_2(OH)COCH(OH)CH(OH)(OO^•)$		$2.0\ 10^9$			3
Pathway 2: $CH_2(OH)COCH(OH)CH_2(OH) + HO^• \rightarrow C^•H(OH)COCH(OH)CH_2(OH) + H_2O$		$3.9\ 10^8$			BR: 30% - 23

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$C^{\bullet}H(OH)COCH(OH)CH_2(OH)+ O_2 \rightarrow CH_2(OH)CH(OH)COCH(OH)(OO^{\bullet})$		$2.0\ 10^9$			3
Pathway 3: $CH_2(OH)COCH(OH)CH_2(OH) + HO^{\bullet} \rightarrow CH_2(OH)COC^{\bullet}(OH)CH_2(OH) + H_2O$		$1.6\ 10^8$			BR: 12% - 23
$CH_2(OH)COC^{\bullet}(OH)CH_2(OH)+ O_2 \rightarrow CH_2(OH)COC(OH)(OO^{\bullet})CH_2(OH)$		$2.0\ 10^9$			3
$CH_2(OH)COCH(OH)CH_2(OH) + HO^{\bullet} \rightarrow 0.58\ CH_2(OH)COCH(OH)CH(OH)(OO^{\bullet}) + 0.30\ CH_2(OH)CH(OH)COCH(OH)(OO^{\bullet}) + 0.12\ CH_2(OH)COC(OH)(OO^{\bullet})CH_2(OH) + H_2O - O_2$	R(641)	$1.3\ 10^9$			12
Pathway 1: $CH_2(OH)COCH(OH)CH_2(OH) + NO_3^{\bullet} \rightarrow CH_2(OH)COCH(OH)C^{\bullet}H(OH) + NO_3^- + H^+$		$3.8\ 10^6$			BR: 58%
$CH_2(OH)COCH(OH)C^{\bullet}H(OH)+ O_2 \rightarrow CH_2(OH)COCH(OH)CH(OH)(OO^{\bullet})$		$2.0\ 10^9$			3
Pathway 2: $CH_2(OH)COCH(OH)CH_2(OH) + NO_3^{\bullet} \rightarrow C^{\bullet}H(OH)COCH(OH)CH_2(OH) + NO_3^- + H^+$		$2.0\ 10^6$			BR: 30%
$C^{\bullet}H(OH)COCH(OH)CH_2(OH)+ O_2 \rightarrow CH_2(OH)CH(OH)COCH(OH)(OO^{\bullet})$		$2.0\ 10^9$			3
Pathway 3: $CH_2(OH)COCH(OH)CH_2(OH) + NO_3^{\bullet} \rightarrow CH_2(OH)COC^{\bullet}(OH)CH_2(OH) + NO_3^- + H^+$		$8.0\ 10^5$			BR: 12%
$CH_2(OH)COC^{\bullet}(OH)CH_2(OH)+ O_2 \rightarrow CH_2(OH)COC(OH)(OO^{\bullet})CH_2(OH)$		$2.0\ 10^9$			3
$CH_2(OH)COCH(OH)CH_2(OH) + NO_3^{\bullet} \rightarrow 0.58\ CH_2(OH)COCH(OH)CH(OH)(OO^{\bullet}) + 0.30\ CH_2(OH)CH(OH)COCH(OH)(OO^{\bullet}) + 0.12\ CH_2(OH)COC(OH)(OO^{\bullet})CH_2(OH) + NO_3^- + H^+ - O_2$	R(642)	$6.6\ 10^6$	2117		= k($CH_2(OH)CH_2(OH) + NO_3^{\bullet}$) - 13
$CH_2(OH)COCH(OH)CH(OH)(OO^{\bullet}) + OH^- \rightarrow CH_2(OH)COCH(OH)CH(O^-)(OO^{\bullet}) + H_2O$		$4.0\ 10^9$			
$CH_2(OH)COCH(OH)CH(O^-)(OO^{\bullet}) \rightarrow CH_2(OH)COCH(OH)CHO + O_2^{\bullet-}$					16
$CH_2(OH)COCH(OH)CH(OH)(OO^{\bullet}) + OH^- \rightarrow CH_2(OH)COCH(OH)CHO + O_2^{\bullet-} + H_2O$	R(643)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^{\bullet}) + OH^-$)
$CH_2(OH)COCH(OH)CH(OH)(OO^{\bullet}) \rightarrow CH_2(OH)COCH(OH)CHO + HO_2^{\bullet}$	R(644)	$1.9\ 10^2$			17
$CH_2(OH)CH(OH)COCH(OH)(OO^{\bullet}) + OH^- \rightarrow CH_2(OH)CH(OH)COCH(O^-)(OO^{\bullet}) + H_2O$		$4.0\ 10^9$			
$CH_2(OH)CH(OH)COCH(O^-)(OO^{\bullet}) \rightarrow CH_2(OH)CH(OH)COCHO + O_2^{\bullet-}$					16
$CH_2(OH)CH(OH)COCH(OH)(OO^{\bullet}) + OH^- \rightarrow CH_2(OH)CH(OH)COCHO + O_2^{\bullet-} + H_2O$	R(645)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^{\bullet}) + OH^-$)
$CH_2(OH)CH(OH)COCH(OH)(OO^{\bullet}) \rightarrow CH_2(OH)CH(OH)COCHO + HO_2^{\bullet}$	R(646)	$1.9\ 10^2$			17
$CH_2(OH)COC(OH)(OO^{\bullet})CH_2(OH) + OH^- \rightarrow CH_2(OH)COC(O^-)(OO^{\bullet})CH_2(OH) + H_2O$		$4.0\ 10^9$			
$CH_2(OH)COC(O^-)(OO^{\bullet})CH_2(OH) \rightarrow CH_2(OH)COCOCH_2(OH) + O_2^{\bullet-}$					16
$CH_2(OH)COC(OH)(OO^{\bullet})CH_2(OH) + OH^- \rightarrow CH_2(OH)COCOCH_2(OH) + O_2^{\bullet-} + H_2O$	R(647)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^{\bullet}) + OH^-$)
$CH_2(OH)COC(OH)(OO^{\bullet})CH_2(OH) \rightarrow CH_2(OH)COCOCH_2(OH) + HO_2^{\bullet}$	R(648)	$1.9\ 10^2$			17
Oxidation of 2,4-dihydroxy-3-oxobutanal					24
Pathway 1: $CH_2(OH)COCH(OH)CH(OH)(OH) + HO^{\bullet} \rightarrow CH_2(OH)COCH(OH)CH(OH)(O^{\bullet})+ H_2O$		$4.5\ 10^8$			BR: 38% - 25
$CH_2(OH)COCH(OH)CH(OH)(O^{\bullet}) \rightarrow CH_2(OH)COC^{\bullet}H(OH) + CHO(OH)$					4 - 5
$CH_2(OH)COC^{\bullet}H(OH) + O_2 \rightarrow CH_2(OH)COCH(OH)(OO^{\bullet})$		$2.0\ 10^9$			3
Pathway 2: $CH_2(OH)COCH(OH)CH(OH)(OH) + HO^{\bullet} \rightarrow C^{\bullet}H(OH)COCH(OH)CH(OH)(OH) + H_2O$		$4.0\ 10^8$			BR: 33% - 25
$C^{\bullet}H(OH)COCH(OH)CH(OH)(OH) + O_2 \rightarrow CH(OH)(OH)CH(OH)COCH(OH)(OO^{\bullet})$		$2.0\ 10^9$			3
Pathway 3: $CH_2(OH)COCH(OH)CH(OH)(OH) + HO^{\bullet} \rightarrow CH_2(OH)COCH(OH)C^{\bullet}(OH)(OH) + H_2O$		$3.5\ 10^8$			BR: 29% - 25
$CH_2(OH)COCH(OH)C^{\bullet}(OH)(OH) + O_2 \rightarrow CH_2(OH)COCH(OH)C(OH)(OH)(OO^{\bullet})$		$2.0\ 10^9$			3
$CH_2(OH)COCH(OH)CH(OH)(OH) + HO^{\bullet} \rightarrow 0.38\ CH_2(OH)COCH(OH)(OO^{\bullet}) + 0.38\ CHO(OH) + 0.33\ CH(OH)(OH)CH(OH)COCH(OH)(OO^{\bullet}) + 0.29\ CH_2(OH)COCH(OH)C(OH)(OH)(OO^{\bullet}) + H_2O - O_2$	R(649)	$1.2\ 10^9$			12
Pathway 1: $CH_2(OH)COCH(OH)CH(OH)(OH) + NO_3^{\bullet} \rightarrow C^{\bullet}H(OH)COCH(OH)CH(OH)(OH)+ NO_3^- + H^+$		$5.3\ 10^5$			BR: 53%
$C^{\bullet}H(OH)COCH(OH)CH(OH)(OH) + O_2 \rightarrow CH(OH)(OH)CH(OH)COCH(OH)(OO^{\bullet})$		$2.0\ 10^9$			3
Pathway 2: $CH_2(OH)COCH(OH)CH(OH)(OH) + NO_3^{\bullet} \rightarrow CH_2(OH)COCH(OH)C^{\bullet}(OH)(OH) + NO_3^- + H^+$		$4.7\ 10^5$			BR: 47%
$CH_2(OH)COCH(OH)C^{\bullet}(OH)(OH) + O_2 \rightarrow CH_2(OH)COCH(OH)C(OH)(OH)(OO^{\bullet})$		$2.0\ 10^9$			3
$CH_2(OH)COCH(OH)CH(OH)(OH) + NO_3^{\bullet} \rightarrow 0.53\ CH(OH)(OH)CH(OH)COCH(OH)(OO^{\bullet}) + 0.47\ CH_2(OH)COCH(OH)C(OH)(OH)(OO^{\bullet}) + NO_3^- + H^+ - O_2$	R(650)	$1.0\ 10^6$			= k($CH(OH)(OH)CH(OH)(OH) + NO_3^{\bullet}$) - 13
Pathway 1: $CH_2(OH)C(OH)(OH)CH(OH)CH(OH)(OH) + HO^{\bullet} \rightarrow CH_2(OH)C(OH)(OH)CH(OH)CH(OH)(O^{\bullet}) + H_2O$		$4.5\ 10^8$			BR: 28% - 26
$CH_2(OH)C(OH)(OH)CH(OH)CH(OH)(O^{\bullet}) \rightarrow CH_2(OH)C(OH)(OH)C^{\bullet}H(OH) + CHO(OH)$					4 - 5
$CH_2(OH)C(OH)(OH)C^{\bullet}H(OH) + O_2 \rightarrow CH_2(OH)C(OH)(OH)CH(OH)(OO^{\bullet})$		$2.0\ 10^9$			3
Pathway 2: $CH_2(OH)C(OH)(OH)CH(OH)CH(OH)(OH) + HO^{\bullet} \rightarrow CH_2(OH)C(OH)(O^{\bullet})CH(OH)CH(OH)(OH) + H_2O$		$4.5\ 10^8$			BR: 28% - 26
$CH_2(OH)C(OH)(O^{\bullet})CH(OH)CH(OH)(OH) \rightarrow CH_2(OH)CO(OH) + CH(OH)(OH)C^{\bullet}H(OH)$					4 - 5
$CH(OH)(OH)C^{\bullet}H(OH)+ O_2 \rightarrow CH(OH)(OO^{\bullet})CH(OH)(OH)$		$2.0\ 10^9$			3

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
Pathway 3: $CH_2(OH)C(OH)(OH)CH(OH)CH(OH)(OH) + HO^\bullet \rightarrow CH_2(OH)C(OH)(OH)CH(OH)C^\bullet(OH)(OH) + H_2O$		$3.7\ 10^8$			BR: 23% - 26
$CH_2(OH)C(OH)(OH)CH(OH)C^\bullet(OH)(OH) + O_2 \rightarrow CH_2(OH)C(OH)(OH)CH(OH)C(OH)(OH)(OO^\bullet)$		$2.0\ 10^9$			3
Pathway 4: $CH_2(OH)C(OH)(OH)CH(OH)CH(OH)(OH) + HO^\bullet \rightarrow C^\bullet H(OH)C(OH)(OH)CH(OH)CH(OH)(OH) + H_2O$		$3.3\ 10^8$			BR: 21% - 26
$C^\bullet H(OH)C(OH)(OH)CH(OH)CH(OH)(OH) + O_2 \rightarrow CH(OH)(OH)CH(OH)C(OH)(OH)CH(OH)(OO^\bullet)$		$2.0\ 10^9$			3
$CH_2(OH)C(OH)(OH)CH(OH)CH(OH)(OH) + HO^\bullet \rightarrow 0.28\ CH_2(OH)C(OH)(OH)CH(OH)(OO^\bullet) + 0.28\ CHO(OH) + 0.28\ CH_2(OH)CO(OH) + 0.28\ CH(OH)(OO^\bullet)CH(OH)(OH) + 0.23\ CH_2(OH)C(OH)(OH)CH(OH)C(OH)(OH)(OO^\bullet) + 0.21\ CH(OH)(OH)CH(OH)C(OH)(OH)CH(OH)(OO^\bullet) + H_2O - O_2$	R(651)	$1.6\ 10^9$			12
Pathway 1: $CH_2(OH)C(OH)(OH)CH(OH)CH(OH)(OH) + NO_3^\bullet \rightarrow CH_2(OH)C(OH)(OH)CH(OH)C^\bullet(OH)(OH) + NO_3^- + H^+$		$5.3\ 10^5$			BR: 53%
$CH_2(OH)C(OH)(OH)CH(OH)C^\bullet(OH)(OH) + O_2 \rightarrow CH_2(OH)C(OH)(OH)CH(OH)C(OH)(OH)(OO^\bullet)$		$2.0\ 10^9$			3
Pathway 2: $CH_2(OH)C(OH)(OH)CH(OH)CH(OH)(OH) + NO_3^\bullet \rightarrow C^\bullet H(OH)C(OH)(OH)CH(OH)CH(OH)(OH) + NO_3^- + H^+$		$4.7\ 10^5$			BR: 47%
$C^\bullet H(OH)C(OH)(OH)CH(OH)CH(OH)(OH) + O_2 \rightarrow CH(OH)(OH)CH(OH)C(OH)(OH)CH(OH)(OO^\bullet)$		$2.0\ 10^9$			3
$CH_2(OH)C(OH)(OH)CH(OH)CH(OH)(OH) + NO_3^\bullet \rightarrow 0.53\ CH_2(OH)C(OH)(OH)CH(OH)C(OH)(OH)(OO^\bullet) + 0.47\ CH(OH)(OH)CH(OH)C(OH)(OH)CH(OH)(OO^\bullet) + NO_3^- + H^+ - O_2$	R(652)	$1.0\ 10^6$			= k($CH(OH)(OH)CH(OH)(OH) + NO_3^\bullet$) - 13
$CH(OH)(OH)CH(OH)COCH(OH)(OO^\bullet) + OH^- \rightarrow CH(OH)(OH)CH(OH)COCH(O^-)(OO^\bullet) + H_2O$		$4.0\ 10^9$			
$CH(OH)(OH)CH(OH)COCH(O^-)(OO^\bullet) \rightarrow CH(OH)(OH)CH(OH)COCHO + O_2^{\bullet-}$					16
$CH(OH)(OH)CH(OH)COCH(OH)(OO^\bullet) + OH^- \rightarrow CH(OH)(OH)CH(OH)COCHO + O_2^{\bullet-} + H_2O$	R(653)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^\bullet) + OH^-$)
$CH(OH)(OH)CH(OH)COCH(OH)(OO^\bullet) \rightarrow CH(OH)(OH)CH(OH)COCHO + HO_2^\bullet$	R(654)	$1.9\ 10^2$			17
$CH(OH)(OH)CH(OH)C(OH)(OH)CH(OH)(OO^\bullet) + OH^- \rightarrow CH(OH)(OH)CH(OH)C(OH)(OH)CH(O^-)(OO^\bullet) + H_2O$		$4.0\ 10^9$			
$CH(OH)(OH)CH(OH)C(OH)(OH)CH(O^-)(OO^\bullet) \rightarrow CH(OH)(OH)CH(OH)C(OH)(OH)CHO + O_2^{\bullet-}$					16
$CH(OH)(OH)CH(OH)C(OH)(OH)CH(OH)(OO^\bullet) + OH^- \rightarrow CH(OH)(OH)CH(OH)C(OH)(OH)CHO + O_2^{\bullet-} + H_2O$	R(655)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^\bullet) + OH^-$)
$CH(OH)(OH)CH(OH)C(OH)(OH)CH(OH)(OO^\bullet) \rightarrow CH(OH)(OH)CH(OH)C(OH)(OH)CHO + HO_2^\bullet$	R(656)	$1.9\ 10^2$			17
$CH_2(OH)COCH(OH)C(OH)(OH)(OO^\bullet) + OH^- \rightarrow CH_2(OH)COCH(OH)C(OH)(O^-)(OO^\bullet) + H_2O$		$4.0\ 10^9$			
$CH_2(OH)COCH(OH)C(OH)(O^-)(OO^\bullet) \rightarrow CH_2(OH)COCH(OH)CO(OH) + O_2^{\bullet-}$					16
$CH_2(OH)COCH(OH)C(OH)(OH)(OO^\bullet) + OH^- \rightarrow CH_2(OH)COCH(OH)CO(OH) + O_2^{\bullet-} + H_2O$	R(657)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^\bullet) + OH^-$)
$CH_2(OH)COCH(OH)C(OH)(OH)(OO^\bullet) \rightarrow CH_2(OH)COCH(OH)CO(OH) + HO_2^\bullet$	R(658)	$1.0\ 10^6$			27
$CH_2(OH)C(OH)(OH)CH(OH)C(OH)(OH)(OO^\bullet) + OH^- \rightarrow CH_2(OH)C(OH)(OH)CH(OH)C(OH)(O^-)(OO^\bullet) + H_2O$		$4.0\ 10^9$			
$CH_2(OH)C(OH)(OH)CH(OH)C(OH)(O^-)(OO^\bullet) \rightarrow CH_2(OH)C(OH)(OH)CH(OH)CO(OH) + O_2^{\bullet-}$					16
$CH_2(OH)C(OH)(OH)CH(OH)C(OH)(OH)(OO^\bullet) + OH^- \rightarrow CH_2(OH)C(OH)(OH)CH(OH)CO(OH) + O_2^{\bullet-} + H_2O$	R(659)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^\bullet) + OH^-$)
$CH_2(OH)C(OH)(OH)CH(OH)C(OH)(OH)(OO^\bullet) \rightarrow CH_2(OH)C(OH)(OH)CH(OH)CO(OH) + HO_2^\bullet$	R(660)	$1.0\ 10^6$			27
Oxidation of 2-oxo-3,4-dihydroxybutanal					28
Pathway 1: $CH_2(OH)CH(OH)C(OH)(OH)CH(OH)(OH) + HO^\bullet \rightarrow C^\bullet H(OH)CH(OH)C(OH)(OH)CH(OH)(OH) + H_2O$		$8.6\ 10^8$			BR: 48% - 29
$C^\bullet H(OH)CH(OH)C(OH)(OH)CH(OH)(OH) + O_2 \rightarrow CH(OH)(OH)C(OH)(OH)CH(OH)CH(OH)(OO^\bullet)$		$2.0\ 10^9$			3
Pathway 2: $CH_2(OH)CH(OH)C(OH)(OH)CH(OH)(OH) + HO^\bullet \rightarrow CH_2(OH)CH(OH)C(OH)(OH)CH(OH)(O^\bullet) + H_2O$		$4.7\ 10^8$			BR: 26% - 29
$CH_2(OH)CH(OH)C(OH)(OH)CH(OH)(O^\bullet) \rightarrow CH_2(OH)CH(OH)C^\bullet(OH)(OH) + CHO(OH)$					4 - 5
$CH_2(OH)CH(OH)C^\bullet(OH)(OH) + O_2 \rightarrow CH_2(OH)CH(OH)C(OH)(OH)(OO^\bullet)$		$2.0\ 10^9$			3
Pathway 3: $CH_2(OH)CH(OH)C(OH)(OH)CH(OH)(OH) + HO^\bullet \rightarrow CH_2(OH)CH(OH)C(OH)(O^\bullet)CH(OH)(OH) + H_2O$		$4.7\ 10^8$			BR: 26% - 29
$CH_2(OH)CH(OH)C(OH)(O^\bullet)CH(OH)(OH) \rightarrow CH_2(OH)C^\bullet H(OH) + CH(OH)(OH)CO(OH)$					4 - 5
$CH_2(OH)C^\bullet H(OH) + O_2 \rightarrow CH_2(OH)CH(OH)(OO^\bullet)$		$2.0\ 10^9$			3
$CH_2(OH)CH(OH)C(OH)(OH)CH(OH)(OH) + HO^\bullet \rightarrow 0.48\ CH(OH)(OH)C(OH)(OH)CH(OH)CH(OH)(OO^\bullet) + 0.26\ CH_2(OH)CH(OH)C(OH)(OH)(OO^\bullet) + 0.26\ CHO(OH) + 0.26\ CH_2(OH)CH(OH)(OO^\bullet) + 0.26\ CH(OH)(OH)CO(OH) + H_2O - O_2$	R(661)	$1.8\ 10^9$			12
Pathway 1: $CH_2(OH)CH(OH)C(OH)(OH)CH(OH)(OH) + NO_3^\bullet \rightarrow C^\bullet H(OH)CH(OH)C(OH)(OH)CH(OH)(OH) + NO_3^- + H^+$		$1.0\ 10^6$			BR: 100%
$C^\bullet H(OH)CH(OH)C(OH)(OH)CH(OH)(OH) + O_2 \rightarrow CH(OH)(OH)C(OH)(OH)CH(OH)CH(OH)(OO^\bullet)$		$2.0{\cdot}10^9$			3
$CH_2(OH)CH(OH)C(OH)(OH)CH(OH)(OH) + NO_3^\bullet \rightarrow CH(OH)(OH)C(OH)(OH)CH(OH)CH(OH)(OO^\bullet) + NO_3^- + H^+ - O_2$	R(662)	$1.0\ 10^6$			= k($CH(OH)(OH)CH(OH)(OH) + NO_3^\bullet$) - 13
$CH(OH)(OH)C(OH)(OH)CH(OH)CH(OH)(OO^\bullet) + OH^- \rightarrow CH(OH)(OH)C(OH)(OH)CH(OH)CH(O^-)(OO^\bullet) + H_2O$		$4.0\ 10^9$			

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CH(OH)(OH)C(OH)(OH)CH(OH)CH(O^-)(OO^\bullet) \rightarrow CHOCH(OH)C(OH)(OH)CH(OH)(OH) + O_2^{\bullet-}$					16
$CH(OH)(OH)C(OH)(OH)CH(OH)CH(OH)(OO^\bullet) + OH^- \rightarrow CHOCH(OH)C(OH)(OH)CH(OH)(OH) + O_2^{\bullet-} + H_2O$	R(663)	$4.0\ 10^9$			= $k(CH_3CH(OH)(OO^\bullet) + OH^-)$
$CH(OH)(OH)C(OH)(OH)CH(OH)CH(OH)(OO^\bullet) \rightarrow CHOCH(OH)C(OH)(OH)CH(OH)(OH) + HO_2^\bullet$	R(664)	$1.9\ 10^2$			17
Oxidation of 2-oxo-3-hydroxybutanedial					30
Pathway 1: $CH(OH)(OH)CH(OH)C(OH)(OH)CH(OH)(OH) + HO^\bullet \rightarrow CH(OH)(O^\bullet)CH(OH)C(OH)(OH)CH(OH)(OH) + H_2O$		$4.6\ 10^8$			BR: 27% - 31
$CH(OH)(O^\bullet)CH(OH)C(OH)(OH)CH(OH)(OH) \rightarrow CHO(OH) + CH(OH)(OH)C(OH)(OH)C^\bullet H(OH)$					4 - 5
$CH(OH)(OH)C(OH)(OH)C^\bullet H(OH) + O_2 \rightarrow CH(OH)(OH)C(OH)(OH)CH(OH)(OO^\bullet)$		$2.0\ 10^9$			3
Pathway 2: $CH(OH)(OH)CH(OH)C(OH)(OH)CH(OH)(OH) + HO^\bullet \rightarrow CH(OH)(OH)CH(OH)C(OH)(OH)CH(OH)(O^\bullet) + H_2O$		$4.4\ 10^8$			BR: 26% - 31
$CH(OH)(OH)CH(OH)C(OH)(OH)CH(OH)(O^\bullet) \rightarrow CH(OH)(OH)CH(OH)C^\bullet(OH)(OH) + CHO(OH)$					4 - 5
$CH(OH)(OH)CH(OH)C^\bullet(OH)(OH) + O_2 \rightarrow CH(OH)(OH)CH(OH)C(OH)(OH)(OO^\bullet)$		$2.0\ 10^9$			3
Pathway 3: $CH(OH)(OH)CH(OH)C(OH)(OH)CH(OH)(OH) + HO^\bullet \rightarrow CH(OH)(OH)CH(OH)C(OH)(O^\bullet)CH(OH)(OH) + H_2O$		$4.3\ 10^8$			BR: 25% - 31
$CH(OH)(OH)CH(OH)C(OH)(O^\bullet)CH(OH)(OH) \rightarrow CH(OH)(OH)C^\bullet H(OH) + CH(OH)(OH)CO(OH)$					4 - 5
$CH(OH)(OH)C^\bullet H(OH) + O_2 \rightarrow CH(OH)(OO^\bullet)CH(OH)(OH)$		$2.0\ 10^9$			3
Pathway 4: $CH(OH)(OH)CH(OH)C(OH)(OH)CH(OH)(OH) + HO^\bullet \rightarrow C^\bullet(OH)(OH)CH(OH)C(OH)(OH)CH(OH)(OH) + H_2O$		$3.7\ 10^8$			BR: 22% - 31
$C^\bullet(OH)(OH)CH(OH)C(OH)(OH)CH(OH)(OH) + O_2 \rightarrow CH(OH)(OH)C(OH)(OH)CH(OH)C(OH)(OH)(OO^\bullet)$		$2.0\ 10^9$			3
$CH(OH)(OH)CH(OH)C(OH)(OH)CH(OH)(OH) + HO^\bullet \rightarrow 0.27\ CH(OH)(OH)C(OH)(OH)CH(OH)(OO^\bullet) + 0.26\ CH(OH)(OH)CH(OH)C(OH)(OH)(OO^\bullet) + 0.53\ CHO(OH) + 0.25\ CH(OH)(OH)CO(OH) + 0.25\ CH(OH)(OO^\bullet)CH(OH)(OH) + 0.22\ CH(OH)(OH)C(OH)(OH)CH(OH)C(OH)(OH)(OO^\bullet) + H_2O - O_2$	R(665)	$1.7\ 10^9$			12
Pathway 1: $CH(OH)(OH)CH(OH)C(OH)(OH)CH(OH)(OH) + NO_3^\bullet \rightarrow C^\bullet(OH)(OH)CH(OH)C(OH)(OH)CH(OH)(OH) + NO_3^- + H^+$		$1.0\ 10^6$			BR: 100%
$C^\bullet(OH)(OH)CH(OH)C(OH)(OH)CH(OH)(OH) + O_2 \rightarrow CH(OH)(OH)C(OH)(OH)CH(OH)C(OH)(OH)(OO^\bullet)$		$2.0{\cdot}10^9$			3
$CH(OH)(OH)CH(OH)C(OH)(OH)CH(OH)(OH) + NO_3^\bullet \rightarrow CH(OH)(OH)C(OH)(OH)CH(OH)C(OH)(OH)(OO^\bullet) + NO_3^- + H^+ - O_2$	R(666)	$1.0\ 10^6$			= $k(CH(OH)(OH)CH(OH)(OH) + NO_3^\bullet)$ - 13
$CH(OH)(OH)C(OH)(OH)CH(OH)C(OH)(OH)(OO^\bullet) + OH^- \rightarrow CH(OH)(OH)C(OH)(OH)CH(OH)C(OH)(O^-)(OO^\bullet) + H_2O$		$4.0\ 10^9$			
$CH(OH)(OH)C(OH)(OH)CH(OH)C(OH)(O^-)(OO^\bullet) \rightarrow CO(OH)CH(OH)C(OH)(OH)CH(OH)(OH) + O_2^{\bullet-}$					16
$CH(OH)(OH)C(OH)(OH)CH(OH)C(OH)(OH)(OO^\bullet) + OH^- \rightarrow CO(OH)CH(OH)C(OH)(OH)CH(OH)(OH) + O_2^{\bullet-} + H_2O$	R(667)	$4.0\ 10^9$			= $k(CH_3CH(OH)(OO^\bullet) + OH^-)$
$CH(OH)(OH)C(OH)(OH)CH(OH)C(OH)(OH)(OO^\bullet) \rightarrow CO(OH)CH(OH)C(OH)(OH)CH(OH)(OH) + HO_2^\bullet$	R(668)	$1.0\ 10^6$			27
Oxidation of 2,4-dioxo-3-hydroxybutanoic acid					32
Pathway 1: $CO(OH)C(OH)(OH)CH(OH)CH(OH)(OH) + HO^\bullet \rightarrow CH(OH)(O^\bullet)CH(OH)C(OH)(OH)CO(OH) + H_2O$		$4.1\ 10^8$			BR: 41% - 33
$CH(OH)(O^\bullet)CH(OH)C(OH)(OH)CO(OH) \rightarrow CHO(OH) + C^\bullet H(OH)C(OH)(OH)CO(OH)$					4 -5
$C^\bullet H(OH)C(OH)(OH)CO(OH) + O_2 \rightarrow CH(OH)(OO^\bullet)C(OH)(OH)CO(OH)$		$2.0\ 10^9$			3
Pathway 2: $CO(OH)C(OH)(OH)CH(OH)CH(OH)(OH) + HO^\bullet \rightarrow C^\bullet(OH)(OH)CH(OH)C(OH)(OH)CO(OH) + H_2O$		$3.3\ 10^8$			BR: 33% - 33
$C^\bullet(OH)(OH)CH(OH)C(OH)(OH)CO(OH) + O_2 \rightarrow C(OH)(OH)(OO^\bullet)CH(OH)C(OH)(OH)CO(OH)$		$2.0\ 10^9$			3
Pathway 3: $CO(OH)C(OH)(OH)CH(OH)CH(OH)(OH) + HO^\bullet \rightarrow CH(OH)(OH)CH(OH)C(OH)(O^\bullet)CO(OH) + H_2O$		$2.6\ 10^8$			BR: 26% - 33
$CH(OH)(OH)CH(OH)C(OH)(O^\bullet)CO(OH) \rightarrow CH(OH)(OH)C^\bullet H(OH) + CO(OH)CO(OH)$					4 -5
$CH(OH)(OH)C^\bullet H(OH) + O_2 \rightarrow CH(OH)(OH)CH(OH)(OO^\bullet)$		$2.0\ 10^9$			3
$CO(OH)C(OH)(OH)CH(OH)CH(OH)(OH) + HO^\bullet \rightarrow 0.41\ CHO(OH) + 0.41\ CH(OH)(OO^\bullet)C(OH)(OH)CO(OH) + 0.33\ C(OH)(OH)(OO^\bullet)CH(OH)C(OH)(OH)CO(OH) + 0.26\ CH(OH)(OH)CH(OH)(OO^\bullet) + 0.26\ CO(OH)CO(OH) + H_2O - O_2$	R(669)	$1.0\ 10^9$			12
Pathway 1: $CO(OH)C(OH)(OH)CH(OH)CH(OH)(OH) + NO_3^\bullet \rightarrow C^\bullet(OH)(OH)CH(OH)C(OH)(OH)CO(OH) + NO_3^- + H^+$		$1.0\ 10^6$			BR: 100%
$C^\bullet(OH)(OH)CH(OH)C(OH)(OH)CO(OH) + O_2 \rightarrow C(OH)(OH)(OO^\bullet)CH(OH)C(OH)(OH)CO(OH)$		$2.0\ 10^9$			3
$CO(OH)C(OH)(OH)CH(OH)CH(OH)(OH) + NO_3^\bullet \rightarrow C(OH)(OH)(OO^\bullet)CH(OH)C(OH)(OH)CO(OH) + NO_3^- + H^+ - O_2$	R(670)	$1.0\ 10^6$			= $k(CH(OH)(OH)CH(OH)(OH) + NO_3^\bullet)$ - 13
Pathway 1: $CO(O^-)COCH(OH)CH(OH)(OH) + HO^\bullet \rightarrow CH(OH)(O^\bullet)CH(OH)COCO(O^-) + H_2O$		$4.9\ 10^8$			BR: 58% - 34
$CH(OH)(O^\bullet)CH(OH)COCO(O^-) \rightarrow CHO(OH) + C^\bullet H(OH)COCO(O^-)$					4 -5
$C^\bullet H(OH)COCO(O^-) + O_2 \rightarrow CH(OH)(OO^\bullet)COCO(O^-)$		$2.0\ 10^9$			3
Pathway 2: $CO(O^-)COCH(OH)CH(OH)(OH) + HO^\bullet \rightarrow C^\bullet(OH)(OH)CH(OH)COCO(O^-) + H_2O$		$3.5\ 10^8$			BR: 42% - 34
$C^\bullet(OH)(OH)CH(OH)COCO(O^-) + O_2 \rightarrow C(OH)(OH)(OO^\bullet)CH(OH)COCO(O^-)$		$2.0\ 10^9$			3

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CO(O^-)COCH(OH)CH(OH)(OH) + HO^\bullet \rightarrow 0.58\ CHO(OH) + 0.58\ CH(OH)(OO^\bullet)COCO(O^-) + 0.42\ C(OH)(OH)(OO^\bullet)CH(OH)COCO(O^-) + H_2O - O_2$	R(671)	$8.4\ 10^8$			12
Pathway 1: $CO(O^-)COCH(OH)CH(OH)(OH) + NO_3^\bullet \rightarrow C^\bullet(OH)(OH)CH(OH)COCO(O^-) + NO_3^- + H^+$		$1.0\ 10^6$			BR: 100%
$C^\bullet(OH)(OH)CH(OH)COCO(O^-) + O_2 \rightarrow C(OH)(OH)(OO^\bullet)CH(OH)COCO(O^-)$		$2.0\ 10^9$			3
$CO(O^-)COCH(OH)CH(OH)(OH) + NO_3^\bullet \rightarrow C(OH)(OH)(OO^\bullet)CH(OH)COCO(O^-) + NO_3^- + H^+ - O_2$	R(672)	$1.0\ 10^6$			= k(CH(OH)(OH)CH(OH)(OH) + $NO_3^\bullet$) - 13
$C(OH)(OH)(OO^\bullet)CH(OH)C(OH)(OH)CO(OH) + OH^- \rightarrow C(OH)(O^-)(OO^\bullet)CH(OH)C(OH)(OH)CO(OH) + H_2O$		$4.0\ 10^9$			
$C(OH)(O^-)(OO^\bullet)CH(OH)C(OH)(OH)CO(OH) \rightarrow CO(OH)CH(OH)C(OH)(OH)CO(OH) + O_2^{\bullet-}$					16
$C(OH)(OH)(OO^\bullet)CH(OH)C(OH)(OH)CO(OH) + OH^- \rightarrow CO(OH)CH(OH)C(OH)(OH)CO(OH) + O_2^{\bullet-} + H_2O$	R(673)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^\bullet)$ + OH^-)
$C(OH)(OH)(OO^\bullet)CH(OH)C(OH)(OH)CO(OH) \rightarrow CO(OH)CH(OH)C(OH)(OH)CO(OH) + HO_2^\bullet$	R(674)	$1.0\ 10^6$			27
$C(OH)(OH)(OO^\bullet)CH(OH)COCO(O^-) + OH^- \rightarrow C(OH)(O^-)(OO^\bullet)CH(OH)COCO(O^-) + H_2O$		$4.0\ 10^9$			
$C(OH)(O^-)(OO^\bullet)CH(OH)COCO(O^-) \rightarrow CO(O^-)CH(OH)C(OH)(OH)CO(OH) + O_2^{\bullet-}$					16
$C(OH)(OH)(OO^\bullet)CH(OH)COCO(O^-) + OH^- \rightarrow CO(O^-)CH(OH)C(OH)(OH)CO(OH) + O_2^{\bullet-} + H_2O$	R(675)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^\bullet)$ + OH^-)
$C(OH)(OH)(OO^\bullet)CH(OH)COCO(O^-) \rightarrow CO(O^-)CH(OH)C(OH)(OH)CO(OH) + HO_2^\bullet$	R(676)	$1.0\ 10^6$			27
Oxidation of 2,3-dioxobutanal					35
Pathway 1: $CH_3COC(OH)(OH)CH(OH)(OH) + HO^\bullet \rightarrow CH_3COC(OH)(OH)CH(OH)(O^\bullet) + H_2O$		$4.6\ 10^8$			BR: 54% - 36
$CH_3COC(OH)(OH)CH(OH)(O^\bullet) \rightarrow CH_3COC^\bullet(OH)(OH) + CHO(OH)$					4 - 5
$CH_3COC^\bullet(OH)(OH) + O_2 \rightarrow CH_3COC(OH)(OH)(OO^\bullet)$		$2.0\ 10^9$			3
Pathway 2: $CH_3COC(OH)(OH)CH(OH)(OH) + HO^\bullet \rightarrow CH_3COC(OH)(O^\bullet)CH(OH)(OH) + H_2O$		$4.0\ 10^8$			BR: 46% - 36
$CH_3COC(OH)(O^\bullet)CH(OH)(OH) \rightarrow CH_3C^\bullet O + CH(OH)(OH)CO(OH)$					4 - 5
$CH_3C^\bullet O + O_2 \rightarrow CH_3CO(OO^\bullet)$		$2.0\ 10^9$			3
$CH_3COC(OH)(OH)CH(OH)(OH) + HO^\bullet \rightarrow 0.54\ CH_3COC(OH)(OH)(OO^\bullet) + 0.54\ CHO(OH) + 0.46\ CH_3CO(OO^\bullet) + 0.46\ CH(OH)(OH)CO(OH) + H_2O - O_2$	R(677)	$8.6\ 10^8$			12
Pathway 1: $CH_3C(OH)(OH)C(OH)(OH)CH(OH)(OH) + HO^\bullet \rightarrow CH_3C(OH)(O^\bullet)C(OH)(OH)CH(OH)(OH) + H_2O$		$4.5\ 10^8$			BR: 35% - 37
$CH_3C(OH)(O^\bullet)C(OH)(OH)CH(OH)(OH) \rightarrow CH_3CO(OH) + C^\bullet(OH)(OH)CH(OH)(OH)$					4 - 5
$C^\bullet(OH)(OH)CH(OH)(OH) + O_2 \rightarrow CH(OH)(OH)C(OH)(OH)(OO^\bullet)$		$2.0\ 10^9$			3
Pathway 2: $CH_3C(OH)(OH)C(OH)(OH)CH(OH)(OH) + HO^\bullet \rightarrow CH_3C(OH)(OH)C(OH)(OH)CH(OH)(O^\bullet) + H_2O$		$4.3\ 10^8$			BR: 33% - 37
$CH_3C(OH)(OH)C(OH)(OH)CH(OH)(O^\bullet) \rightarrow CH_3C(OH)(OH)C^\bullet(OH)(OH) + CHO(OH)$					4 - 5
$CH_3C(OH)(OH)C^\bullet(OH)(OH) + O_2 \rightarrow CH_3C(OH)(OH)C(OH)(OH)(OO^\bullet)$		$2.0\ 10^9$			3
Pathway 3: $CH_3C(OH)(OH)C(OH)(OH)CH(OH)(OH) + HO^\bullet \rightarrow CH_3C(OH)(OH)C(OH)(O^\bullet)CH(OH)(OH) + H_2O$		$4.2\ 10^8$			BR: 32% - 37
$CH_3C(OH)(OH)C(OH)(O^\bullet)CH(OH)(OH) \rightarrow CH_3C^\bullet(OH)(OH) + CH(OH)(OH)CO(OH)$					4 - 5
$CH_3C^\bullet(OH)(OH) + O_2 \rightarrow CH_3C(OH)(OH)(OO^\bullet)$		$2.0\ 10^9$			3
$CH_3C(OH)(OH)C(OH)(OH)CH(OH)(OH) + HO^\bullet \rightarrow 0.35\ CH_3CO(OH) + 0.35\ CH(OH)(OH)C(OH)(OH)(OO^\bullet) + 0.33\ CH_3C(OH)(OH)C(OH)(OH)(OO^\bullet) + 0.33\ CHO(OH) + 0.32\ CH_3C(OH)(OH)(OO^\bullet) + 0.32\ CH(OH)(OH)CO(OH) + H_2O - O_2$	R(678)	$1.3\ 10^9$			12
Oxidation of 2-hydroxy, 3-oxobutanal					38
Pathway 1: $CH_3COCH(OH)CH(OH)(OH) + HO^\bullet \rightarrow CH_3COCH(OH)CH(OH)(O^\bullet) + H_2O$		$5.0\ 10^8$			BR: 58% - 39
$CH_3COCH(OH)CH(OH)(O^\bullet) \rightarrow CH_3COC^\bullet H(OH) + CHO(OH)$					4 - 5
$CH_3COC^\bullet H(OH) + O_2 \rightarrow CH_3COCH(OH)(OO^\bullet)$		$2.0\ 10^9$			3
Pathway 2: $CH_3COCH(OH)CH(OH)(OH) + HO^\bullet \rightarrow CH_3COCH(OH)C^\bullet(OH)(OH) + H_2O$		$3.7\ 10^8$			BR: 42% - 39
$CH_3COCH(OH)C^\bullet(OH)(OH) + O_2 \rightarrow CH_3COCH(OH)C(OH)(OH)(OO^\bullet)$		$2.0\ 10^9$			3
$CH_3COCH(OH)CH(OH)(OH) + HO^\bullet \rightarrow 0.58\ CH_3COCH(OH)(OO^\bullet) + 0.58\ CHO(OH) + 0.42\ CH_3COCH(OH)C(OH)(OH)(OO^\bullet) + H_2O - O_2$	R(679)	$8.7\ 10^8$			12
Pathway 1: $CH_3COCH(OH)CH(OH)(OH) + NO_3^\bullet \rightarrow CH_3COCH(OH)C^\bullet(OH)(OH) + NO_3^- + H^+$		$1.0\ 10^6$			BR: 100%
$CH_3COCH(OH)C^\bullet(OH)(OH) + O_2 \rightarrow CH_3COCH(OH)C(OH)(OH)(OO^\bullet)$		$2.0\ 10^9$			3

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CH_3COCH(OH)CH(OH)(OH) + NO_3^\bullet \rightarrow CH_3COCH(OH)C(OH)(OH)(OO^\bullet) + NO_3^- + H^+ - O_2$	R(680)	$1.0\ 10^6$			= k(CH(OH)(OH)CH(OH)(OH) + $NO_3^\bullet$) - 13
$CH_3COCH(OH)C(OH)(OH)(OO^\bullet) + OH^- \rightarrow CH_3COCH(OH)C(O^-)(OH)(OO^\bullet) + H_2O$		$4.0\ 10^9$			
$CH_3COCH(OH)C(O^-)(OH)(OO^\bullet) \rightarrow CH_3COCH(OH)CO(OH) + O_2^{\bullet-}$					16
$CH_3COCH(OH)C(OH)(OH)(OO^\bullet) + OH^- \rightarrow CH_3COCH(OH)CO(OH) + O_2^{\bullet-} + H_2O$	R(681)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^\bullet)$ + OH^-)
$CH_3COCH(OH)C(OH)(OH)(OO^\bullet) \rightarrow CH_3COCH(OH)CO(OH) + HO_2^\bullet$	R(682)	$1.0\ 10^6$			27
Oxidation of 2-hydroxy,3-oxobutanoïc acid					40
Pathway 1: $CH_3COCH(OH)CO(OH) + HO^\bullet \rightarrow C^\bullet H_2COCH(OH)CO(OH) + H_2O$		$9.4\ 10^7$			BR: 63% - 41
$C^\bullet H_2COCH(OH)CO(OH) + O_2 \rightarrow CO(OH)CH(OH)COCH_2(OO^\bullet)$		$2.0\ 10^9$			3
Pathway 2: $CH_3COCH(OH)CO(OH) + HO^\bullet \rightarrow CH_3COCH(O^\bullet)CO(OH) + H_2O$		$5.6\ 10^7$			BR: 37% - 41
$CH_3COCH(O^\bullet)CO(OH) \rightarrow CH_3COCHO + C^\bullet O(OH)$					4 - 5
$C^\bullet O(OH) + O_2 \rightarrow CO(OH)(OO^\bullet)$		$2.0\ 10^9$			3
$CH_3COCH(OH)CO(OH) + HO^\bullet \rightarrow 0.63\ CO(OH)CH(OH)COCH_2(OO^\bullet) + 0.37\ CH_3COCHO + 0.37\ CO(OH)(OO^\bullet) + H_2O - O_2$	R(683)	$1.5\ 10^8$			12
Pathway 1: $CH_3COCH(OH)CO(OH) + NO_3^\bullet \rightarrow C^\bullet H_2COCH(OH)CO(OH) + NO_3^- + H^+$		$2.1\ 10^6$			BR: 100%
$C^\bullet H_2COCH(OH)CO(OH) + O_2 \rightarrow CO(OH)CH(OH)COCH_2(OO^\bullet)$		$2.0\ 10^9$			3
$CH_3COCH(OH)CO(OH) + NO_3^\bullet \rightarrow CO(OH)CH(OH)COCH_2(OO^\bullet) + NO_3^- + H^+ - O_2$	R(684)	$2.1\ 10^6$	3248		= k($CH_3CH(OH)CO(OH)$ + $NO_3^\bullet$) - 13
Pathway 1: $CH_3C(OH)(OH)CH(OH)CO(OH) + HO^\bullet \rightarrow CH_3C(OH)(O^\bullet)CH(OH)CO(OH) + H_2O$		$4.6\ 10^8$			BR: 85% - 42
$CH_3C(OH)(O^\bullet)CH(OH)CO(OH) \rightarrow CH_3CO(OH) + C^\bullet H(OH)CO(OH)$					4 - 5
$C^\bullet H(OH)CO(OH) + O_2 \rightarrow CH(OH)(OO^\bullet)CO(OH)$		$2.0\ 10^9$			3
Pathway 2: $CH_3C(OH)(OH)CH(OH)CO(OH) + HO^\bullet \rightarrow C^\bullet H_2C(OH)(OH)CH(OH)CO(OH) + H_2O$		$8.0\ 10^7$			BR: 15% - 42
$C^\bullet H_2C(OH)(OH)CH(OH)CO(OH) + O_2 \rightarrow CO(OH)CH(OH)C(OH)(OH)CH_2(OO^\bullet)$		$2.0\ 10^9$			3
$CH_3C(OH)(OH)CH(OH)CO(OH) + HO^\bullet \rightarrow 0.85\ CH_3CO(OH) + 0.85\ CH(OH)(OO^\bullet)CO(OH) + 0.15\ CO(OH)CH(OH)C(OH)(OH)CH_2(OO^\bullet) + H_2O - O_2$	R(685)	$5.4\ 10^8$			12
$CH_3C(OH)(OH)CH(OH)CO(OH) + NO_3^\bullet \rightarrow C^\bullet H_2C(OH)(OH)CH(OH)CO(OH) + NO_3^- + H^+$		$2.1\ 10^6$			BR: 100%
$C^\bullet H_2C(OH)(OH)CH(OH)CO(OH) + O_2 \rightarrow CO(OH)CH(OH)C(OH)(OH)CH_2(OO^\bullet)$		$2.0\ 10^9$			3
$CH_3C(OH)(OH)CH(OH)CO(OH) + NO_3^\bullet \rightarrow CO(OH)CH(OH)C(OH)(OH)CH_2(OO^\bullet) + NO_3^- + H^+ - O_2$	R(686)	$2.1\ 10^6$	3248		= k($CH_3CH(OH)CO(OH)$ + $NO_3^\bullet$) - 13
Pathway 1: $CH_3COCH(OH)CO(O^-) + HO^\bullet \rightarrow CH_3COCH(OH)CO(O^\bullet) + OH^-$		$1.1\ 10^8$			BR: 36% - 43
$CH_3COCH(OH)CO(O^\bullet) \rightarrow CH_3COC^\bullet H(OH) + CO_2$					4 - 5
$CH_3COC^\bullet H(OH) + O_2 \rightarrow CH_3COCH(OH)(OO^\bullet)$		$2.0\ 10^9$			3
Pathway 2: $CH_3COCH(OH)CO(O^-) + HO^\bullet \rightarrow CH_3COCH(O^\bullet)CO(O^-) + H_2O$		$1.1\ 10^8$			BR: 33% - 43
$CH_3COCH(O^\bullet)CO(O^-) \rightarrow CH_3COCHO + C^\bullet O(O^-)$					4 - 5
$C^\bullet O(O^-) + O_2 \rightarrow CO(O^-)(OO^\bullet)$		$2.0\ 10^9$			3
Pathway 3: $CH_3COCH(OH)CO(O^-) + HO^\bullet \rightarrow C^\bullet H_2COCH(OH)CO(O^-) + H_2O$		$1.0\ 10^8$			BR: 31% - 43
$C^\bullet H_2COCH(OH)CO(O^-) + O_2 \rightarrow CO(O^-)CH(OH)COCH_2(OO^\bullet)$		$2.0\ 10^9$			3
$CH_3COCH(OH)CO(O^-) + HO^\bullet \rightarrow 0.36\ CH_3COCH(OH)(OO^\bullet) + 0.33\ CH_3COCHO + 0.31\ CO(O^-)CH(OH)COCH_2(OO^\bullet) + 0.33\ CO(O^-)(OO^\bullet) + 0.36\ CO_2 + 0.64\ H_2O + 0.36\ OH^- - O_2$	R(687)	$3.2\ 10^8$			12
Pathway 1: $CH_3COCH(OH)CO(O^-) + NO_3^\bullet \rightarrow C^\bullet H_2COCH(OH)CO(O^-) + NO_3^- + H^+$		$1.0{\cdot}10^7$			BR: 100%
$C^\bullet H_2COCH(OH)CO(O^-) + O_2 \rightarrow CO(O^-)CH(OH)COCH_2(OO^\bullet)$		$2.0\ 10^9$			3
$CH_3COCH(OH)CO(O^-) + NO_3^\bullet \rightarrow CO(O^-)CH(OH)COCH_2(OO^\bullet) + NO_3^- + H^+ - O_2$	R(688)	$1.0{\cdot}10^7$	2646		= k($CH_3CH(OH)CO(O^-)$ + $NO_3^\bullet$) - 13
Pathway 1: $2\ CO(OH)CH(OH)COCH_2(OO^\bullet) \rightarrow 2\ CO(OH)CH(OH)COCHO + H_2O_2$		$1.8\ 10^8$			BR: 45%
Pathway 2: $2\ CO(OH)CH(OH)COCH_2(OO^\bullet) \rightarrow CO(OH)CH(OH)COCHO + CO(OH)CH(OH)COCH_2(OH) + O_2$		$8.0\ 10^7$			BR: 20%
Pathway 3: $2\ CO(OH)CH(OH)COCH_2(OO^\bullet) \rightarrow 2\ CO(OH)CH(OH)COCH_2(O^\bullet) + O_2$		$1.4\ 10^8$			BR: 35%
$CO(OH)CH(OH)COCH_2(O^\bullet) \rightarrow CO(OH)CH(OH)C^\bullet O + CH_2O$					4 - 5

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CO(OH)CH(OH)C^{\bullet}O + O_2 \rightarrow CO(OH)CH(OH)CO(OO^{\bullet})$		$2.0\ 10^9$			3
$2\ CO(OH)CH(OH)COCH_2(OO^{\bullet}) \rightarrow 1.10\ CO(OH)CH(OH)COCHO + 0.20\ CO(OH)CH(OH)COCH_2(OH) + 0.70\ CH_2O + 0.70\ CO(OH)CH(OH)CO(OO^{\bullet}) + 0.45\ H_2O_2 - 0.15\ O_2$	R(689)	$4.0\ 10^8$			= k(2 $CH_3COCH_2(OO^{\bullet})$) - 6
Pathway 1: $2\ CO(OH)CH(OH)C(OH)(OH)CH_2(OO^{\bullet}) \rightarrow 2\ CO(OH)CH(OH)C(OH)(OH)CHO + H_2O_2$		$1.8\ 10^8$			BR: 45%
Pathway 2: $2\ CO(OH)CH(OH)C(OH)(OH)CH_2(OO^{\bullet}) \rightarrow CO(OH)CH(OH)C(OH)(OH)CHO + CO(OH)CH(OH)C(OH)(OH)CH_2(OH) + O_2$		$8.0\ 10^7$			BR: 20%
Pathway 3: $2\ CO(OH)CH(OH)C(OH)(OH)CH_2(OO^{\bullet}) \rightarrow 2\ CO(OH)CH(OH)C(OH)(OH)CH_2(O^{\bullet}) + O_2$		$1.4\ 10^8$			BR: 35%
$CO(OH)CH(OH)C(OH)(OH)CH_2(O^{\bullet}) \rightarrow CO(OH)CH(OH)C^{\bullet}(OH)(OH) + CH_2O$					4 - 5
$CO(OH)CH(OH)C^{\bullet}(OH)(OH) + O_2 \rightarrow CO(OH)CH(OH)C(OH)(OH)(OO^{\bullet})$		$2.0\ 10^9$			3
$2\ CO(OH)CH(OH)C(OH)(OH)CH_2(OO^{\bullet}) \rightarrow 1.10\ CO(OH)CH(OH)C(OH)(OH)CHO + 0.20\ CO(OH)CH(OH)C(OH)(OH)CH_2(OH) + 0.70\ CH_2O + 0.70\ CO(OH)CH(OH)C(OH)(OH)(OO^{\bullet}) + 0.45\ H_2O_2 - 0.15\ O_2$	R(690)	$4.0\ 10^8$			= k(2 $CH_3COCH_2(OO^{\bullet})$) - 6
Pathway 1: $2\ CO(O^-)CH(OH)COCH_2(OO^{\bullet}) \rightarrow 2\ CO(O^-)CH(OH)COCHO + H_2O_2$		$1.8\ 10^8$			BR: 45%
Pathway 2: $2\ CO(O^-)CH(OH)COCH_2(OO^{\bullet}) \rightarrow CO(O^-)CH(OH)COCHO + CO(O^-)CH(OH)COCH_2(OH) + O_2$		$8.0\ 10^7$			BR: 20%
Pathway 3: $2\ CO(O^-)CH(OH)COCH_2(OO^{\bullet}) \rightarrow 2\ CO(O^-)CH(OH)COCH_2(O^{\bullet}) + O_2$		$1.4\ 10^8$			BR: 35%
$CO(O^-)CH(OH)COCH_2(O^{\bullet}) \rightarrow CO(O^-)CH(OH)C^{\bullet}O + CH_2O$					4 - 5
$CO(O^-)CH(OH)C^{\bullet}O + O_2 \rightarrow CO(O^-)CH(OH)CO(OO^{\bullet})$		$2.0\ 10^9$			3
$2\ CO(O^-)CH(OH)COCH_2(OO^{\bullet}) \rightarrow 1.10\ CO(O^-)CH(OH)COCHO + 0.20\ CO(O^-)CH(OH)COCH_2(OH) + 0.70\ CH_2O + 0.70\ CO(O^-)CH(OH)CO(OO^{\bullet}) + 0.45\ H_2O_2 - 0.15\ O_2$	R(691)	$4.0\ 10^8$			= k(2 $CH_3COCH_2(OO^{\bullet})$) -6
Oxidation of 2,4-dihydroxy-3-oxobutanoic acid					44
Pathway 1: $CH_2(OH)C(OH)(OH)CH(OH)CO(OH) + HO^{\bullet} \rightarrow CH_2(OH)C(OH)(O^{\bullet})CH(OH)CO(OH) + H_2O$		$4.7\ 10^7$			BR: 58% - 45
$CH_2(OH)C(OH)(O^{\bullet})CH(OH)CO(OH) \rightarrow CH_2(OH)CO(OH) + CO(OH)C^{\bullet}H(OH)$					4 - 5
$CO(OH)C^{\bullet}H(OH) + O_2 \rightarrow CH(OH)(OO^{\bullet})CO(OH)$		$2.0\ 10^9$			3
Pathway 2: $CH_2(OH)C(OH)(OH)CH(OH)CO(OH) + HO^{\bullet} \rightarrow C^{\bullet}H(OH)C(OH)(OH)CH(OH)CO(OH) + H_2O$		$3.4\ 10^7$			BR: 42% - 45
$C^{\bullet}H(OH)C(OH)(OH)CH(OH)CO(OH) + O_2 \rightarrow CO(OH)CH(OH)C(OH)(OH)CH(OH)(OO^{\bullet})$		$2.0\ 10^9$			3
$CH_2(OH)C(OH)(OH)CH(OH)CO(OH) + HO^{\bullet} \rightarrow 0.58\ CH_2(OH)CO(OH) + 0.58\ CH(OH)(OO^{\bullet})CO(OH) + 0.42\ CO(OH)CH(OH)C(OH)(OH)CH(OH)(OO^{\bullet}) + H_2O - O_2$	R(692)	$8.1\ 10^8$			12
Pathway 1: $CH_2(OH)C(OH)(OH)CH(OH)CO(OH) + NO_3^{\bullet} \rightarrow C^{\bullet}H(OH)C(OH)(OH)CH(OH)CO(OH) + NO_3^- + H^+$		$1.0\ 10^6$			BR: 100%
$C^{\bullet}H(OH)C(OH)(OH)CH(OH)CO(OH) + O_2 \rightarrow CO(OH)CH(OH)C(OH)(OH)CH(OH)(OO^{\bullet})$		$2.0\ 10^9$			3
$CH_2(OH)C(OH)(OH)CH(OH)CO(OH) + NO_3^{\bullet} \rightarrow CO(OH)CH(OH)C(OH)(OH)CH(OH)(OO^{\bullet}) + NO_3^- + H^+ - O_2$	R(693)	$1.0\ 10^6$			= k(CH(OH)(OH)CH(OH)(OH) + $NO_3^{\bullet}$) - 13
Pathway 1: $CH_2(OH)COCH(OH)CO(O^-) + HO^{\bullet} \rightarrow C^{\bullet}H(OH)COCH(OH)CO(O^-) + H_2O$		$3.9\ 10^8$			BR: 63% - 46
$C^{\bullet}H(OH)COCH(OH)CO(O^-) + O_2 \rightarrow CO(O^-)CH(OH)COCH(OH)(OO^{\bullet})$		$2.0\ 10^9$			3
Pathway 2: $CH_2(OH)COCH(OH)CO(O^-) + HO^{\bullet} \rightarrow CH_2(OH)COCH(OH)CO(O^{\bullet}) + OH^-$		$1.2\ 10^8$			BR: 19% - 46
$CH_2(OH)COCH(OH)CO(O^{\bullet}) \rightarrow CH_2(OH)COC^{\bullet}H(OH) + CO_2$					4 - 5
$CH_2(OH)COC^{\bullet}H(OH) + O_2 \rightarrow CH_2(OH)COCH(OH)(OO^{\bullet})$		$2.0\ 10^9$			3
Pathway 3: $CH_2(OH)COCH(OH)CO(O^-) + HO^{\bullet} \rightarrow CH_2(OH)COCH(O^{\bullet})CO(O^-) + H_2O$		$1.1\ 10^8$			BR: 18% - 46
$CH_2(OH)COCH(O^{\bullet})CO(O^-) \rightarrow CH_2(OH)C^{\bullet}O + CHOCO(O^-)$					4 - 5
$CH_2(OH)C^{\bullet}O + O_2 \rightarrow CH_2(OH)CO(OO^{\bullet})$		$2.0{\cdot}10^9$			3
$CH_2(OH)COCH(OH)CO(O^-) + HO^{\bullet} \rightarrow 0.63\ CO(O^-)CH(OH)COCH(OH)(OO^{\bullet}) + 0.19 CH_2(OH)COCH(OH)(OO^{\bullet}) + 0.18\ CHOCO(O^-) + 0.18\ CH_2(OH)CO(OO^{\bullet}) + 0.19\ CO_2 + 0.19\ OH^- + 0.81\ H_2O - O_2$	R(694)	$6.2\ 10^8$			12
Pathway 1: $CH_2(OH)COCH(OH)CO(O^-) + NO_3^{\bullet} \rightarrow C^{\bullet}H(OH)COCH(OH)CO(O^-) + NO_3^- + H^+$		$1.0\ 10^6$			BR: 100%
$C^{\bullet}H(OH)COCH(OH)CO(O^-) + O_2 \rightarrow CO(O^-)CH(OH)COCH(OH)(OO^{\bullet})$		$2.0{\cdot}10^9$			3
$CH_2(OH)COCH(OH)CO(O^-) + NO_3^{\bullet} \rightarrow CO(O^-)CH(OH)COCH(OH)(OO^{\bullet}) + NO_3^- + H^+ - O_2$	R(695)	$1.0\ 10^6$			= k(CH(OH)(OH)CH(OH)(OH) + $NO_3^{\bullet}$) - 13
$CO(OH)CH(OH)C(OH)(OH)CH(OH)(OO^{\bullet}) + OH^- \rightarrow CO(OH)CH(OH)C(OH)(OH)CH(O^-)(OO^{\bullet}) + H_2O$		$4.0\ 10^9$			
$CO(OH)CH(OH)C(OH)(OH)CH(O^-)(OO^{\bullet}) \rightarrow CO(OH)CH(OH)C(OH)(OH)CHO + O_2^{\bullet-}$					16
$CO(OH)CH(OH)C(OH)(OH)CH(OH)(OO^{\bullet}) + OH^- \rightarrow CO(OH)CH(OH)C(OH)(OH)CHO + O_2^{\bullet-} + H_2O$	R(696)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^{\bullet}) + OH^-$)
$CO(OH)CH(OH)C(OH)(OH)CH(OH)(OO^{\bullet}) \rightarrow CO(OH)CH(OH)C(OH)(OH)CHO + HO_2^{\bullet}$	R(697)	$1.9\ 10^2$			17

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CO(O^-)CH(OH)COCH(OH)(OO^\bullet) + OH^- \rightarrow CO(O^-)CH(OH)COCH(O^-)(OO^\bullet) + H_2O$		4.0 10^9			
$CO(O^-)CH(OH)COCH(O^-)(OO^\bullet) \rightarrow CO(O^-)CH(OH)COCHO + O_2^{\bullet-}$					16
$CO(O^-)CH(OH)COCH(OH)(OO^\bullet) + OH^- \rightarrow CO(O^-)CH(OH)COCHO + O_2^{\bullet-} + H_2O$	R(698)	4.0 10^9			= $k(CH_3CH(OH)(OO^\bullet) + OH^-)$
$CO(O^-)CH(OH)COCH(OH)(OO^\bullet) \rightarrow CO(O^-)CH(OH)COCHO + HO_2^\bullet$	R(699)	1.9 10^2			17
Oxidation of 2-hydroxy, 3,4-dioxobutanoic acid					47
Pathway 1: $CO(OH)CH(OH)C(OH)(OH)CH(OH)(OH) + HO^\bullet \rightarrow CO(OH)CH(OH)C(OH)(OH)CH(OH)(O^\bullet) + H_2O$		4.6 10^8			BR: 50% - 48
$CO(OH)CH(OH)C(OH)(OH)CH(OH)(O^\bullet) \rightarrow CO(OH)CH(OH)C^\bullet(OH)(OH) + CHO(OH)$					4 - 5
$CO(OH)CH(OH)C^\bullet(OH)(OH) + O_2 \rightarrow CO(OH)CH(OH)C(OH)(OH)(OO^\bullet)$		2.0 10^9			3
Pathway 2: $CO(OH)CH(OH)C(OH)(OH)CH(OH)(OH) + HO^\bullet \rightarrow CO(OH)CH(OH)C(OH)(O^\bullet)CH(OH)(OH) + H_2O$		4.6 10^8			BR: 50% - 48
$CO(OH)CH(OH)C(OH)(O^\bullet)CH(OH)(OH) \rightarrow CO(OH)C^\bullet H(OH) + CH(OH)(OH)CO(OH)$					4 - 5
$CO(OH)C^\bullet H(OH) + O_2 \rightarrow CH(OH)(OO^\bullet)CO(OH)$		2.0 10^9			3
$CO(OH)CH(OH)C(OH)(OH)CH(OH)(OH) + HO^\bullet \rightarrow 0.50\ CO(OH)CH(OH)C(OH)(OH)(OO^\bullet) + 0.50\ CHO(OH) + 0.50\ CH(OH)(OO^\bullet)CO(OH) + 0.50\ CH(OH)(OH)CO(OH) + H_2O - O_2$	R(700)	9.2 10^8			12
Pathway 1: $CO(O^-)CH(OH)COCH(OH)(OH) + HO^\bullet \rightarrow CO(O^-)CH(OH)COCH(OH)(O^\bullet) + H_2O$		4.1 10^8			BR: 58% - 49
$CO(O^-)CH(OH)COCH(OH)(O^\bullet) \rightarrow CO(O^-)CH(OH)C^\bullet O + CHO(OH)$					4 - 5
$CO(O^-)CH(OH)C^\bullet O + O_2 \rightarrow CO(O^-)CH(OH)CO(OO^\bullet)$		2.0 10^9			3
Pathway 2: $CO(O^-)CH(OH)COCH(OH)(OH) + HO^\bullet \rightarrow CO(O^-)CH(OH)COC^\bullet(OH)(OH) + H_2O$		1.9 10^8			BR: 26% - 49
$CO(O^-)CH(OH)COC^\bullet(OH)(OH) + O_2 \rightarrow CO(O^-)CH(OH)COC(OH)(OH)(OO^\bullet)$		2.0 10^9			3
Pathway 3: $CO(O^-)CH(OH)COCH(OH)(OH) + HO^\bullet \rightarrow CO(O^\bullet)CH(OH)COCH(OH)(OH) + OH^-$		1.1 10^8			BR: 16% - 49
$CO(O^\bullet)CH(OH)COCH(OH)(OH) \rightarrow CO_2 + C^\bullet H(OH)COCH(OH)(OH)$					4 - 5
$C^\bullet H(OH)COCH(OH)(OH) + O_2 \rightarrow CH(OH)(OH)COCH(OH)(OO^\bullet)$		2.0 10^9			3
$CO(O^-)CH(OH)COCH(OH)(OH) + HO^\bullet \rightarrow 0.58\ CO(O^-)CH(OH)CO(OO^\bullet) + 0.58\ CHO(OH) + 0.26\ CO(O^-)CH(OH)COC(OH)(OH)(OO^\bullet) + 0.16\ CH(OH)(OH)COCH(OH)(OO^\bullet) + 0.16\ CO_2 + 0.84\ H_2O + 0.16\ OH^- - O_2$	R(701)	7.1 10^8			12
Pathway 1: $CO(O^-)CH(OH)COCH(OH)(OH) + NO_3^\bullet \rightarrow CO(O^-)CH(OH)COC^\bullet(OH)(OH) + NO_3^- + H^+$		1.8 10^5			BR: 100%
$CO(O^-)CH(OH)COC^\bullet(OH)(OH) + O_2 \rightarrow CO(O^-)CH(OH)COC(OH)(OH)(OO^\bullet)$		2.0 10^9			3
$CO(O^-)CH(OH)COCH(OH)(OH) + NO_3^\bullet \rightarrow CO(O^-)CH(OH)COC(OH)(OH)(OO^\bullet) + NO_3^- + H^+ - O_2$	R(702)	1.8 10^5			= $k(CH(OH)(OH)CO(O^-) + NO_3^\bullet)$ - 13
Pathway 1: $CO(O^-)CH(OH)C(OH)(OH)CH(OH)(OH) + HO^\bullet \rightarrow CO(O^-)CH(OH)C(OH)(OH)CH(OH)(O^\bullet) + H_2O$		4.6 10^8			BR: 42% - 50
$CO(O^-)CH(OH)C(OH)(OH)CH(OH)(O^\bullet) \rightarrow CO(O^-)CH(OH)C^\bullet(OH)(OH) + CHO(OH)$					4 - 5
$CO(O^-)CH(OH)C^\bullet(OH)(OH) + O_2 \rightarrow CO(O^-)CH(OH)C(OH)(OH)(OO^\bullet)$		2.0 10^9			3
Pathway 2: $CO(O^-)CH(OH)C(OH)(OH)CH(OH)(OH) + HO^\bullet \rightarrow CO(O^-)CH(OH)C(OH)(O^\bullet)CH(OH)(OH) + H_2O$		4.6 10^8			BR: 42% - 50
$CO(O^-)CH(OH)C(OH)(O^\bullet)CH(OH)(OH) \rightarrow CO(O^-)C^\bullet H(OH) + CH(OH)(OH)CO(OH)$					4 - 5
$CO(O^-)C^\bullet H(OH) + O_2 \rightarrow CH(OH)(OO^\bullet)CO(O^-)$		2.0 10^9			3
Pathway 3: $CO(O^-)CH(OH)C(OH)(OH)CH(OH)(OH) + HO^\bullet \rightarrow CO(O^-)CH(OH)C(OH)(OH)C^\bullet(OH)(OH) + H_2O$		1.8 10^8			BR: 16% - 50
$CO(O^-)CH(OH)C(OH)(OH)C^\bullet(OH)(OH) + O_2 \rightarrow CO(O^-)CH(OH)C(OH)(OH)C(OH)(OH)(OO^\bullet)$		2.0 10^9			3
$CO(O^-)CH(OH)C(OH)(OH)CH(OH)(OH) + HO^\bullet \rightarrow 0.42\ CO(O^-)CH(OH)C(OH)(OH)(OO^\bullet) + 0.42\ CHO(OH) + 0.42\ CH(OH)(OO^\bullet)CO(O^-) + 0.42\ CH(OH)(OH)CO(OH) + 0.16\ CO(O^-)CH(OH)C(OH)(OH)C(OH)(OH)(OO^\bullet) + H_2O - O_2$	R(703)	1.1 10^9			12
Pathway 1: $CO(O^-)CH(OH)C(OH)(OH)CH(OH)(OH) + NO_3^\bullet \rightarrow CO(O^-)CH(OH)C(OH)(OH)C^\bullet(OH)(OH) + NO_3^- + H^+$		1.8 10^5			BR: 100%
$CO(O^-)CH(OH)C(OH)(OH)C^\bullet(OH)(OH) + O_2 \rightarrow CO(O^-)CH(OH)C(OH)(OH)C(OH)(OH)(OO^\bullet)$		2.0 10^9			3
$CO(O^-)CH(OH)C(OH)(OH)CH(OH)(OH) + NO_3^\bullet \rightarrow CO(O^-)CH(OH)C(OH)(OH)C(OH)(OH)(OO^\bullet) + NO_3^- + H^+ - O_2$	R(704)	1.8 10^5			= $k(CH(OH)(OH)CO(O^-) + NO_3^\bullet)$ - 13
$CO(O^-)CH(OH)COC(OH)(OH)(OO^\bullet) + OH^- \rightarrow CO(O^-)CH(OH)COC(O^-)(OH)(OO^\bullet) + H_2O$		4.0 10^9			
$CO(O^-)CH(OH)COC(O^-)(OH)(OO^\bullet) \rightarrow CO(O^-)CH(OH)COCO(OH) + O_2^{\bullet-}$					16
$CO(O^-)CH(OH)COC(OH)(OH)(OO^\bullet) + OH^- \rightarrow CO(O^-)CH(OH)COCO(OH) + O_2^{\bullet-} + H_2O$	R(705)	4.0 10^9			= $k(CH_3CH(OH)(OO^\bullet) + OH^-)$
$CO(O^-)CH(OH)COC(OH)(OH)(OO^\bullet) \rightarrow CO(O^-)CH(OH)COCO(OH) + HO_2^\bullet$	R(706)	1.0 10^6			27
$CO(OH)CH(OH)C(OH)(OH)C(OH)(OH)(OO^\bullet) + OH^- \rightarrow CO(OH)CH(OH)C(OH)(OH)C(O^-)(OH)(OO^\bullet) + H_2O$		4.0 10^9			
$CO(OH)CH(OH)C(OH)(OH)C(O^-)(OH)(OO^\bullet) \rightarrow CO(OH)CH(OH)C(OH)(OH)CO(OH) + O_2^{\bullet-}$					16

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CO(OH)CH(OH)C(OH)(OH)C(OH)(OH)(OO^{\bullet})$ + OH^- → $CO(OH)CH(OH)C(OH)(OH)CO(OH)$ + $O_2^{\bullet-}$ + H_2O	R(707)	$4.0\ 10^9$			= $k(CH_3CH(OH)(OO^{\bullet}) + OH^-)$
$CO(OH)CH(OH)C(OH)(OH)C(OH)(OH)(OO^{\bullet})$ → $CO(OH)CH(OH)C(OH)(OH)CO(OH)$ + $HO_2^{\bullet}$	R(708)	$1.0\ 10^6$			27
$CO(O^-)CH(OH)C(OH)(OH)C(OH)(OH)(OO^{\bullet})$ + OH^- → $CO(O^-)CH(OH)C(OH)(OH)C(O^-)(OH)(OO^{\bullet})$ + H_2O		$4.0\ 10^9$			
$CO(O^-)CH(OH)C(OH)(OH)C(O^-)(OH)(OO^{\bullet})$ → $CO(O^-)CH(OH)C(OH)(OH)CO(OH)$ + $O_2^{\bullet-}$					16
$CO(O^-)CH(OH)C(OH)(OH)C(OH)(OH)(OO^{\bullet})$ + OH^- → $CO(O^-)CH(OH)C(OH)(OH)CO(OH)$ + $O_2^{\bullet-}$ + H_2O	R(709)	$4.0\ 10^9$			= $k(CH_3CH(OH)(OO^{\bullet}) + OH^-)$
$CO(O^-)CH(OH)C(OH)(OH)C(OH)(OH)(OO^{\bullet})$ → $CO(O^-)CH(OH)C(OH)(OH)CO(OH)$ + $HO_2^{\bullet}$	R(710)	$1.0\ 10^6$			27
Oxidation of 2-oxomalic acid					51
Pathway 1: $CO(OH)CH(OH)C(OH)(OH)CO(OH)$ + $HO^{\bullet}$ → $CO(OH)CH(OH)C(OH)(O^{\bullet})CO(OH)$ + H_2O		$3.0\ 10^8$			BR: 100% - 52
$CO(OH)CH(OH)C(OH)(O^{\bullet})CO(OH)$ → $CO(OH)CH(OH)CO(OH)$ + $C^{\bullet}O(OH)$					4 - 5
$C^{\bullet}O(OH)$ + O_2 → $CO(OH)(OO^{\bullet})$		$2.0\ 10^9$			3
$CO(OH)CH(OH)C(OH)(OH)CO(OH)$ + $HO^{\bullet}$ → $CO(OH)CH(OH)CO(OH)$ + $CO(OH)(OO^{\bullet})$ + H_2O - O_2	R(711)	$3.0\ 10^8$			12
Pathway 1: $CO(OH)CH(OH)COCO(O^-)$ + $HO^{\bullet}$ → $CO(OH)CH(OH)COCO(O^{\bullet})$ + OH^-		$6.0\ 10^7$			BR: 50% - 53
$CO(OH)CH(OH)COCO(O^{\bullet})$ → $CO(OH)CH(OH)C^{\bullet}O$ + CO_2					4 - 5
$CO(OH)CH(OH)C^{\bullet}O$ + O_2 → $CO(OH)CH(OH)CO(OO^{\bullet})$		$2.0\ 10^9$			3
Pathway 2: $CO(OH)CH(OH)COCO(O^-)$ + $HO^{\bullet}$ → $CO(OH)CH(O^{\bullet})COCO(O^-)$ + H_2O		$6.0\ 10^7$			BR: 50% - 53
$CO(OH)CH(O^{\bullet})COCO(O^-)$ → $C^{\bullet}O(OH)$ + $CO(O^-)COCHO$					4 - 5
$C^{\bullet}O(OH)$ + O_2 → $CO(OH)(OO^{\bullet})$		$2.0\ 10^9$			3
$CO(OH)CH(OH)COCO(O^-)$ + $HO^{\bullet}$ → 0.50 $CO(OH)CH(OH)CO(OO^{\bullet})$ + 0.50 $CO(O^-)COCHO$ + 0.50 $CO(OH)(OO^{\bullet})$ + 0.50 H_2O + 0.50 OH^- - O_2	R(712)	$1.2\ 10^8$			12
Pathway 1: $CO(OH)CH(OH)C(OH)(OH)CO(O^-)$ + $HO^{\bullet}$ → $CO(OH)CH(OH)C(OH)(O^{\bullet})CO(O^-)$ + H_2O		$5.4\ 10^8$			BR: 100% - 54
$CO(OH)CH(OH)C(OH)(O^{\bullet})CO(O^-)$ → $CO(OH)CH(OH)CO(OH)$ + $C^{\bullet}O(O^-)$					4 - 5
$C^{\bullet}O(O^-)$ + O_2 → $CO(O^-)(OO^{\bullet})$		$2.0\ 10^9$			3
$CO(OH)CH(OH)C(OH)(OH)CO(O^-)$ + $HO^{\bullet}$ → $CO(OH)CH(OH)CO(OH)$ + $CO(O^-)(OO^{\bullet})$ + H_2O - O_2	R(713)	$5.4\ 10^8$			
Pathway 1: $CO(O^-)CH(OH)C(OH)(OH)CO(OH)$ + $HO^{\bullet}$ → $CO(O^-)CH(OH)C(OH)(O^{\bullet})CO(OH)$ + H_2O		$2.6\ 10^8$			BR: 55% - 55
$CO(O^-)CH(OH)C(OH)(O^{\bullet})CO(OH)$ → $CO(OH)CH(OH)CO(O^-)$ + $C^{\bullet}O(OH)$					4 - 5
$C^{\bullet}O(OH)$ + O_2 → $CO(OH)(OO^{\bullet})$		$2.0\ 10^9$			3
Pathway 2: $CO(O^-)CH(OH)C(OH)(OH)CO(OH)$ + $HO^{\bullet}$ → $CO(O^{\bullet})CH(OH)C(OH)(OH)CO(OH)$ + OH^-		$1.1\ 10^8$			BR: 24% - 55
$CO(O^{\bullet})CH(OH)C(OH)(OH)CO(OH)$ → CO_2 + $C^{\bullet}H(OH)C(OH)(OH)CO(OH)$					4 - 5
$C^{\bullet}H(OH)C(OH)(OH)CO(OH)$ + O_2 → $CH(OH)(OO^{\bullet})C(OH)(OH)CO(OH)$		$2.0\ 10^9$			3
Pathway 3: $CO(O^-)CH(OH)C(OH)(OH)CO(OH)$ + $HO^{\bullet}$ → $CO(O^-)CH(O^{\bullet})C(OH)(OH)CO(OH)$ + H_2O		$1.0\ 10^8$			BR: 21% - 55
$CO(O^-)CH(O^{\bullet})C(OH)(OH)CO(OH)$ → $C^{\bullet}O(O^-)$ + $CO(OH)C(OH)(OH)CHO$					4 - 5
$C^{\bullet}O(O^-)$ + O_2 → $CO(O^-)(OO^{\bullet})$		$2.0\ 10^9$			3
$CO(O^-)CH(OH)C(OH)(OH)CO(OH)$ + $HO^{\bullet}$ → 0.55 $CO(OH)CH(OH)CO(O^-)$ + 0.24 $CH(OH)(OO^{\bullet})C(OH)(OH)CO(OH)$ + 0.21 $CO(OH)C(OH)(OH)CHO$ + 0.24 CO_2 + 0.55 $CO(OH)(OO^{\bullet})$ + 0.21 $CO(O^-)(OO^{\bullet})$ + 0.76 H_2O + 0.24 OH^- - O_2	R(714)	$4.7\ 10^8$			12
Pathway 1: $CO(O^-)CH(OH)COCO(O^-)$ + $HO^{\bullet}$ → $CO(O^{\bullet})CH(OH)COCO(O^-)$ + OH^-		$1.1\ 10^8$			BR: 39% - 56
$CO(O^{\bullet})CH(OH)COCO(O^-)$ → CO_2 + $C^{\bullet}H(OH)COCO(O^-)$					4 - 5
$C^{\bullet}H(OH)COCO(O^-)$ + O_2 → $CH(OH)(OO^{\bullet})COCO(O^-)$		$2.0\ 10^9$			3
Pathway 2: $CO(O^-)CH(OH)COCO(O^-)$ + $HO^{\bullet}$ → $CO(O^-)CH(O^{\bullet})COCO(O^-)$ + H_2O		$1.0\ 10^8$			BR: 35% - 56
$CO(O^-)CH(O^{\bullet})COCO(O^-)$ → $C^{\bullet}O(O^-)$ + $CO(O^-)COCHO$					4 - 5
$C^{\bullet}O(O^-)$ + O_2 → $CO(O^-)(OO^{\bullet})$		$2.0\ 10^9$			3
Pathway 3: $CO(O^-)CH(OH)COCO(O^-)$ + $HO^{\bullet}$ → $CO(O^-)C^{\bullet}(OH)COCO(O^-)$ + H_2O		$8.0\ 10^7$			BR: 26% - 56
$CO(O^-)C^{\bullet}(OH)COCO(O^-)$ + O_2 → $CO(O^-)C(OH)(OO^{\bullet})COCO(O^-)$		$2.0\ 10^9$			3
$CO(O^-)CH(OH)COCO(O^-)$ + $HO^{\bullet}$ → 0.39 $CH(OH)(OO^{\bullet})COCO(O^-)$ + 0.35 $CO(O^-)COCHO$ + 0.26 $CO(O^-)C(OH)(OO^{\bullet})COCO(O^-)$ + 0.39 CO_2 + 0.35 $CO(O^-)(OO^{\bullet})$ + 0.39 OH^- + 0.61 H_2O - O_2	R(715)	$2.9\ 10^8$			12
Pathway 1: $CO(O^-)CH(OH)COCO(O^-)$ + $NO_3^{\bullet}$ → $CO(O^-)C^{\bullet}(OH)COCO(O^-)$ + NO_3^- + H^+		$2.3\ 10^7$			BR: 100%
$CO(O^-)C^{\bullet}(OH)COCO(O^-)$ + O_2 → $CO(O^-)C(OH)(OO^{\bullet})COCO(O^-)$		$2.0\ 10^9$			3

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CO(O^-)CH(OH)COCO(O^-) + NO_3^\bullet \rightarrow CO(O^-)C(OH)(OO^\bullet)COCO(O^-) + NO_3^- + H^+ - O_2$	R(716)	$2.3\ 10^7$			= k($CO(O^-)CH_2CO(O^-) + NO_3^\bullet$) - 13
$CO(OH)C(OH)(OO^\bullet)C(OH)(OH)CO(OH) + OH^- \rightarrow CO(OH)C(O^-)(OO^\bullet)C(OH)(OH)CO(OH) + H_2O$		$4.0\ 10^9$			
$CO(OH)C(O^-)(OO^\bullet)C(OH)(OH)CO(OH) \rightarrow CO(OH)COC(OH)(OH)CO(OH) + O_2^{\bullet-}$					16
$CO(OH)C(OH)(OO^\bullet)C(OH)(OH)CO(OH) + OH^- \rightarrow CO(OH)COC(OH)(OH)CO(OH) + O_2^{\bullet-} + H_2O$	R(717)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^\bullet) + OH^-$)
$CO(OH)C(OH)(OO^\bullet)C(OH)(OH)CO(OH) \rightarrow CO(OH)COC(OH)(OH)CO(OH) + HO_2^\bullet$	R(718)	$1.9\ 10^2$			17
$CO(OH)C(OH)(OO^\bullet)COCO(O^-) + OH^- \rightarrow CO(OH)C(O^-)(OO^\bullet)COCO(O^-) + H_2O$		$4.0\ 10^9$			
$CO(OH)C(O^-)(OO^\bullet)COCO(O^-) \rightarrow CO(OH)COCOCO(O^-) + O_2^{\bullet-}$					16
$CO(OH)C(OH)(OO^\bullet)COCO(O^-) + OH^- \rightarrow CO(OH)COCOCO(O^-) + O_2^{\bullet-} + H_2O$	R(719)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^\bullet) + OH^-$)
$CO(OH)C(OH)(OO^\bullet)COCO(O^-) \rightarrow CO(OH)COCOCO(O^-) + HO_2^\bullet$	R(720)	$1.9\ 10^2$			17
$CO(OH)C(OH)(OO^\bullet)C(OH)(OH)CO(O^-) + OH^- \rightarrow CO(OH)C(O^-)(OO^\bullet)C(OH)(OH)CO(O^-) + H_2O$		$4.0\ 10^9$			
$CO(OH)C(O^-)(OO^\bullet)C(OH)(OH)CO(O^-) \rightarrow CO(OH)COC(OH)(OH)CO(O^-) + O_2^{\bullet-}$					16
$CO(OH)C(OH)(OO^\bullet)C(OH)(OH)CO(O^-) + OH^- \rightarrow CO(OH)COC(OH)(OH)CO(O^-) + O_2^{\bullet-} + H_2O$	R(721)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^\bullet) + OH^-$)
$CO(OH)C(OH)(OO^\bullet)C(OH)(OH)CO(O^-) \rightarrow CO(OH)COC(OH)(OH)CO(O^-) + HO_2^\bullet$	R(722)	$1.9\ 10^2$			17
$CO(O^-)C(OH)(OO^\bullet)C(OH)(OH)CO(OH) + OH^- \rightarrow CO(O^-)C(O^-)(OO^\bullet)C(OH)(OH)CO(OH) + H_2O$		$4.0\ 10^9$			
$CO(O^-)C(O^-)(OO^\bullet)C(OH)(OH)CO(OH) \rightarrow CO(OH)C(OH)(OH)COCO(O^-) + O_2^{\bullet-}$					16
$CO(O^-)C(OH)(OO^\bullet)C(OH)(OH)CO(OH) + OH^- \rightarrow CO(OH)C(OH)(OH)COCO(O^-) + O_2^{\bullet-} + H_2O$	R(723)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^\bullet) + OH^-$)
$CO(O^-)C(OH)(OO^\bullet)C(OH)(OH)CO(OH) \rightarrow CO(OH)C(OH)(OH)COCO(O^-) + HO_2^\bullet$	R(724)	$1.9\ 10^2$			17
$CO(O^-)C(OH)(OO^\bullet)COCO(O^-) + OH^- \rightarrow CO(O^-)C(O^-)(OO^\bullet)COCO(O^-) + H_2O$		$4.0\ 10^9$			
$CO(O^-)C(O^-)(OO^\bullet)COCO(O^-) \rightarrow CO(O^-)COCOCO(O^-) + O_2^{\bullet-}$					16
$CO(O^-)C(OH)(OO^\bullet)COCO(O^-) + OH^- \rightarrow CO(O^-)COCOCO(O^-) + O_2^{\bullet-} + H_2O$	R(725)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^\bullet) + OH^-$)
$CO(O^-)C(OH)(OO^\bullet)COCO(O^-) \rightarrow CO(O^-)COCOCO(O^-) + HO_2^\bullet$	R(726)	$1.9\ 10^2$			17
Oxidation of Dioxosuccinic acid					57
Pathway 1: $CO(OH)C(OH)(OH)C(OH)(OH)CO(OH) + HO^\bullet \rightarrow CO(OH)C(OH)(OH)C(OH)(O^\bullet)CO(OH) + H_2O$		$4.6\ 10^8$			BR: 100% - 58
$CO(OH)C(OH)(OH)C(OH)(O^\bullet)CO(OH) \rightarrow CO(OH)C(OH)(OH)CO(OH) + C^\bullet O(OH)$					4 - 5
$C^\bullet O(OH) + O_2 \rightarrow CO(OH)(OO^\bullet)$		$2.0\ 10^9$			3
$CO(OH)C(OH)(OH)C(OH)(OH)CO(OH) + HO^\bullet \rightarrow CO(OH)C(OH)(OH)CO(OH) + CO(OH)(OO^\bullet) + H_2O - O_2$	R(727)	$4.6\ 10^8$			12
Pathway 1: $CO(OH)C(OH)(OH)COCO(O^-) + HO^\bullet \rightarrow CO(OH)C(OH)(O^\bullet)COCO(O^-) + H_2O$		$2.5\ 10^8$			BR: 100% - 59
$CO(OH)C(OH)(O^\bullet)COCO(O^-) \rightarrow C^\bullet O(OH) + CO(OH)COCO(O^-)$					4 - 5
$C^\bullet O(OH) + O_2 \rightarrow CO(OH)(OO^\bullet)$		$2.0\ 10^9$			3
$CO(OH)C(OH)(OH)COCO(O^-) + HO^\bullet \rightarrow CO(OH)COCO(O^-) + CO(OH)(OO^\bullet) + H_2O - O_2$	R(728)	$2.5\ 10^8$			12
Pathway 1: $CO(OH)C(OH)(OH)C(OH)(OH)CO(O^-) + HO^\bullet \rightarrow CO(OH)C(OH)(OH)C(OH)(O^\bullet)CO(O^-) + H_2O$		$4.3\ 10^8$			BR: 64% - 60
$CO(OH)C(OH)(OH)C(OH)(O^\bullet)CO(O^-) \rightarrow CO(OH)C(OH)(OH)CO(OH) + C^\bullet O(O^-)$					4 - 5
$C^\bullet O(O^-) + O_2 \rightarrow CO(O^-)(OO^\bullet)$		$2.0\ 10^9$			3
Pathway 2: $CO(OH)C(OH)(OH)C(OH)(OH)CO(O^-) + HO^\bullet \rightarrow CO(OH)C(OH)(O^\bullet)C(OH)(OH)CO(O^-) + H_2O$		$2.4\ 10^8$			BR: 36% - 60
$CO(OH)C(OH)(O^\bullet)C(OH)(OH)CO(O^-) \rightarrow C^\bullet O(OH) + CO(OH)C(OH)(OH)CO(O^-)$					4 - 5
$C^\bullet O(OH) + O_2 \rightarrow CO(OH)(OO^\bullet)$		$2.0\ 10^9$			3
$CO(OH)C(OH)(OH)C(OH)(OH)CO(O^-) + HO^\bullet \rightarrow 0.64\ CO(OH)C(OH)(OH)CO(OH) + 0.36\ CO(OH)C(OH)(OH)CO(O^-) + 0.64\ CO(O^-)(OO^\bullet) + 0.36\ CO(OH)(OO^\bullet) + H_2O - O_2$	R(729)	$6.7\ 10^8$			12
Pathway 1: $CO(O^-)COCOCO(O^-) + HO^\bullet \rightarrow CO(O^-)COCOCO(O^\bullet) + OH^-$		$8.3\ 10^7$			BR: 100% - 61
$CO(O^-)COCOCO(O^\bullet) \rightarrow CO(O^-)COC^\bullet O + CO_2$					4 - 5
$CO(O^-)COC^\bullet O + O_2 \rightarrow CO(O^-)COCO(OO^\bullet)$		$2.0\ 10^9$			3
$CO(O^-)COCOCO(O^-) + HO^\bullet \rightarrow CO(O^-)COCO(OO^\bullet) + CO_2 + OH^- - O_2$	R(730)	$8.3\ 10^7$			12
Pathway 1: $CO(O^-)COC(OH)(OH)CO(O^-) + HO^\bullet \rightarrow CO(O^-)COC(OH)(O^\bullet)CO(O^-) + H_2O$		$4.4\ 10^8$			BR: 100% - 62
$CO(O^-)COC(OH)(O^\bullet)CO(O^-) \rightarrow CO(OH)COCO(O^-) + C^\bullet O(O^-)$					4 - 5
$C^\bullet O(O^-) + O_2 \rightarrow CO(O^-)(OO^\bullet)$		$2.0\ 10^9$			3

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CO(O^-)COC(OH)(OH)CO(O^-) + HO^\bullet \rightarrow CO(OH)COCO(O^-) + CO(O^-)(OO^\bullet) + H_2O - O_2$	R(731)	4.4 10^8			12
Oxidation of 2,3-dioxobutanedial					63
$CH(OH)(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OH) + HO^\bullet \rightarrow CH(OH)(OH)C(OH)(OH)C(OH)(OH)CH(OH)(O^\bullet) + H_2O$		8.8 10^8			BR: 52% - 64
$CH(OH)(OH)C(OH)(OH)C(OH)(OH)CH(OH)(O^\bullet) \rightarrow CH(OH)(OH)C(OH)(OH)C^\bullet(OH)(OH) + CHO(OH)$					4 - 5
$CH(OH)(OH)C(OH)(OH)C^\bullet(OH)(OH) + O_2 \rightarrow CH(OH)(OH)C(OH)(OH)C(OH)(OH)(OO^\bullet)$		2.0 10^9			3
$CH(OH)(OH)C(OH)(OH)C(OH)(O^\bullet)CH(OH)(OH) \rightarrow CH(OH)(OH)C^\bullet(OH)(OH) + CH(OH)(OH)CO(OH)$					4 - 5
$CH(OH)(OH)C^\bullet(OH)(OH) + O_2 \rightarrow CH(OH)(OH)C(OH)(OH)(OO^\bullet)$		2.0 10^9			3
$CH(OH)(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OH) + HO^\bullet \rightarrow 0.52\ CH(OH)(OH)C(OH)(OH)C(OH)(OH)(OO^\bullet) + 0.52\ CHO(OH) + 0.48\ CH(OH)(OH)C(OH)(OH)(OO^\bullet) + 0.48\ CH(OH)(OH)CO(OH) + H_2O - O_2$	R(732)	1.7 10^9			12
Oxidation of 2,3-dioxobutanoic acid					65
$CH_3C(OH)(OH)C(OH)(OH)CO(OH) + HO^\bullet \rightarrow CH_3C(OH)(O^\bullet)C(OH)(OH)CO(OH) + H_2O$		6.2 10^8			BR: 62% - 66
$CH_3C(OH)(O^\bullet)C(OH)(OH)CO(OH) \rightarrow CH_3CO(OH) + CO(OH)C^\bullet(OH)(OH)$					4 - 5
$CO(OH)C^\bullet(OH)(OH) + O_2 \rightarrow CO(OH)C(OH)(OH)(OO^\bullet)$		2.0 10^9			3
$CH_3C(OH)(OH)C(OH)(OH)C(OH)(O^\bullet)CO(OH) + HO^\bullet \rightarrow CH_3C(OH)(OH)C(OH)(OH)C(OH)(O^\bullet)CO(OH) + H_2O$		2.6 10^8			BR: 38% - 66
$CH_3C(OH)(OH)C(OH)(O^\bullet)CO(OH) \rightarrow CH_3C^\bullet(OH)(OH) + CO(OH)CO(OH)$					4 - 5
$CH_3C^\bullet(OH)(OH) + O_2 \rightarrow CH_3C(OH)(OH)(OO^\bullet)$		2.0 10^9			3
$CH_3C(OH)(OH)C(OH)(OH)CO(OH) + HO^\bullet \rightarrow 0.62\ CH_3CO(OH) + 0.62\ CO(OH)C(OH)(OH)(OO^\bullet) + 0.38\ CO(OH)CO(OH) + 0.38\ CH_3C(OH)(OH)(OO^\bullet) + H_2O - O_2$	R(733)	6.8 10^8			12
$CH_3COCOCO(O^-) + HO^\bullet \rightarrow C^\bullet H_2COCOCO(O^-) + H_2O$		6.9 10^7			BR: 63% - 67
$C^\bullet H_2COCOCO(O^-) + O_2 \rightarrow CH_2(OO^\bullet)COCOCO(O^-)$		2.0 10^9			3
$CH_3COCOCO(O^-) + HO^\bullet \rightarrow CH_3COCOCO(O^\bullet) + OH^-$		4.1 10^7			BR: 37% - 67
$CH_3COCOCO(O^\bullet) \rightarrow CH_3COC^\bullet O + CO_2$					4 - 5
$CH_3COC^\bullet O + O_2 \rightarrow CH_3COCO(OO^\bullet)$		2.0 10^9			3
$CH_3COCOCO(O^-) + HO^\bullet \rightarrow 0.63\ CH_2(OO^\bullet)COCOCO(O^-) + 0.37\ CH_3COCO(OO^\bullet) + 0.37\ CO_2 + 0.63\ H_2O + 0.37\ OH^- - O_2$	R(734)	1.1 10^8			12
$CH_3COCOCO(O^-) + NO_3^\bullet \rightarrow C^\bullet H_2COCOCO(O^-) + NO_3^- + H^+$		1.9 10^7			BR: 100%
$C^\bullet H_2COCOCO(O^-) + O_2 \rightarrow CH_2(OO^\bullet)COCOCO(O^-)$		2.0 10^9			3
$CH_3COCOCO(O^-) + NO_3^\bullet \rightarrow CH_2(OO^\bullet)COCOCO(O^-) + NO_3^- + H^+ - O_2$	R(735)	1.9 10^7	2887		= k($CH_3COCO(O^-) + NO_3^\bullet$) - 13
$CH_3C(OH)(OH)COCO(O^-) + HO^\bullet \rightarrow CH_3C(OH)(O^\bullet)COCO(O^-) + H_2O$		4.5 10^8			BR: 100% - 68
$CH_3C(OH)(O^\bullet)COCO(O^-) \rightarrow CH_3CO(OH) + CO(O^-)C^\bullet O$					4 - 5
$CO(O^-)C^\bullet O + O_2 \rightarrow CO(O^-)CO(OO^\bullet)$		2.0 10^9			3
$CH_3C(OH)(OH)COCO(O^-) + HO^\bullet \rightarrow CH_3CO(OH) + CO(O^-)CO(OO^\bullet) + H_2O - O_2$	R(736)	4.5 10^8			12
$CH_3COC(OH)(OH)CO(O^-) + HO^\bullet \rightarrow CH_3COC(OH)(O^\bullet)CO(O^-) + H_2O$		4.8 10^8			BR: 100% - 69
$CH_3COC(OH)(O^\bullet)CO(O^-) \rightarrow CH_3COCO(OH) + C^\bullet O(O^-)$					4 - 5
$C^\bullet O(O^-) + O_2 \rightarrow CO(O^-)(OO^\bullet)$		2.0 10^9			3
$CH_3COC(OH)(OH)CO(O^-) + HO^\bullet \rightarrow CH_3COCO(OH) + CO(O^-)(OO^\bullet) + H_2O - O_2$	R(737)	4.8 10^8			12
$2\ CH_2(OO^\bullet)C(OH)(OH)C(OH)(OH)CO(OH) \rightarrow 2\ CHOC(OH)(OH)C(OH)(OH)CO(OH) + H_2O_2$		1.8 10^8			BR: 45%
$2\ CH_2(OO^\bullet)C(OH)(OH)C(OH)(OH)CO(OH) \rightarrow CHOC(OH)(OH)C(OH)(OH)CO(OH) + CH_2(OH)C(OH)(OH)C(OH)(OH)CO(OH) + O_2$		8.0 10^7			BR: 20%
$2\ CH_2(OO^\bullet)C(OH)(OH)C(OH)(OH)CO(OH) \rightarrow 2\ CH_2(O^\bullet)C(OH)(OH)C(OH)(OH)CO(OH) + O_2$		1.4 10^8			BR: 35%
$CH_2(O^\bullet)C(OH)(OH)C(OH)(OH)CO(OH) \rightarrow CO(OH)C(OH)(OH)C^\bullet(OH)(OH) + CH_2O$					4 - 5
$CO(OH)C(OH)(OH)C^\bullet(OH)(OH) + O_2 \rightarrow CO(OH)C(OH)(OH)C(OH)(OH)(OO^\bullet)$		2.0 10^9			3
$2\ CH_2(OO^\bullet)C(OH)(OH)C(OH)(OH)CO(OH) \rightarrow 1.10\ CHOC(OH)(OH)C(OH)(OH)CO(OH) + 0.20\ CH_2(OH)C(OH)(OH)C(OH)(OH)CO(OH) + 0.70\ CO(OH)C(OH)(OH)C(OH)(OH)(OO^\bullet) + 0.70\ CH_2O + 0.45\ H_2O_2 - 0.15\ O_2$	R(738)	4.0 10^8			= k(2 $CH_3COCH_2(OO^\bullet)$) - 6

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
Pathway 1: $2\ CH_2(OO^\bullet)COCOCO(O^-) \rightarrow 2\ CHOCOCOCO(O^-) + H_2O_2$		$1.8\ 10^8$			BR: 45%
Pathway 2: $2\ CH_2(OO^\bullet)COCOCO(O^-) \rightarrow CHOCOCOCO(O^-) + CH_2(OH)COCOCO(O^-) + O_2$		$8.0\ 10^7$			BR: 20%
Pathway 3: $2\ CH_2(OO^\bullet)COCOCO(O^-) \rightarrow 2\ CH_2(O^\bullet)COCOCO(O^-) + O_2$		$1.4\ 10^8$			BR: 35%
$CH_2(O^\bullet)COCOCO(O^-) \rightarrow CO(O^-)COC^\bullet O + CH_2O$					4 -5
$CO(O^-)COC^\bullet O + O_2 \rightarrow CO(O^-)COCO(OO^\bullet)$		$2.0\ 10^9$			3
$2\ CH_2(OO^\bullet)COCOCO(O^-) \rightarrow 1.10\ CHOCOCOCO(O^-) + 0.20\ CH_2(OH)COCOCO(O^-) + 0.70\ CO(O^-)COCO(OO^\bullet) + 0.70\ CH_2O + 0.45\ H_2O_2 - 0.15\ O_2$	R(739)	$4.0\ 10^8$			= k(2 $CH_3COCH_2(OO^\bullet)$) - 6
Pathway 1: $2\ CH_2(OO^\bullet)C(OH)(OH)COCO(O^-) \rightarrow 2\ CHOC(OH)(OH)COCO(O^-) + H_2O_2$		$1.8\ 10^8$			BR: 45%
Pathway 2: $2\ CH_2(OO^\bullet)C(OH)(OH)COCO(O^-) \rightarrow CHOC(OH)(OH)COCO(O^-) + CH_2(OH)C(OH)(OH)COCO(O^-) + O_2$		$8.0\ 10^7$			BR: 20%
Pathway 3: $2\ CH_2(OO^\bullet)C(OH)(OH)COCO(O^-) \rightarrow 2\ CH_2(O^\bullet)C(OH)(OH)COCO(O^-) + O_2$		$1.4\ 10^8$			BR: 35%
$CH_2(O^\bullet)C(OH)(OH)COCO(O^-) \rightarrow CO(O^-)COC^\bullet(OH)(OH) + CH_2O$					4 - 5
$CO(O^-)COC^\bullet(OH)(OH) + O_2 \rightarrow CO(O^-)COC(OH)(OH)(OO^\bullet)$		$2.0\ 10^9$			3
$2\ CH_2(OO^\bullet)C(OH)(OH)COCO(O^-) \rightarrow 1.10\ CHOC(OH)(OH)COCO(O^-) + 0.20\ CH_2(OH)C(OH)(OH)COCO(O^-) + 0.70\ CO(O^-)COC(OH)(OH)(OO^\bullet) + 0.70\ CH_2O + 0.45\ H_2O_2 - 0.15\ O_2$	R(740)	$4.0\ 10^8$			= k(2 $CH_3COCH_2(OO^\bullet)$) - 6
Pathway 1: $2\ CH_2(OO^\bullet)COC(OH)(OH)CO(O^-) \rightarrow 2\ CHOCOC(OH)(OH)CO(O^-) + H_2O_2$		$1.8\ 10^8$			BR: 45%
Pathway 2: $2\ CH_2(OO^\bullet)COC(OH)(OH)CO(O^-) \rightarrow CHOCOC(OH)(OH)CO(O^-) + CH_2(OH)COC(OH)(OH)CO(O^-) + O_2$		$8.0\ 10^7$			BR: 20%
Pathway 3: $2\ CH_2(OO^\bullet)COC(OH)(OH)CO(O^-) \rightarrow 2\ CH_2(O^\bullet)COC(OH)(OH)CO(O^-) + O_2$		$1.4\ 10^8$			BR: 35%
$CH_2(O^\bullet)COC(OH)(OH)CO(O^-) \rightarrow CO(O^-)C(OH)(OH)C^\bullet O + CH_2O$					4 - 5
$CO(O^-)C(OH)(OH)C^\bullet O + O_2 \rightarrow CO(O^-)C(OH)(OH)CO(OO^\bullet)$		$2.0\ 10^9$			3
$2\ CH_2(OO^\bullet)COC(OH)(OH)CO(O^-) \rightarrow 1.10\ CHOCOC(OH)(OH)CO(O^-) + 0.20\ CH_2(OH)COC(OH)(OH)CO(O^-) + 0.70\ CO(O^-)C(OH)(OH)CO(OO^\bullet) + 0.70\ CH_2O + 0.45\ H_2O_2 - 0.15\ O_2$	R(741)	$4.0\ 10^8$			= k(2 $CH_3COCH_2(OO^\bullet)$) - 6
Oxidation of 2,3-dioxo-4-hydroxybutanal					70
Pathway 1: $CH_2(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OH) + HO^\bullet \rightarrow CH_2(OH)C(OH)(OH)C(OH)(OH)CH(OH)(O^\bullet) + H_2O$		$4.2\ 10^8$			BR: 28% - 71
$CH_2(OH)C(OH)(OH)C(OH)(OH)CH(OH)(O^\bullet) \rightarrow CH_2(OH)C(OH)(OH)C^\bullet(OH)(OH) + CHO(OH)$					4 - 5
$CH_2(OH)C(OH)(OH)C^\bullet(OH)(OH) + O_2 \rightarrow CH_2(OH)C(OH)(OH)C(OH)(OH)(OO^\bullet)$		$2.0\ 10^9$			3
Pathway 2: $CH_2(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OH) + HO^\bullet \rightarrow CH_2(OH)C(OH)(O^\bullet)C(OH)(OH)CH(OH)(OH) + H_2O$		$4.0\ 10^8$			BR: 27% - 71
$CH_2(OH)C(OH)(O^\bullet)C(OH)(OH)CH(OH)(OH) \rightarrow CH_2(OH)CO(OH) + CH(OH)(OH)C^\bullet(OH)(OH)$					4 - 5
$CH(OH)(OH)C^\bullet(OH)(OH) + O_2 \rightarrow CH(OH)(OH)C(OH)(OH)(OO^\bullet)$		$2.0\ 10^9$			3
Pathway 3: $CH_2(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OH) + HO^\bullet \rightarrow CH_2(OH)C(OH)(OH)C(OH)(O^\bullet)CH(OH)(OH) + H_2O$		$3.8\ 10^8$			BR: 25% - 71
$CH_2(OH)C(OH)(OH)C(OH)(O^\bullet)CH(OH)(OH) \rightarrow CH_2(OH)C^\bullet(OH)(OH) + CH(OH)(OH)CO(OH)$					4 - 5
$CH_2(OH)C^\bullet(OH)(OH) + O_2 \rightarrow CH_2(OH)C(OH)(OH)(OO^\bullet)$		$2.0\ 10^9$			3
Pathway 4: $CH_2(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OH) + HO^\bullet \rightarrow C^\bullet H(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OH) + H_2O$		$3.0\ 10^8$			BR: 20% - 71
$C^\bullet H(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OH) + O_2 \rightarrow CH(OH)(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OO^\bullet)$		$2.0\ 10^9$			3
$CH_2(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OH) + HO^\bullet \rightarrow 0.28\ CH_2(OH)C(OH)(OH)C(OH)(OH)(OO^\bullet) + 0.28\ CHO(OH) + 0.27\ CH_2(OH)CO(OH) + 0.27\ CH(OH)(OH)C(OH)(OH)(OO^\bullet) + 0.25\ CH_2(OH)C(OH)(OH)(OO^\bullet) + 0.25\ CH(OH)(OH)CO(OH) + 0.20\ CH(OH)(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OO^\bullet) + H_2O - O_2$	R(742)	$1.5\ 10^9$			12
Pathway 1: $CH_2(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OH) + NO_3^\bullet \rightarrow C^\bullet H(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OH) + NO_3^- + H^+$		$1.0\ 10^6$			BR: 100%
$C^\bullet H(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OH) + O_2 \rightarrow CH(OH)(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OO^\bullet)$		$2.0\ 10^9$			3
$CH_2(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OH) + NO_3^\bullet \rightarrow CH(OH)(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OO^\bullet) + NO_3^- + H^+ - O_2$	R(743)	$1.0\ 10^6$			= k(CH(OH)(OH)CH(OH)(OH) + $NO_3^\bullet$) - 13
$CH(OH)(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OO^\bullet) + OH^- \rightarrow CH(OH)(OH)C(OH)(OH)C(OH)(OH)CH(O^-)(OO^\bullet) + H_2O$		$4.0\ 10^9$			
$CH(OH)(OH)C(OH)(OH)C(OH)(OH)CH(O^-)(OO^\bullet) \rightarrow CHOC(OH)(OH)C(OH)(OH)CH(OH)(OH) + O_2^{\bullet-}$					16
$CH(OH)(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OO^\bullet) + OH^- \rightarrow CHOC(OH)(OH)C(OH)(OH)CH(OH)(OH) + O_2^{\bullet-} + H_2O$	R(744)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^\bullet) + OH^-$)
$CH(OH)(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OO^\bullet) \rightarrow CHOC(OH)(OH)C(OH)(OH)CH(OH)(OH) + HO_2^\bullet$		$1.9\ 10^2$			17
Oxidation of 2,3-dioxo-4-hydroxybutanoic acid					72
Pathway 1: $CH_2(OH)C(OH)(OH)C(OH)(OH)CO(OH) + HO^\bullet \rightarrow CH_2(OH)C(OH)(O^\bullet)C(OH)(OH)CO(OH) + H_2O$		$4.0\ 10^8$			BR: 42% - 73

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CH_2(OH)C(OH)(O^•)C(OH)(OH)CO(OH) \rightarrow CH_2(OH)CO(OH) + CO(OH)C^•(OH)(OH)$					4 - 5
$CO(OH)C^•(OH)(OH) + O_2 \rightarrow CO(OH)C(OH)(OH)(OO^•)$		$2.0\ 10^9$			3
Pathway 2: $CH_2(OH)C(OH)(OH)C(OH)(OH)CO(OH) + HO^• \rightarrow C^•H(OH)C(OH)(OH)C(OH)(OH)CO(OH) + H_2O$		$2.9\ 10^8$			BR: 31% - 73
$C^•H(OH)C(OH)(OH)C(OH)(OH)CO(OH) + O_2 \rightarrow CO(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OO^•)$		$2.0\ 10^9$			3
Pathway 3: $CH_2(OH)C(OH)(OH)C(OH)(OH)CO(OH) + HO^• \rightarrow CH_2(OH)C(OH)(OH)C(OH)(O^•)CO(OH) + H_2O$		$2.5\ 10^8$			BR: 27% - 73
$CH_2(OH)C(OH)(OH)C(OH)(O^•)CO(OH) \rightarrow CH_2(OH)C^•(OH)(OH) + CO(OH)CO(OH)$					4 - 5
$CH_2(OH)C^•(OH)(OH) + O_2 \rightarrow CH_2(OH)C(OH)(OH)(OO^•)$		$2.0\ 10^9$			3
$CH_2(OH)C(OH)(OH)C(OH)(OH)CO(OH) + HO^• \rightarrow 0.42\ CH_2(OH)CO(OH) + 0.42\ CO(OH)C(OH)(OH)(OO^•) + 0.31CO(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OO^•) + 0.27\ CO(OH)CO(OH) + 0.27\ CH_2(OH)C(OH)(OH)(OO^•) + H_2O - O_2$	R(745)	$9.4\ 10^8$			12
Pathway 1: $CH_2(OH)C(OH)(OH)C(OH)(OH)CO(OH) + NO_3^• \rightarrow C^•H(OH)C(OH)(OH)C(OH)(OH)CO(OH) + NO_3^- + H^+$		$1.0\ 10^6$			BR: 100%
$C^•H(OH)C(OH)(OH)C(OH)(OH)CO(OH) + O_2 \rightarrow CO(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OO^•)$		$2.0\ 10^9$			3
$CH_2(OH)C(OH)(OH)C(OH)(OH)CO(OH) + NO_3^• \rightarrow CO(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OO^•) + NO_3^- + H^+ - O_2$	R(746)	$1.0\ 10^6$			= k(CH(OH)(OH)CH(OH)(OH) + $NO_3^•$) - 13
Pathway 1: $CH_2(OH)C(OH)(OH)COCO(O^-) + HO^• \rightarrow CH_2(OH)C(OH)(O^•)COCO(O^-) + H_2O$		$4.0\ 10^8$			BR: 58% - 74
$CH_2(OH)C(OH)(O^•)COCO(O^-) \rightarrow CH_2(OH)CO(OH) + CO(O^-)C^•O$					4 - 5
$CO(O^-)C^•O + O_2 \rightarrow CO(O^-)CO(OO^•)$		$2.0\ 10^9$			3
Pathway 2: $CH_2(OH)C(OH)(OH)COCO(O^-) + HO^• \rightarrow C^•H(OH)C(OH)(OH)COCO(O^-) + H_2O$		$2.9\ 10^8$			BR: 42% - 74
$C^•H(OH)C(OH)(OH)COCO(O^-) + O_2 \rightarrow CO(O^-)COC(OH)(OH)CH(OH)(OO^•)$		$2.0\ 10^9$			3
$CH_2(OH)C(OH)(OH)COCO(O^-) + HO^• \rightarrow 0.58\ CH_2(OH)CO(OH) + 0.58\ CO(O^-)CO(OO^•) + 0.42\ CO(O^-)COC(OH)(OH)CH(OH)(OO^•) + H_2O - O_2$	R(747)	$6.9\ 10^8$			12
Pathway 1: $CH_2(OH)C(OH)(OH)COCO(O^-) + NO_3^• \rightarrow C^•H(OH)C(OH)(OH)COCO(O^-) + NO_3^- + H^+$		$1.0\ 10^6$			BR: 100%
$C^•H(OH)C(OH)(OH)COCO(O^-) + O_2 \rightarrow CO(O^-)COC(OH)(OH)CH(OH)(OO^•)$		$2.0\ 10^9$			3
$CH_2(OH)C(OH)(OH)COCO(O^-) + NO_3^• \rightarrow CO(O^-)COC(OH)(OH)CH(OH)(OO^•) + NO_3^- + H^+ - O_2$	R(748)	$1.0\ 10^6$			= k(CH(OH)(OH)CH(OH)(OH) + $NO_3^•$) - 13
Pathway 1: $CH_2(OH)C(OH)(OH)C(OH)(OH)CO(O^-) + HO^• \rightarrow CH_2(OH)C(OH)(OH)C(OH)(O^•)CO(O^-) + H_2O$		$4.7\ 10^8$			BR: 39% - 75
$CH_2(OH)C(OH)(OH)C(OH)(O^•)CO(O^-) \rightarrow CH_2(OH)C^•(OH)(OH) + CO(OH)CO(O^-)$					4 - 5
$CH_2(OH)C^•(OH)(OH) + O_2 \rightarrow CH_2(OH)C(OH)(OH)(OO^•)$		$2.0\ 10^9$			3
Pathway 2: $CH_2(OH)C(OH)(OH)C(OH)(OH)CO(O^-) + HO^• \rightarrow CH_2(OH)C(OH)(O^•)C(OH)(OH)CO(O^-) + H_2O$		$4.2\ 10^8$			BR: 35% - 75
$CH_2(OH)C(OH)(O^•)C(OH)(OH)CO(O^-) \rightarrow CH_2(OH)CO(OH) + CO(O^-)C^•(OH)(OH)$					4 - 5
$CO(O^-)C^•(OH)(OH) + O_2 \rightarrow CO(O^-)C(OH)(OH)(OO^•)$		$2.0\ 10^9$			3
Pathway 3: $CH_2(OH)C(OH)(OH)C(OH)(OH)CO(O^-) + HO^• \rightarrow C^•H(OH)C(OH)(OH)C(OH)(OH)CO(O^-) + H_2O$		$3.1\ 10^8$			BR: 26% - 75
$C^•H(OH)C(OH)(OH)C(OH)(OH)CO(O^-) + O_2 \rightarrow CO(O^-)C(OH)(OH)C(OH)(OH)CH(OH)(OO^•)$		$2.0\ 10^9$			3
$CH_2(OH)C(OH)(OH)C(OH)(OH)CO(O^-) + HO^• \rightarrow 0.39\ CO(OH)CO(O^-) + 0.39\ CH_2(OH)C(OH)(OH)(OO^•) + 0.35\ CH_2(OH)CO(OH) + 0.35\ CO(O^-)C(OH)(OH)(OO^•) + 0.26\ CO(O^-)C(OH)(OH)C(OH)(OH)CH(OH)(OO^•) + H_2O - O_2$	R(749)	$1.2\ 10^9$			12
Pathway 1: $CH_2(OH)C(OH)(OH)C(OH)(OH)CO(O^-) + NO_3^• \rightarrow C^•H(OH)C(OH)(OH)C(OH)(OH)CO(O^-) + NO_3^- + H^+$		$1.0\ 10^6$			BR: 100%
$C^•H(OH)C(OH)(OH)C(OH)(OH)CO(O^-) + O_2 \rightarrow CO(O^-)C(OH)(OH)C(OH)(OH)CH(OH)(OO^•)$		$2.0\ 10^9$			3
$CH_2(OH)C(OH)(OH)C(OH)(OH)CO(O^-) + NO_3^• \rightarrow CO(O^-)C(OH)(OH)C(OH)(OH)CH(OH)(OO^•) + NO_3^- + H^+ - O_2$	R(750)	$1.0\ 10^6$			= k(CH(OH)(OH)CH(OH)(OH) + $NO_3^•$) - 13
$CO(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OO^•) + OH^- \rightarrow CO(OH)C(OH)(OH)C(OH)(OH)CH(O^-)(OO^•) + H_2O$		$4.0\ 10^9$			
$CO(OH)C(OH)(OH)C(OH)(OH)CH(O^-)(OO^•) \rightarrow CHOC(OH)(OH)C(OH)(OH)CO(OH) + O_2^{•-}$					16
$CO(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OO^•) + OH^- \rightarrow CHOC(OH)(OH)C(OH)(OH)CO(OH) + O_2^{•-} + H_2O$	R(751)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^•)$ + OH^-)
$CO(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OO^•) \rightarrow CHOC(OH)(OH)C(OH)(OH)CO(OH) + HO_2^•$	R(752)	$1.9\ 10^2$			17
$CO(O^-)COC(OH)(OH)CH(OH)(OO^•) + OH^- \rightarrow CO(O^-)COC(OH)(OH)CH(O^-)(OO^•) + H_2O$		$4.0\ 10^9$			
$CO(O^-)COC(OH)(OH)CH(O^-)(OO^•) \rightarrow CHOC(OH)(OH)COCO(O^-) + O_2^{•-}$					16
$CO(O^-)COC(OH)(OH)CH(OH)(OO^•) + OH^- \rightarrow CHOC(OH)(OH)COCO(O^-) + O_2^{•-} + H_2O$	R(753)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^•)$ + OH^-)
$CO(O^-)COC(OH)(OH)CH(OH)(OO^•) \rightarrow CHOC(OH)(OH)COCO(O^-) + HO_2^•$	R(754)	$1.9\ 10^2$			17

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CO(O^-)C(OH)(OH)C(OH)(OH)CH(OH)(OO^\bullet) + OH^- \rightarrow CO(O^-)C(OH)(OH)C(OH)(OH)CH(O^-)(OO^\bullet) + H_2O$		$4.0\ 10^9$			
$CO(O^-)C(OH)(OH)C(OH)(OH)CH(O^-)(OO^\bullet) \rightarrow CH(OH)(OH)C(OH)(OH)COCO(O^-) + O_2^{\bullet-}$					16
$CO(O^-)C(OH)(OH)C(OH)(OH)CH(OH)(OO^\bullet) \rightarrow CHOC(OH)(OH)C(OH)(OH)CO(O^-) + O_2^{\bullet-} + H_2O$	R(755)	$4.0\ 10^9$			$= k(CH_3CH(OH)(OO^\bullet) + OH^-)$
$CO(O^-)C(OH)(OH)C(OH)(OH)CH(OH)(OO^\bullet) \rightarrow CHOC(OH)(OH)C(OH)(OH)CO(O^-) + HO_2^\bullet$	R(756)	$1.9\ 10^2$			17
Oxidation of 2,3,4-trioxobutanoic acid					76
Pathway 1: $CH(OH)(OH)C(OH)(OH)C(OH)(OH)CO(OH) + HO^\bullet \rightarrow CH(OH)(O^\bullet)C(OH)(OH)C(OH)(OH)CO(OH) + H_2O$		$4.3\ 10^8$			BR: 39% - 77
$CH(OH)(O^\bullet)C(OH)(OH)C(OH)(OH)CO(OH) \rightarrow CHO(OH) + CO(OH)C(OH)(OH)C^\bullet(OH)(OH)$					4 - 5
$CO(OH)C(OH)(OH)C^\bullet(OH)(OH) + O_2 \rightarrow CO(OH)C(OH)(OH)C(OH)(OH)(OO^\bullet)$		$2.0\ 10^9$			3
Pathway 2: $CH(OH)(OH)C(OH)(OH)C(OH)(OH)CO(OH) + HO^\bullet \rightarrow CH(OH)(OH)C(OH)(O^\bullet)C(OH)(OH)CO(OH) + H_2O$		$4.0\ 10^8$			BR: 36% - 77
$CH(OH)(OH)C(OH)(O^\bullet)C(OH)(OH)CO(OH) \rightarrow CH(OH)(OH)CO(OH) + CO(OH)C^\bullet(OH)(OH)$					4 - 5
$CO(OH)C^\bullet(OH)(OH) + O_2 \rightarrow CO(OH)C(OH)(OH)(OO^\bullet)$		$2.0\ 10^9$			3
Pathway 3: $CH(OH)(OH)C(OH)(OH)C(OH)(OH)CO(OH) + HO^\bullet \rightarrow CH(OH)(OH)C(OH)(OH)C(OH)(O^\bullet)CO(OH) + H_2O$		$2.7\ 10^8$			BR: 25% - 77
$CH(OH)(OH)C(OH)(OH)C(OH)(O^\bullet)CO(OH) \rightarrow CH(OH)(OH)C^\bullet(OH)(OH) + CO(OH)CO(OH)$					4 - 5
$CH(OH)(OH)C^\bullet(OH)(OH) + O_2 \rightarrow CH(OH)(OH)C(OH)(OH)(OO^\bullet)$		$2.0\ 10^9$			3
$CH(OH)(OH)C(OH)(OH)C(OH)(OH)CO(OH) + HO^\bullet \rightarrow 0.39\ CHO(OH) + 0.39\ CO(OH)C(OH)(OH)C(OH)(OH)(OO^\bullet) + 0.36\ CH(OH)(OH)CO(OH) + 0.36\ CO(OH)C(OH)(OH)(OO^\bullet) + 0.25\ CO(OH)CO(OH) + 0.25\ CH(OH)(OH)C(OH)(OH)(OO^\bullet) + H_2O - O_2$	R(757)	$1.1\ 10^9$			12
Pathway 1: $CH(OH)(OH)C(OH)(OH)COCO(O^-) + HO^\bullet \rightarrow CH(OH)(O^\bullet)C(OH)(OH)COCO(O^-) + H_2O$		$4.5\ 10^8$			BR: 54% - 78
$CH(OH)(O^\bullet)C(OH)(OH)COCO(O^-) \rightarrow CHO(OH) + CO(O^-)COC^\bullet(OH)(OH)$					4 - 5
$CO(O^-)COC^\bullet(OH)(OH) + O_2 \rightarrow CO(O^-)COC(OH)(OH)(OO^\bullet)$		$2.0\ 10^9$			3
Pathway 2: $CH(OH)(OH)C(OH)(OH)COCO(O^-) + HO^\bullet \rightarrow CH(OH)(OH)C(OH)(O^\bullet)COCO(O^-) + H_2O$		$3.8\ 10^8$			BR: 46% - 78
$CH(OH)(OH)C(OH)(O^\bullet)COCO(O^-) \rightarrow CH(OH)(OH)CO(OH) + CO(O^-)C^\bullet O$					4 - 5
$CO(O^-)C^\bullet O + O_2 \rightarrow CO(O^-)CO(OO^\bullet)$		$2.0\ 10^9$			3
$CH(OH)(OH)C(OH)(OH)COCO(O^-) + HO^\bullet \rightarrow 0.54\ CHO(OH) + 0.54\ CO(O^-)COC(OH)(OH)(OO^\bullet) + 0.46\ CH(OH)(OH)CO(OH) + 0.46\ CO(O^-)CO(OO^\bullet) + H_2O - O_2$	R(758)	$8.3\ 10^8$			12
Pathway 1: $CH(OH)(OH)C(OH)(OH)C(OH)(OH)CO(O^-) + HO^\bullet \rightarrow CH(OH)(OH)C(OH)(OH)C(OH)(O^\bullet)CO(O^-) + H_2O$		$4.7\ 10^8$			BR: 36% - 79
$CH(OH)(OH)C(OH)(OH)C(OH)(O^\bullet)CO(O^-) \rightarrow CH(OH)(OH)C^\bullet(OH)(OH) + CO(OH)CO(O^-)$					4 - 5
$CH(OH)(OH)C^\bullet(OH)(OH) + O_2 \rightarrow CH(OH)(OH)C(OH)(OH)(OO^\bullet)$		$2.0\ 10^9$			3
Pathway 2: $CH(OH)(OH)C(OH)(OH)C(OH)(OH)CO(O^-) + HO^\bullet \rightarrow CH(OH)(O^\bullet)C(OH)(OH)C(OH)(OH)CO(O^-) + H_2O$		$4.3\ 10^8$			BR: 33% - 79
$CH(OH)(O^\bullet)C(OH)(OH)C(OH)(OH)CO(O^-) \rightarrow CHO(OH) + CO(O^-)C(OH)(OH)C^\bullet(OH)(OH)$					4 - 5
$CO(O^-)C(OH)(OH)C^\bullet(OH)(OH) + O_2 \rightarrow CO(O^-)C(OH)(OH)C(OH)(OH)(OO^\bullet)$		$2.0\ 10^9$			3
Pathway 3: $CH(OH)(OH)C(OH)(OH)C(OH)(OH)CO(O^-) + HO^\bullet \rightarrow CH(OH)(OH)C(OH)(O^\bullet)C(OH)(OH)CO(O^-) + H_2O$		$4.0\ 10^8$			BR: 31% - 79
$CH(OH)(OH)C(OH)(O^\bullet)C(OH)(OH)CO(O^-) \rightarrow CH(OH)(OH)CO(OH) + CO(O^-)C^\bullet(OH)(OH)$					4 - 5
$CO(O^-)C^\bullet(OH)(OH) + O_2 \rightarrow CO(O^-)C(OH)(OH)(OO^\bullet)$		$2.0\ 10^9$			3
$CH(OH)(OH)C(OH)(OH)C(OH)(OH)CO(O^-) + HO^\bullet \rightarrow 0.36\ CO(OH)CO(O^-) + 0.36\ CH(OH)(OH)C(OH)(OH)(OO^\bullet) + 0.33\ CHO(OH) + 0.33\ CO(O^-)C(OH)(OH)C(OH)(OH)(OO^\bullet) + 0.31\ CH(OH)(OH)CO(OH) + 0.31\ CO(O^-)C(OH)(OH)(OO^\bullet) + H_2O - O_2$	R(759)	$1.3\ 10^9$			12
Hydrolysis of Methacrylic Acid Epoxide (MAE)					80
$CH_3C1(CO(OH))\text{-}O\text{-}C1H_2 + H^+ \rightarrow CH_2(OH)C(OH)(CH_3)CO(OH) - H_2O + H^+$	R(760)	$5.9\ 10^{-5}$		Birdsall et al., 2014	
Hydrolysis of Hydroxymethyl-methyl-α-lactone (HMML)					81
$CH_3C1(CH_2(OH))\text{-}O\text{-}C1O \rightarrow CH_2(OH)C(OH)(CH_3)CO(OH) - H_2O$	R(761)	$1.0\ 10^6$			82
Oxidation of 2- Methylglyceric Acid (2-MG)					83
Pathway 1: $CH_2(OH)C(OH)(CH_3)CO(OH) + HO^\bullet \rightarrow C^\bullet H(OH)C(OH)(CH_3)CO(OH) + H_2O$		$6.1\ 10^8$			BR: 80% - 84
$C^\bullet H(OH)C(OH)(CH_3)CO(OH) + O_2 \rightarrow CH(OH)(OO^\bullet)C(OH)(CH_3)CO(OH)$		$2.0\ 10^9$			3
Pathway 2: $CH_2(OH)C(OH)(CH_3)CO(OH) + HO^\bullet \rightarrow CH_2(OH)C(OH)(C^\bullet H_2)CO(OH) + H_2O$		$1.5\ 10^8$			BR: 20% - 84

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CH_2(OH)C(OH)(C^{\bullet}H_2)CO(OH)+ O_2 \rightarrow CH_2(OH)C(OH)(CH_2(OO^{\bullet}))CO(OH)$		$2.0\ 10^9$			3
$CH_2(OH)C(OH)(CH_3)CO(OH) + HO^{\bullet} \rightarrow 0.80\ CH(OH)(OO^{\bullet})C(OH)(CH_3)CO(OH) + 0.20\ CH_2(OH)C(OH)(CH_2(OO^{\bullet}))CO(OH) + H_2O - O_2$	R(762)	$7.6\ 10^8$			12
Pathway 1: $CH_2(OH)C(OH)(CH_3)CO(OH) + NO_3^{\bullet} \rightarrow C^{\bullet}H(OH)C(OH)(CH_3)CO(OH) + NO_3^- + H^+$		$8.0\ 10^5$			BR: 80%
$C^{\bullet}H(OH)C(OH)(CH_3)CO(OH) + O_2 \rightarrow CH(OH)(OO^{\bullet})C(OH)(CH_3)CO(OH)$		$2.0\ 10^9$			3
Pathway 2: $CH_2(OH)C(OH)(CH_3)CO(OH) + NO_3^{\bullet} \rightarrow CH_2(OH)C(OH)(C^{\bullet}H_2)CO(OH) + NO_3^- + H^+$		$2.0\ 10^5$			BR:20%
$CH_2(OH)C(OH)(C^{\bullet}H_2)CO(OH)+ O_2 \rightarrow CH_2(OH)C(OH)(CH_2(OO^{\bullet}))CO(OH)$		$2.0\ 10^9$			3
$CH_2(OH)C(OH)(CH_3)CO(OH) + NO_3^{\bullet} \rightarrow 0.80\ CH(OH)(OO^{\bullet})C(OH)(CH_3)CO(OH) + 0.20\ CH_2(OH)C(OH)(CH_2(OO^{\bullet}))CO(OH) + NO_3^- + H^+ - O_2$	R(763)	$1.0\ 10^6$			= k(CH(OH)(OH)CH(OH)(OH) + $NO_3^{\bullet}$) - 13
Pathway 1: $CH_2(OH)C(OH)(CH_3)CO(O^-) + HO^{\bullet} \rightarrow C^{\bullet}H(OH)C(OH)(CH_3)CO(O^-) + H_2O$		$1.1\ 10^9$			BR: 81% - 85
$C^{\bullet}H(OH)C(OH)(CH_3)CO(O^-) + O_2 \rightarrow CH(OH)(OO^{\bullet})C(OH)(CH_3)CO(O^-)$		$2.0\ 10^9$			3
Pathway 2: $CH_2(OH)C(OH)(CH_3)CO(O^-) + HO^{\bullet} \rightarrow CH_2(OH)C(OH)(C^{\bullet}H_2)CO(O^-) + H_2O$		$3.0\ 10^8$			BR: 19% - 85
$CH_2(OH)C(OH)(C^{\bullet}H_2)CO(O^-) + O_2 \rightarrow CH_2(OH)C(OH)(CH_2(OO^{\bullet}))CO(O^-)$		$2.0\ 10^9$			3
$CH_2(OH)C(OH)(CH_3)CO(O^-) + HO^{\bullet} \rightarrow 0.81\ CH(OH)(OO^{\bullet})C(OH)(CH_3)CO(O^-) + 0.19\ CH_2(OH)C(OH)(CH_2(OO^{\bullet}))CO(O^-) + H_2O - O_2$	R(764)	$1.4\ 10^9$			12
Pathway 1: $CH_2(OH)C(OH)(CH_3)CO(O^-) + NO_3^{\bullet} \rightarrow C^{\bullet}H(OH)C(OH)(CH_3)CO(O^-) + NO_3^- + H^+$		$8.1\ 10^5$			BR: 81%
$C^{\bullet}H(OH)C(OH)(CH_3)CO(O^-) + O_2 \rightarrow CH(OH)(OO^{\bullet})C(OH)(CH_3)CO(O^-)$		$2.0\ 10^9$			3
Pathway 2: $CH_2(OH)C(OH)(CH_3)CO(O^-) + NO_3^{\bullet} \rightarrow CH_2(OH)C(OH)(C^{\bullet}H_2)CO(O^-) + NO_3^- + H^+$		$1.9\ 10^5$			BR: 19%
$CH_2(OH)C(OH)(C^{\bullet}H_2)CO(O^-) + O_2 \rightarrow CH_2(OH)C(OH)(CH_2(OO^{\bullet}))CO(O^-)$		$2.0\ 10^9$			3
$CH_2(OH)C(OH)(CH_3)CO(O^-) + NO_3^{\bullet} \rightarrow 0.81\ CH(OH)(OO^{\bullet})C(OH)(CH_3)CO(O^-) + 0.19\ CH_2(OH)C(OH)(CH_2(OO^{\bullet}))CO(O^-) + NO_3^- + H^+ - O_2$		$1.0\ 10^6$			= k(CH(OH)(OH)CH(OH)(OH) + $NO_3^{\bullet}$) - 13
$CH(OH)(OO^{\bullet})C(OH)(CH_3)CO(OH) + OH^- \rightarrow CH(O^-)(OO^{\bullet})C(OH)(CH_3)CO(OH) + H_2O$		$4.0\ 10^9$			
$CH(O^-)(OO^{\bullet})C(OH)(CH_3)CO(OH) \rightarrow CHOC(OH)(CH_3)CO(OH) + O_2^{\bullet-}$					16
$CH(OH)(OO^{\bullet})C(OH)(CH_3)CO(OH) + OH^- \rightarrow CHOC(OH)(CH_3)CO(OH) + O_2^{\bullet-} + H_2O$	R(765)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^{\bullet}) + OH^-$)
$CH(OH)(OO^{\bullet})C(OH)(CH_3)CO(OH) \rightarrow CHOC(OH)(CH_3)CO(OH) + HO_2^{\bullet}$	R(766)	$1.9\ 10^2$			17
$CH(OH)(OO^{\bullet})C(OH)(CH_3)CO(O^-) + OH^- \rightarrow CH(O^-)(OO^{\bullet})C(OH)(CH_3)CO(O^-) + H_2O$		$4.0\ 10^9$			
$CH(O^-)(OO^{\bullet})C(OH)(CH_3)CO(O^-) \rightarrow CHOC(OH)(CH_3)CO(O^-) + O_2^{\bullet-}$					16
$CH(OH)(OO^{\bullet})C(OH)(CH_3)CO(O^-) + OH^- \rightarrow CHOC(OH)(CH_3)CO(O^-) + O_2^{\bullet-} + H_2O$	R(767)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^{\bullet}) + OH^-$)
$CH(OH)(OO^{\bullet})C(OH)(CH_3)CO(O^-) \rightarrow CHOC(OH)(CH_3)CO(O^-) + HO_2^{\bullet}$	R(768)	$1.9\ 10^2$			17
Pathway 1: $2\ CH_2(OH)C(OH)(CH_2(OO^{\bullet}))CO(OH) \rightarrow 2\ CHOC(OH)(CH_2(OH))CO(OH) + H_2O_2$		$5.0\ 10^7$			BR: 50%
Pathway 2:2 $CH_2(OH)C(OH)(CH_2(OO^{\bullet}))CO(OH) \rightarrow CHOC(OH)(CH_2(OH))CO(OH) + CH_2(OH)C(OH)(CH_2(OH))CO(OH) + O_2$		$3.3\ 10^7$			BR: 33%
Pathway 3: $2\ CH_2(OH)C(OH)(CH_2(OO^{\bullet}))CO(OH) \rightarrow 2\ CH_2(OH)C(OH)(CH_2(O^{\bullet}))CO(OH) + O_2$		$1.7\ 10^7$			BR: 17%
$CH_2(OH)C(OH)(CH_2(O^{\bullet}))CO(OH) \rightarrow CH_2(OH)C^{\bullet}(OH)CO(OH) + CH_2O$					4 - 5
$CH_2(OH)C^{\bullet}(OH)CO(OH) + O_2 \rightarrow CH_2(OH)C(OH)(OO^{\bullet})CO(OH)$		$2.0\ 10^9$			3
$2\ CH_2(OH)C(OH)(CH_2(OO^{\bullet}))CO(OH) \rightarrow 1.33\ CHOC(OH)(CH_2(OH))CO(OH) + 0.33\ CH_2(OH)C(OH)(CH_2(OH))CO(OH) + 0.34\ CH_2(OH)C(OH)(OO^{\bullet})CO(OH) + 0.34\ CH_2O + 0.50\ H_2O_2 + 0.16\ O_2$	R(769)	$1.0\ 10^8$			= k($2\ CH_2(OH)CH_2(OO^{\bullet})$) - 6
Pathway 1: $2\ CH_2(OH)C(OH)(CH_2(OO^{\bullet}))CO(O^-) \rightarrow 2\ CHOC(OH)(CH_2(OH))CO(O^-) + H_2O_2$		$5.0\ 10^7$			BR: 50%
Pathway 2:2 $CH_2(OH)C(OH)(CH_2(OO^{\bullet}))CO(O^-) \rightarrow CHOC(OH)(CH_2(OH))CO(O^-) + CH_2(OH)C(OH)(CH_2(OH))CO(O^-) + O_2$		$3.3\ 10^7$			BR: 33%
Pathway 3: $2\ CH_2(OH)C(OH)(CH_2(OO^{\bullet}))CO(O^-) \rightarrow 2\ CH_2(OH)C(OH)(CH_2(O^{\bullet}))CO(O^-) + O_2$		$1.7\ 10^7$			BR: 17%
$CH_2(OH)C(OH)(CH_2(O^{\bullet}))CO(O^-) \rightarrow CH_2(OH)C^{\bullet}(OH)CO(O^-) + CH_2O$					4 - 5
$CH_2(OH)C^{\bullet}(OH)CO(O^-) + O_2 \rightarrow CH_2(OH)C(OH)(OO^{\bullet})CO(O^-)$		$2.0\ 10^9$			3
$2\ CH_2(OH)C(OH)(CH_2(OO^{\bullet}))CO(O^-) \rightarrow 1.33\ CHOC(OH)(CH_2(OH))CO(O^-) + 0.33\ CH_2(OH)C(OH)(CH_2(OH))CO(O^-) + 0.34\ CH_2(OH)C(OH)(OO^{\bullet})CO(O^-) + 0.34\ CH_2O + 0.50\ H_2O_2 + 0.16\ O_2$	R(770)	$1.0\ 10^8$			= k($2\ CH_2(OH)CH_2(OO^{\bullet})$) - 6
2-hydroxy,3-oxomethylpropanoic acid					86
Pathway 1: $CH(OH)(OH)C(OH)(CH_3)CO(OH) + HO^{\bullet} \rightarrow CH(OH)(O^{\bullet})C(OH)(CH_3)CO(OH) + H_2O$		$4.7\ 10^8$			BR: 61% - 87
$CH(OH)(O^{\bullet})C(OH)(CH_3)CO(OH) \rightarrow CHO(OH) + CH_3C^{\bullet}(OH)CO(OH)$					4 - 5

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CH_3C^{\bullet}(OH)CO(OH) + O_2 \rightarrow CH_3C(OH)(OO^{\bullet})CO(OH)$		$2.0\ 10^9$			3
Pathway 2: $CH(OH)(OH)C(OH)(CH_3)CO(OH) + HO^{\bullet} \rightarrow C^{\bullet}(OH)(OH)C(OH)(CH_3)CO(OH) + H_2O$		$3.0\ 10^8$			BR: 39% - 87
$C^{\bullet}(OH)(OH)C(OH)(CH_3)CO(OH) + O_2 \rightarrow C(OH)(OH)(OO^{\bullet})C(OH)(CH_3)CO(OH)$		$2.0\ 10^9$			3
$CH(OH)(OH)C(OH)(CH_3)CO(OH) + HO^{\bullet} \rightarrow 0.61\ CHO(OH) + 0.61\ CH_3C(OH)(OO^{\bullet})CO(OH) + 0.39\ C(OH)(OH)(OO^{\bullet})C(OH)(CH_3)CO(OH) + H_2O - O_2$	R(771)	$7.7\ 10^8$			12
Pathway 1: $CH(OH)(OH)C(OH)(CH_3)CO(OH) + NO_3^{\bullet} \rightarrow C^{\bullet}(OH)(OH)C(OH)(CH_3)CO(OH) + NO_3^- + H^+$		$1.0\ 10^6$			BR: 100%
$C^{\bullet}(OH)(OH)C(OH)(CH_3)CO(OH) + O_2 \rightarrow C(OH)(OH)(OO^{\bullet})C(OH)(CH_3)CO(OH)$		$2.0\ 10^9$			3
$CH(OH)(OH)C(OH)(CH_3)CO(OH) + NO_3^{\bullet} \rightarrow C(OH)(OH)(OO^{\bullet})C(OH)(CH_3)CO(OH) + NO_3^- + H^+ - O_2$	R(772)	$1.0\ 10^6$			= k(CH(OH)(OH)CH(OH)(OH) + $NO_3^{\bullet}$) - 13
Pathway 1: $CH(OH)(OH)C(OH)(CH_3)CO(O^-) + HO^{\bullet} \rightarrow C^{\bullet}(OH)(OH)C(OH)(CH_3)CO(O^-) + H_2O$		$4.9\ 10^8$			BR: 41% - 88
$C^{\bullet}(OH)(OH)C(OH)(CH_3)CO(O^-) + O_2 \rightarrow C(OH)(OH)(OO^{\bullet})C(OH)(CH_3)CO(O^-)$		$2.0\ 10^9$			3
Pathway 2: $CH(OH)(OH)C(OH)(CH_3)CO(O^-) + HO^{\bullet} \rightarrow CH(OH)(O^{\bullet})C(OH)(CH_3)CO(O^-) + H_2O$		$4.6\ 10^8$			BR: 38% - 88
$CH(OH)(O^{\bullet})C(OH)(CH_3)CO(O^-) \rightarrow CHO(OH) + CH_3C^{\bullet}(OH)CO(O^-)$					4 - 5
$CH_3C^{\bullet}(OH)CO(O^-) + O_2 \rightarrow CH_3C(OH)(OO^{\bullet})CO(O^-)$		$2.0\ 10^9$			3
Pathway 3: $CH(OH)(OH)C(OH)(CH_3)CO(O^-) + HO^{\bullet} \rightarrow CH(OH)(OH)C(OH)(C^{\bullet}H_2)CO(O^-) + H_2O$		$2.5\ 10^8$			BR: 21% - 88
$CH(OH)(OH)C(OH)(C^{\bullet}H_2)CO(O^-) + O_2 \rightarrow CH(OH)(OH)C(OH)(CH_2(OO^{\bullet}))CO(O^-)$		$2.0\ 10^9$			3
$CH(OH)(OH)C(OH)(CH_3)CO(O^-) + HO^{\bullet} \rightarrow 0.41\ C(OH)(OH)(OO^{\bullet})C(OH)(CH_3)CO(O^-) + 0.38\ CHO(OH) + 0.38\ CH_3C(OH)(OO^{\bullet})CO(O^-) + 0.21\ CH(OH)(OH)C(OH)(CH_2(OO^{\bullet}))CO(O^-) + H_2O - O_2$	R(773)	$1.2\ 10^9$			12
Pathway 1: $CH(OH)(OH)C(OH)(CH_3)CO(O^-) + NO_3^{\bullet} \rightarrow C^{\bullet}(OH)(OH)C(OH)(CH_3)CO(O^-) + NO_3^- + H^+$		$6.7\ 10^5$			BR: 67%
$C^{\bullet}(OH)(OH)C(OH)(CH_3)CO(O^-) + O_2 \rightarrow C(OH)(OH)(OO^{\bullet})C(OH)(CH_3)CO(O^-)$		$2.0\ 10^9$			3
Pathway 2: $CH(OH)(OH)C(OH)(CH_3)CO(O^-) + NO_3^{\bullet} \rightarrow CH(OH)(OH)C(OH)(C^{\bullet}H_2)CO(O^-) + NO_3^- + H^+$		$3.3\ 10^5$			BR: 33%
$CH(OH)(OH)C(OH)(C^{\bullet}H_2)CO(O^-) + O_2 \rightarrow CH(OH)(OH)C(OH)(CH_2(OO^{\bullet}))CO(O^-)$		$2.0\ 10^9$			3
$CH(OH)(OH)C(OH)(CH_3)CO(O^-) + NO_3^{\bullet} \rightarrow 0.67\ C(OH)(OH)(OO^{\bullet})C(OH)(CH_3)CO(O^-) + 0.33\ CH(OH)(OH)C(OH)(CH_2(OO^{\bullet}))CO(O^-) + NO_3^- + H^+ - O_2$	R(774)	$1.0\ 10^6$			= k(CH(OH)(OH)CH(OH)(OH) + $NO_3^{\bullet}$) - 13
$C(OH)(OH)(OO^{\bullet})C(OH)(CH_3)CO(OH) + OH^- \rightarrow C(OH)(O^-)(OO^{\bullet})C(OH)(CH_3)CO(OH) + H_2O$		$4.0\ 10^9$			
$C(OH)(O^-)(OO^{\bullet})C(OH)(CH_3)CO(OH) \rightarrow CO(OH)C(OH)(CH_3)CO(OH) + O_2^{\bullet-}$					16
$C(OH)(OH)(OO^{\bullet})C(OH)(CH_3)CO(OH) + OH^- \rightarrow CO(OH)C(OH)(CH_3)CO(OH) + O_2^{\bullet-} + H_2O$	R(775)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^{\bullet})$ + OH^-)
$C(OH)(OH)(OO^{\bullet})C(OH)(CH_3)CO(OH) \rightarrow CO(OH)C(OH)(CH_3)CO(OH) + HO_2^{\bullet}$	R(776)	$1.0\ 10^6$			27
$C(OH)(OH)(OO^{\bullet})C(OH)(CH_3)CO(O^-) + OH^- \rightarrow C(OH)(O^-)(OO^{\bullet})C(OH)(CH_3)CO(O^-) + H_2O$		$4.0\ 10^9$			
$C(OH)(O^-)(OO^{\bullet})C(OH)(CH_3)CO(O^-) \rightarrow CO(OH)C(OH)(CH_3)CO(O^-) + O_2^{\bullet-}$					16
$C(OH)(OH)(OO^{\bullet})C(OH)(CH_3)CO(O^-) + OH^- \rightarrow CO(OH)C(OH)(CH_3)CO(O^-) + O_2^{\bullet-} + H_2O$	R(777)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^{\bullet})$ + OH^-)
$C(OH)(OH)(OO^{\bullet})C(OH)(CH_3)CO(O^-) \rightarrow CO(OH)C(OH)(CH_3)CO(O^-) + HO_2^{\bullet}$	R(778)	$1.0\ 10^6$			27
Pathway 1: $2\ CH(OH)(OH)C(OH)(CH_2(OO^{\bullet}))CO(OH) \rightarrow 2\ CH(OH)(OH)C(OH)(CHO)CO(OH) + H_2O_2$		$5.0\ 10^7$			BR: 50%
Pathway 2:2 $CH(OH)(OH)C(OH)(CH_2(OO^{\bullet}))CO(OH) \rightarrow CH(OH)(OH)C(OH)(CHO)CO(OH) + CH(OH)(OH)C(OH)(CH_2(OH))CO(OH) + O_2$		$3.3\ 10^7$			BR: 33%
Pathway 3: $2\ CH(OH)(OH)C(OH)(CH_2(OO^{\bullet}))CO(OH) \rightarrow 2\ CH(OH)(OH)C(OH)(CH_2(O^{\bullet}))CO(OH) + O_2$		$1.7\ 10^7$			BR: 17%
$CH(OH)(OH)C(OH)(CH_2(O^{\bullet}))CO(OH) \rightarrow CH(OH)(OH)C^{\bullet}(OH)CO(OH) + CH_2O$					4 - 5
$CH(OH)(OH)C^{\bullet}(OH)CO(OH) + O_2 \rightarrow CH(OH)(OH)C(OH)(OO^{\bullet})CO(OH)$		$2.0{\cdot}10^9$			3
$2\ CH(OH)(OH)C(OH)(CH_2(OO^{\bullet}))CO(OH) \rightarrow 1.33\ CH(OH)(OH)C(OH)(CHO)CO(OH) + 0.33\ CH(OH)(OH)C(OH)(CH_2(OH))CO(OH) + 0.34\ CH(OH)(OH)C(OH)(OO^{\bullet})CO(OH) + 0.34\ CH_2O + 0.50\ H_2O_2 + 0.16\ O_2$	R(779)	$1.0\ 10^8$			= k(2 $CH_2(OH)CH_2(OO^{\bullet})$) - 6
Pathway 1: $2\ CH(OH)(OH)C(OH)(CH_2(OO^{\bullet}))CO(O^-) \rightarrow 2\ CH(OH)(OH)C(OH)(CHO)CO(O^-) + H_2O_2$		$5.0\ 10^7$			BR: 50%
Pathway 2:2 $CH(OH)(OH)C(OH)(CH_2(OO^{\bullet}))CO(O^-) \rightarrow CH(OH)(OH)C(OH)(CHO)CO(O^-) + CH(OH)(OH)C(OH)(CH_2(OH))CO(O^-) + O_2$		$3.3\ 10^7$			BR: 33%
Pathway 3: $2\ CH(OH)(OH)C(OH)(CH_2(OO^{\bullet}))CO(O^-) \rightarrow 2\ CH(OH)(OH)C(OH)(CH_2(O^{\bullet}))CO(O^-) + O_2$		$1.7\ 10^7$			BR: 17%
$CH(OH)(OH)C(OH)(CH_2(O^{\bullet}))CO(O^-) \rightarrow CH(OH)(OH)C^{\bullet}(OH)CO(O^-) + CH_2O$					4 - 5
$CH(OH)(OH)C^{\bullet}(OH)CO(O^-) + O_2 \rightarrow CH(OH)(OH)C(OH)(OO^{\bullet})CO(O^-)$		$2.0{\cdot}10^9$			3
$2\ CH(OH)(OH)C(OH)(CH_2(OO^{\bullet}))CO(O^-) \rightarrow 1.33\ CH(OH)(OH)C(OH)(CHO)CO(O^-) + 0.33\ CH(OH)(OH)C(OH)(CH_2(OH))CO(O^-) + 0.34\ CH(OH)(OH)C(OH)(OO^{\bullet})CO(O^-) + 0.34\ CH_2O + 0.50\ H_2O_2 + 0.16\ O_2$	R(780)	$1.0\ 10^8$			= k(2 $CH_2(OH)CH_2(OO^{\bullet})$) - 6

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
2-hydroxy-2-(hydroxymethyl)-3-oxopropanoic acid					89
Pathway 1: CH(OH)(OH)C(OH)(CH_2(OH))CO(OH) + HO$^\bullet$ → CH(OH)(OH)C(OH)(C$^\bullet$H(OH))CO(OH) + H_2O		5.3 10^8			BR: 43% - 90
CH(OH)(OH)C(OH)(C$^\bullet$H(OH))CO(OH) + O_2 → CH(OH)(OH)C(OH)(CH(OH)(OO$^\bullet$))CO(OH)		2.0 10^9			3
Pathway 2: CH(OH)(OH)C(OH)(CH_2(OH))CO(OH) + HO$^\bullet$ → CH(OH)(O$^\bullet$)C(OH)(CH_2(OH))CO(OH) + H_2O		4.2 10^8			BR: 35% - 90
CH(OH)(O$^\bullet$)C(OH)(CH_2(OH))CO(OH) → CHO(OH) + CH_2(OH)C$^\bullet$(OH)CO(OH)					4 - 5
CH_2(OH)C$^\bullet$(OH)CO(OH) + O_2 → CH_2(OH)C(OH)(OO$^\bullet$)CO(OH)		2.0 10^9			3
Pathway 3: CH(OH)(OH)C(OH)(CH_2(OH))CO(OH) + HO$^\bullet$ → C$^\bullet$(OH)(OH)C(OH)(CH_2(OH))CO(OH) + H_2O		2.5 10^8			BR: 22% - 90
C$^\bullet$(OH)(OH)C(OH)(CH_2(OH))CO(OH) + O_2 → C(OH)(OH)(OO$^\bullet$)C(OH)(CH_2(OH))CO(OH)		2.0 10^9			3
CH(OH)(OH)C(OH)(CH_2(OH))CO(OH) + HO$^\bullet$ → 0.43 CH(OH)(OH)C(OH)(CH(OH)(OO$^\bullet$))CO(OH) + 0.35 CHO(OH) + 0.35 CH_2(OH)C(OH)(OO$^\bullet$)CO(OH) + 0.22 C(OH)(OH)(OO$^\bullet$)C(OH)(CH_2(OH))CO(OH) + H_2O - O_2	R(781)	1.2 10^9			12
Pathway 1: CH(OH)(OH)C(OH)(CH_2(OH))CO(OH) + $NO_3^\bullet$ → CH(OH)(OH)C(OH)(C$^\bullet$H(OH))CO(OH) + NO_3^- + H^+		6.7 10^5			BR: 67%
CH(OH)(OH)C(OH)(C$^\bullet$H(OH))CO(OH) + O_2 → CH(OH)(OH)C(OH)(CH(OH)(OO$^\bullet$))CO(OH)		2.0 10^9			3
Pathway 2: CH(OH)(OH)C(OH)(CH_2(OH))CO(OH) + $NO_3^\bullet$ → C$^\bullet$(OH)(OH)C(OH)(CH_2(OH))CO(OH) + NO_3^- + H^+		3.3 10^5			BR: 33%
C$^\bullet$(OH)(OH)C(OH)(CH_2(OH))CO(OH) + O_2 → C(OH)(OH)(OO$^\bullet$)C(OH)(CH_2(OH))CO(OH)		2.0 10^9			3
CH(OH)(OH)C(OH)(CH_2(OH))CO(OH) + $NO_3^\bullet$ → 0.67 CH(OH)(OH)C(OH)(CH(OH)(OO$^\bullet$))CO(OH) + 0.33 C(OH)(OH)(OO$^\bullet$)C(OH)(CH_2(OH))CO(OH) + NO_3^- + H^+ - O_2	R(782)	1.0 10^6			= k(CH(OH)(OH)CH(OH)(OH) + $NO_3^\bullet$) - 13
Pathway 1: CH(OH)(OH)C(OH)(CH_2(OH))CO(O^-) + HO$^\bullet$ → CH(OH)(OH)C(OH)(C$^\bullet$H(OH))CO(O^-) + H_2O		9.2 10^8			BR: 51% - 91
CH(OH)(OH)C(OH)(C$^\bullet$H(OH))CO(O^-) + O_2 → CH(OH)(OH)C(OH)(CH(OH)(OO$^\bullet$))CO(O^-)		2.0 10^9			3
Pathway 2: CH(OH)(OH)C(OH)(CH_2(OH))CO(O^-) + HO$^\bullet$ → C$^\bullet$(OH)(OH)C(OH)(CH_2(OH))CO(O^-) + H_2O		4.5 10^8			BR: 25% - 91
C$^\bullet$(OH)(OH)C(OH)(CH_2(OH))CO(O^-) + O_2 → C(OH)(OH)(OO$^\bullet$)C(OH)(CH_2(OH))CO(O^-)		2.0 10^9			3
Pathway 3: CH(OH)(OH)C(OH)(CH_2(OH))CO(O^-) + HO$^\bullet$ → CH(OH)(O$^\bullet$)C(OH)(CH_2(OH))CO(O^-) + H_2O		4.3 10^8			BR: 24% - 91
CH(OH)(O$^\bullet$)C(OH)(CH_2(OH))CO(O^-) → CHO(OH) + CH_2(OH)C$^\bullet$(OH)CO(O^-)					4 -5
CH_2(OH)C$^\bullet$(OH)CO(O^-) + O_2 → CH_2(OH)C(OH)(OO$^\bullet$)CO(O^-)		2.0 10^9			3
CH(OH)(OH)C(OH)(CH_2(OH))CO(O^-) + HO$^\bullet$ → 0.51 CH(OH)(OH)C(OH)(CH(OH)(OO$^\bullet$))CO(O^-) + 0.25 C(OH)(OH)(OO$^\bullet$)C(OH)(CH_2(OH))CO(O^-) + 0.24 CHO(OH) + 0.24 CH_2(OH)C(OH)(OO$^\bullet$)CO(O^-) + H_2O - O_2	R(783)	1.8 10^9			12
Pathway 1: CH(OH)(OH)C(OH)(CH_2(OH))CO(O^-) + $NO_3^\bullet$ → CH(OH)(OH)C(OH)(C$^\bullet$H(OH))CO(O^-) + NO_3^- + H^+		6.7 10^5			BR: 67%
CH(OH)(OH)C(OH)(C$^\bullet$H(OH))CO(O^-) + O_2 → CH(OH)(OH)C(OH)(CH(OH)(OO$^\bullet$))CO(O^-)		2.0 10^9			3
Pathway 2: CH(OH)(OH)C(OH)(CH_2(OH))CO(O^-) + $NO_3^\bullet$ → C$^\bullet$(OH)(OH)C(OH)(CH_2(OH))CO(O^-) + NO_3^- + H^+		3.3 10^5			BR: 33%
C$^\bullet$(OH)(OH)C(OH)(CH_2(OH))CO(O^-) + O_2 → C(OH)(OH)(OO$^\bullet$)C(OH)(CH_2(OH))CO(O^-)		2.0 10^9			3
CH(OH)(OH)C(OH)(CH_2(OH))CO(O^-) + $NO_3^\bullet$ → 0.67 CH(OH)(OH)C(OH)(CH(OH)(OO$^\bullet$))CO(O^-) + 0.33 C(OH)(OH)(OO$^\bullet$)C(OH)(CH_2(OH))CO(O^-) + NO_3^- + H^+ - O_2	R(784)	1.0 10^6			= k(CH(OH)(OH)CH(OH)(OH) + $NO_3^\bullet$) - 13
CH(OH)(OH)C(OH)(CH(OH)(OO$^\bullet$))CO(OH) + OH^- → CH(OH)(OH)C(OH)(CH(O^-)(OO$^\bullet$))CO(OH) + H_2O		4.0 10^9			
CH(OH)(OH)C(OH)(CH(O^-)(OO$^\bullet$))CO(OH) → CH(OH)(OH)C(OH)(CHO)CO(OH) + $O_2^{\bullet-}$					16
CH(OH)(OH)C(OH)(CH(OH)(OO$^\bullet$))CO(OH) + OH^- → CH(OH)(OH)C(OH)(CHO)CO(OH) + $O_2^{\bullet-}$ + H_2O	R(785)	4.0 10^9			= k(CH_3CH(OH)(OO$^\bullet$) + OH^-)
CH(OH)(OH)C(OH)(CH(OH)(OO$^\bullet$))CO(OH) → CH(OH)(OH)C(OH)(CHO)CO(OH) + $HO_2^\bullet$	R(786)	1.9 10^2			17
CH(OH)(OH)C(OH)(CH(OH)(OO$^\bullet$))CO(O^-) + OH^- → CH(OH)(OH)C(OH)(CH(O^-)(OO$^\bullet$))CO(O^-) + H_2O		4.0 10^9			
CH(OH)(OH)C(OH)(CH(O^-)(OO$^\bullet$))CO(O^-) → CH(OH)(OH)C(OH)(CHO)CO(O^-) + $O_2^{\bullet-}$					16
CH(OH)(OH)C(OH)(CH(OH)(OO$^\bullet$))CO(O^-) + OH^- → CH(OH)(OH)C(OH)(CHO)CO(O^-) + $O_2^{\bullet-}$ + H_2O	R(787)	4.0 10^9			= k(CH_3CH(OH)(OO$^\bullet$) + OH^-)
CH(OH)(OH)C(OH)(CH(OH)(OO$^\bullet$))CO(O^-) → CH(OH)(OH)C(OH)(CHO)CO(O^-) + $HO_2^\bullet$	R(788)	1.9 10^2			17
C(OH)(OH)(OO$^\bullet$)C(OH)(CH_2(OH))CO(OH) + OH^- → C(OH)(O^-)(OO$^\bullet$)C(OH)(CH_2(OH))CO(OH) + H_2O		4.0 10^9			
C(OH)(O^-)(OO$^\bullet$)C(OH)(CH_2(OH))CO(OH) → CO(OH)C(OH)(CH_2(OH))CO(OH) + $O_2^{\bullet-}$					16
C(OH)(OH)(OO$^\bullet$)C(OH)(CH_2(OH))CO(OH) + OH^- → CO(OH)C(OH)(CH_2(OH))CO(OH) + $O_2^{\bullet-}$ + H_2O	R(789)	4.0 10^9			= k(CH_3CH(OH)(OO$^\bullet$) + OH^-)
C(OH)(OH)(OO$^\bullet$)C(OH)(CH_2(OH))CO(OH) → CO(OH)C(OH)(CH_2(OH))CO(OH) + $HO_2^\bullet$	R(790)	1.0 10^6			27
C(OH)(OH)(OO$^\bullet$)C(OH)(CH_2(OH))CO(O^-) + OH^- → C(OH)(O^-)(OO$^\bullet$)C(OH)(CH_2(OH))CO(O^-) + H_2O		4.0 10^9			
C(OH)(O^-)(OO$^\bullet$)C(OH)(CH_2(OH))CO(O^-) → CO(OH)C(OH)(CH_2(OH))CO(O^-) + $O_2^{\bullet-}$					16
C(OH)(OH)(OO$^\bullet$)C(OH)(CH_2(OH))CO(O^-) + OH^- → CO(OH)C(OH)(CH_2(OH))CO(O^-) + $O_2^{\bullet-}$ + H_2O	R(791)	4.0 10^9			= k(CH_3CH(OH)(OO$^\bullet$) + OH^-)

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$C(OH)(OH)(OO^{\bullet})C(OH)(CH_2(OH))CO(O^-) \rightarrow CO(OH)C(OH)(CH_2(OH))CO(O^-) + HO_2^{\bullet}$	R(792)	$1.0\ 10^6$			27
2,3-hydroxy-2-(hydroxymethyl)-propanoic acid					92
Pathway 1: $CH_2(OH)C(OH)(CH_2(OH))CO(OH) + HO^{\bullet} \rightarrow C^{\bullet}H(OH)C(OH)(CH_2(OH))CO(OH) + H_2O$		$1.2\ 10^9$			BR: 100% - 93
$C^{\bullet}H(OH)C(OH)(CH_2(OH))CO(OH) + O_2 \rightarrow CH(OH)(OO^{\bullet})C(OH)(CH_2(OH))CO(OH)$		$2.0\ 10^9$			3
$CH_2(OH)C(OH)(CH_2(OH))CO(OH) + HO^{\bullet} \rightarrow CH(OH)(OO^{\bullet})C(OH)(CH_2(OH))CO(OH) + H_2O - O_2$	R(793)	$1.2\ 10^9$			12
Pathway 1: $CH_2(OH)C(OH)(CH_2(OH))CO(OH) + NO_3^{\bullet} \rightarrow C^{\bullet}H(OH)C(OH)(CH_2(OH))CO(OH) + NO_3^- + H^+$		$1.0\ 10^6$			BR: 100%
$C^{\bullet}H(OH)C(OH)(CH_2(OH))CO(OH) + O_2 \rightarrow CH(OH)(OO^{\bullet})C(OH)(CH_2(OH))CO(OH)$		$2.0\ 10^9$			3
$CH_2(OH)C(OH)(CH_2(OH))CO(OH) + NO_3^{\bullet} \rightarrow CH(OH)(OO^{\bullet})C(OH)(CH_2(OH))CO(OH) + NO_3^- + H^+ - O_2$	R(794)	$1.0\ 10^6$			= k(CH(OH)(OH)CH(OH)(OH) + $NO_3^{\bullet}$) - 13
Pathway 1: $CH_2(OH)C(OH)(CH_2(OH))CO(O^-) + HO^{\bullet} \rightarrow C^{\bullet}H(OH)C(OH)(CH_2(OH))CO(O^-) + H_2O$		$2.0\ 10^9$			BR: 100% - 94
$C^{\bullet}H(OH)C(OH)(CH_2(OH))CO(O^-) + O_2 \rightarrow CH(OH)(OO^{\bullet})C(OH)(CH_2(OH))CO(O^-)$		$2.0\ 10^9$			3
$CH_2(OH)C(OH)(CH_2(OH))CO(O^-) + HO^{\bullet} \rightarrow CH(OH)(OO^{\bullet})C(OH)(CH_2(OH))CO(O^-) + H_2O - O_2$	R(795)	$2.0\ 10^9$			12
Pathway 1: $CH_2(OH)C(OH)(CH_2(OH))CO(O^-) + NO_3^{\bullet} \rightarrow C^{\bullet}H(OH)C(OH)(CH_2(OH))CO(O^-) + NO_3^- + H^+$		$1.0\ 10^6$			BR: 100%
$C^{\bullet}H(OH)C(OH)(CH_2(OH))CO(O^-) + O_2 \rightarrow CH(OH)(OO^{\bullet})C(OH)(CH_2(OH))CO(O^-)$		$2.0\ 10^9$			3
$CH_2(OH)C(OH)(CH_2(OH))CO(O^-) + NO_3^{\bullet} \rightarrow CH(OH)(OO^{\bullet})C(OH)(CH_2(OH))CO(O^-) + NO_3^- + H^+ - O_2$	R(796)	$1.0\ 10^6$			= k(CH(OH)(OH)CH(OH)(OH) + $NO_3^{\bullet}$) - 13
$CH(OH)(OO^{\bullet})C(OH)(CH_2(OH))CO(OH) + OH^- \rightarrow CH(O^-)(OO^{\bullet})C(OH)(CH_2(OH))CO(OH) + H_2O$		$4.0\ 10^9$			
$CH(O^-)(OO^{\bullet})C(OH)(CH_2(OH))CO(OH) \rightarrow CHOC(OH)(CH_2(OH))CO(OH) + O_2^{\bullet-}$					16
$CH(OH)(OO^{\bullet})C(OH)(CH_2(OH))CO(OH) + OH^- \rightarrow CHOC(OH)(CH_2(OH))CO(OH) + O_2^{\bullet-} + H_2O$	R(797)	$4.0\ 10^9$			= $k(CH_3CH(OH)(OO^{\bullet}) + OH^-)$
$CH(OH)(OO^{\bullet})C(OH)(CH_2(OH))CO(OH) \rightarrow CHOC(OH)(CH_2(OH))CO(OH) + HO_2^{\bullet}$	R(798)	$1.9\ 10^2$			17
$CH(OH)(OO^{\bullet})C(OH)(CH_2(OH))CO(O^-) + OH^- \rightarrow CH(O^-)(OO^{\bullet})C(OH)(CH_2(OH))CO(O^-) + H_2O$		$4.0\ 10^9$			
$CH(O^-)(OO^{\bullet})C(OH)(CH_2(OH))CO(O^-) \rightarrow CHOC(OH)(CH_2(OH))CO(O^-) + O_2^{\bullet-}$					16
$CH(OH)(OO^{\bullet})C(OH)(CH_2(OH))CO(O^-) + OH^- \rightarrow CHOC(OH)(CH_2(OH))CO(O^-) + O_2^{\bullet-} + H_2O$	R(799)	$4.0\ 10^9$			= $k(CH_3CH(OH)(OO^{\bullet}) + OH^-)$
$CH(OH)(OO^{\bullet})C(OH)(CH_2(OH))CO(O^-) \rightarrow CHOC(OH)(CH_2(OH))CO(O^-) + HO_2^{\bullet}$	R(800)	$1.9\ 10^2$			17
Methyltartronic acid					95
Pathway 1: $CO(OH)C(OH)(CH_3)CO(OH) + HO^{\bullet} \rightarrow CO(OH)C(OH)(C^{\bullet}H_2)CO(OH) + H_2O$		$8.0\ 10^7$			BR: 66% - 96
$CO(OH)C(OH)(C^{\bullet}H_2)CO(OH) + O_2 \rightarrow CO(OH)C(OH)(CH_2(OO^{\bullet}))CO(OH)$		$2.0\ 10^9$			3
Pathway 2: $CO(OH)C(OH)(CH_3)CO(OH) + HO^{\bullet} \rightarrow CO(OH)C(O^{\bullet})(CH_3)CO(OH) + H_2O$		$4.0\ 10^7$			BR: 34% - 96
$CO(OH)C(O^{\bullet})(CH_3)CO(OH) \rightarrow C^{\bullet}O(OH) + CH_3COCO(OH)$					4 - 5
$C^{\bullet}O(OH) + O_2 \rightarrow CO(OH)(OO^{\bullet})$		$2.0\ 10^9$			3
$CO(OH)C(OH)(CH_3)CO(OH) + HO^{\bullet} \rightarrow 0.66\ CO(OH)C(OH)(CH_2(OO^{\bullet}))CO(OH) + 0.34\ CH_3COCO(OH) + 0.34\ CO(OH)(OO^{\bullet}) + H_2O - O_2$	R(801)	$1.2\ 10^8$			12
Pathway 1: $CO(OH)C(OH)(CH_3)CO(OH) + NO_3^{\bullet} \rightarrow CO(OH)C(OH)(C^{\bullet}H_2)CO(OH) + NO_3^- + H^+$		$2.1\ 10^6$			BR: 100%
$CO(OH)C(OH)(C^{\bullet}H_2)CO(OH) + O_2 \rightarrow CO(OH)C(OH)(CH_2(OO^{\bullet}))CO(OH)$		$2.0\ 10^9$			3
$CO(OH)C(OH)(CH_3)CO(OH) + NO_3^{\bullet} \rightarrow CO(OH)C(OH)(CH_2(OO^{\bullet}))CO(OH) + NO_3^- + H^+ - O_2$	R(802)	$2.1{\cdot}10^6$	3248		= k($CH_3CH(OH)CO(OH) + NO_3^{\bullet}$) - 13
Pathway 1: $CO(OH)C(OH)(CH_3)CO(O^-) + HO^{\bullet} \rightarrow CO(OH)C(OH)(C^{\bullet}H_2)CO(O^-) + H_2O$		$1.8\ 10^8$			BR: 64% - 97
$CO(OH)C(OH)(C^{\bullet}H_2)CO(O^-) + O_2 \rightarrow CO(OH)C(OH)(CH_2(OO^{\bullet}))CO(O^-)$		$2.0\ 10^9$			3
Pathway 2: $CO(OH)C(OH)(CH_3)CO(O^-) + HO^{\bullet} \rightarrow CO(OH)C(OH)(CH_3)CO(O^{\bullet}) + HO^-$		$1.0\ 10^8$			BR: 36% - 97
$CO(OH)C(OH)(CH_3)CO(O^{\bullet}) \rightarrow CH_3C^{\bullet}(OH)CO(OH) + CO_2$					4 - 5
$CH_3C^{\bullet}(OH)CO(OH) + O_2 \rightarrow CH_3C(OH)(OO^{\bullet})CO(OH)$		$2.0\ 10^9$			3
$CO(OH)C(OH)(CH_3)CO(O^-) + HO^{\bullet} \rightarrow 0.64\ CO(OH)C(OH)(CH_2(OO^{\bullet}))CO(O^-) + 0.36\ CH_3C(OH)(OO^{\bullet})CO(OH) + 0.36\ CO_2 + 0.36\ HO^- + 0.64\ H_2O - O_2$	R(803)	$2.8\ 10^8$			12
Pathway 1: $CO(OH)C(OH)(CH_3)CO(O^-) + NO_3^{\bullet} \rightarrow CO(OH)C(OH)(C^{\bullet}H_2)CO(O^-) + NO_3^- + H^+$		$1.0\ 10^7$			BR: 100%
$CO(OH)C(OH)(C^{\bullet}H_2)CO(O^-) + O_2 \rightarrow CO(OH)C(OH)(CH_2(OO^{\bullet}))CO(O^-)$		$2.0\ 10^9$			3

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CO(OH)C(OH)(CH_3)CO(O^-) + NO_3^\bullet \rightarrow CO(OH)C(OH)(CH_2(OO^\bullet))CO(O^-) + NO_3^- + H^+ - O_2$	R(804)	$1.0 \cdot 10^7$	2646		= k($CH_3CH(OH)CO(O^-)$ + $NO_3^\bullet$) - 13
Pathway 1: $CO(O^-)C(OH)(CH_3)CO(O^-) + HO^\bullet \rightarrow CO(O^-)C(OH)(C^\bullet H_2)CO(O^-) + H_2O$		$2.9\ 10^8$			BR: 47% - 98
$CO(O^-)C(OH)(C^\bullet H_2)CO(O^-) + O_2 \rightarrow CO(O^-)C(OH)(CH_2(OO^\bullet))CO(O^-)$		$2.0\ 10^9$			3
Pathway 2: $CO(O^-)C(OH)(CH_3)CO(O^-) + HO^\bullet \rightarrow CO(O^-)C(OH)(CH_3)CO(O^\bullet) + HO^-$		$3.3\ 10^8$			BR: 53% - 98
$CO(O^-)C(OH)(CH_3)CO(O^\bullet) \rightarrow CH_3C^\bullet(OH)CO(O^-) + CO_2$					4 - 5
$CH_3C^\bullet(OH)CO(O^-) + O_2 \rightarrow CH_3C(OH)(OO^\bullet)CO(O^-)$		$2.0\ 10^9$			3
$CO(O^-)C(OH)(CH_3)CO(O^-) + HO^\bullet \rightarrow 0.47\ CO(O^-)C(OH)(CH_2(OO^\bullet))CO(O^-) + 0.53\ CH_3C(OH)(OO^\bullet)CO(O^-) + 0.53\ CO_2 + 0.53\ HO^- + 0.47\ H_2O - O_2$	R(805)	$6.2\ 10^8$			12
Pathway 1: $CO(O^-)C(OH)(CH_3)CO(O^-) + NO_3^\bullet \rightarrow CO(O^-)C(OH)(C^\bullet H_2)CO(O^-) + NO_3^- + H^+$		$1.0\ 10^7$			BR: 100%
$CO(O^-)C(OH)(C^\bullet H_2)CO(O^-) + O_2 \rightarrow CO(O^-)C(OH)(CH_2(OO^\bullet))CO(O^-)$		$2.0\ 10^9$			3
$CO(O^-)C(OH)(CH_3)CO(O^-) + NO_3^\bullet \rightarrow CO(O^-)C(OH)(CH_2(OO^\bullet))CO(O^-) + NO_3^- + H^+ - O_2$	R(806)	$1.0 \cdot 10^7$	2646		= k($CH_3CH(OH)CO(O^-)$ + $NO_3^\bullet$) - 13
Pathway 1: 2 $CO(OH)C(OH)(CH_2(OO^\bullet))CO(OH) \rightarrow 2\ CO(OH)C(OH)(CHO)CO(OH) + H_2O_2$		$5.0\ 10^7$			BR: 50%
Pathway 2:2 $CO(OH)C(OH)(CH_2(OO^\bullet))CO(OH) \rightarrow CO(OH)C(OH)(CHO)CO(OH) + CO(OH)C(OH)(CH_2(OH))CO(OH) + O_2$		$3.3\ 10^7$			BR: 33%
Pathway 3: 2 $CO(OH)C(OH)(CH_2(OO^\bullet))CO(OH) \rightarrow 2\ CO(OH)C(OH)(CH_2(O^\bullet))CO(OH) + O_2$		$1.7\ 10^7$			BR: 17%
$CO(OH)C(OH)(CH_2(O^\bullet))CO(OH) \rightarrow CO(OH)C^\bullet(OH)CO(OH) + CH_2O$					4 - 5
$CO(OH)C^\bullet(OH)CO(OH) + O_2 \rightarrow CO(OH)C(OH)(OO^\bullet)CO(OH)$		$2.0 \cdot 10^9$			3
$2\ CO(OH)C(OH)(CH_2(OO^\bullet))CO(OH) \rightarrow 1.33\ CO(OH)C(OH)(CHO)CO(OH) + 0.33\ CO(OH)C(OH)(CH_2(OH))CO(OH) + 0.34\ CO(OH)C(OH)(OO^\bullet)CO(OH) + 0.34\ CH_2O + 0.50\ H_2O_2 + 0.16\ O_2$	R(807)	$1.0\ 10^8$			= k(2 $CH_2(OH)CH_2(OO^\bullet)$) - 6
Pathway 1: 2 $CO(OH)C(OH)(CH_2(OO^\bullet))CO(O^-) \rightarrow 2\ CO(OH)C(OH)(CHO)CO(O^-) + H_2O_2$		$5.0\ 10^7$			BR: 50%
Pathway 2:2 $CO(OH)C(OH)(CH_2(OO^\bullet))CO(O^-) \rightarrow CO(OH)C(OH)(CHO)CO(O^-) + CO(OH)C(OH)(CH_2(OH))CO(O^-) + O_2$		$3.3\ 10^7$			BR: 33%
Pathway 3: 2 $CO(OH)C(OH)(CH_2(OO^\bullet))CO(O^-) \rightarrow 2\ CO(OH)C(OH)(CH_2(O^\bullet))CO(O^-) + O_2$		$1.7\ 10^7$			BR: 17%
$CO(OH)C(OH)(CH_2(O^\bullet))CO(O^-) \rightarrow CO(OH)C^\bullet(OH)CO(O^-) + CH_2O$					4 - 5
$CO(OH)C^\bullet(OH)CO(O^-) + O_2 \rightarrow CO(OH)C(OH)(OO^\bullet)CO(O^-)$		$2.0 \cdot 10^9$			3
$2\ CO(OH)C(OH)(CH_2(OO^\bullet))CO(O^-) \rightarrow 1.33\ CO(OH)C(OH)(CHO)CO(O^-) + 0.33\ CO(OH)C(OH)(CH_2(OH))CO(O^-) + 0.34\ CO(OH)C(OH)(OO^\bullet)CO(O^-) + 0.34\ CH_2O + 0.50\ H_2O_2 + 0.16\ O_2$	R(808)	$1.0\ 10^8$			= k(2 $CH_2(OH)CH_2(OO^\bullet)$) - 6
Pathway 1: 2 $CO(O^-)C(OH)(CH_2(OO^\bullet))CO(O^-) \rightarrow 2\ CO(O^-)C(OH)(CHO)CO(O^-) + H_2O_2$		$5.0\ 10^7$			BR: 50%
Pathway 2:2 $CO(O^-)C(OH)(CH_2(OO^\bullet))CO(O^-) \rightarrow CO(O^-)C(OH)(CHO)CO(O^-) + CO(O^-)C(OH)(CH_2(OH))CO(O^-) + O_2$		$3.3\ 10^7$			BR: 33%
Pathway 3: 2 $CO(O^-)C(OH)(CH_2(OO^\bullet))CO(O^-) \rightarrow 2\ CO(O^-)C(OH)(CH_2(O^\bullet))CO(O^-) + O_2$		$1.7\ 10^7$			BR: 17%
$CO(O^-)C(OH)(CH_2(O^\bullet))CO(O^-) \rightarrow CO(O^-)C^\bullet(OH)CO(O^-) + CH_2O$					4 - 5
$CO(O^-)C^\bullet(OH)CO(O^-) + O_2 \rightarrow CO(O^-)C(OH)(OO^\bullet)CO(O^-)$		$2.0 \cdot 10^9$			3
$2\ CO(O^-)C(OH)(CH_2(OO^\bullet))CO(O^-) \rightarrow 1.33\ CO(O^-)C(OH)(CHO)CO(O^-) + 0.33\ CO(O^-)C(OH)(CH_2(OH))CO(O^-) + 0.34\ CO(O^-)C(OH)(OO^\bullet)CO(O^-) + 0.34\ CH_2O + 0.50\ H_2O_2 + 0.16\ O_2$	R(809)	$1.0\ 10^8$			= k(2 $CH_2(OH)CH_2(OO^\bullet)$) - 6
2- hydroxy-2-(oxomethyl)-3-oxopropanoic acid					99
Pathway 1: $CH(OH)(OH)C(OH)(CH(OH)(OH))CO(OH) + HO^\bullet \rightarrow CH(OH)(O^\bullet)C(OH)(CH(OH)(OH))CO(OH) + H_2O$		$7.7\ 10^8$			BR: 64% - 100
$CH(OH)(O^\bullet)C(OH)(CH(OH)(OH))CO(OH) \rightarrow CHO(OH) + CH(OH)(OH)C^\bullet(OH)CO(OH)$					4 - 5
$CH(OH)(OH)C^\bullet(OH)CO(OH) + O_2 \rightarrow CH(OH)(OH)C(OH)(OO^\bullet)CO(OH)$		$2.0\ 10^9$			3
Pathway 2: $CH(OH)(OH)C(OH)(CH(OH)(OH))CO(OH) + HO^\bullet \rightarrow C^\bullet(OH)(OH)C(OH)(CH(OH)(OH))CO(OH) + H_2O$		$4.3\ 10^8$			BR: 36% - 100
$C^\bullet(OH)(OH)C(OH)(CH(OH)(OH))CO(OH) + O_2 \rightarrow C(OH)(OH)(OO^\bullet)C(OH)(CH(OH)(OH))CO(OH)$		$2.0\ 10^9$			3
$CH(OH)(OH)C(OH)(CH(OH)(OH))CO(OH) + HO^\bullet \rightarrow 0.64\ CH(OH)(OH)C(OH)(OO^\bullet)CO(OH) + 0.64\ CHO(OH) + 0.36\ C(OH)(OH)(OO^\bullet)C(OH)(CH(OH)(OH))CO(OH) + H_2O - O_2$	R(810)	$1.2\ 10^9$			12
Pathway 1: $CH(OH)(OH)C(OH)(CH(OH)(OH))CO(OH) + NO_3^\bullet \rightarrow C^\bullet(OH)(OH)C(OH)(CH(OH)(OH))CO(OH) + NO_3^- + H^+$		$1.0\ 10^6$			BR: 100%
$C^\bullet(OH)(OH)C(OH)(CH(OH)(OH))CO(OH) + O_2 \rightarrow C(OH)(OH)(OO^\bullet)C(OH)(CH(OH)(OH))CO(OH)$		$2.0\ 10^9$			3
$CH(OH)(OH)C(OH)(CH(OH)(OH))CO(OH) + NO_3^\bullet \rightarrow C(OH)(OH)(OO^\bullet)C(OH)(CH(OH)(OH))CO(OH) + NO_3^- + H^+ - O_2$	R(811)	$1.0\ 10^6$			= k($CH(OH)(OH)CH(OH)(OH)$ + $NO_3^\bullet$) - 13
Pathway 1: $CH(OH)(OH)C(OH)(CH(OH)(OH))CO(O^-) + HO^\bullet \rightarrow CH(OH)(O^\bullet)C(OH)(CH(OH)(OH))CO(O^-) + H_2O$		$8.0\ 10^8$			BR: 50% - 101

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
CH(OH)(O•)C(OH)(CH(OH)(OH))CO(O^-) → CHO(OH) + CH(OH)(OH)C•(OH)CO(O^-)					4 - 5
CH(OH)(OH)C•(OH)CO(O^-) + O_2 → CH(OH)(OH)C(OH)(OO•)CO(O^-)		$2.0\ 10^9$			3
Pathway 2: CH(OH)(OH)C(OH)(CH(OH)(OH))CO(O^-) + HO• → C•(OH)(OH)C(OH)(CH(OH)(OH))CO(O^-) + H_2O		$8.0\ 10^8$			BR: 50% - 101
C•(OH)(OH)C(OH)(CH(OH)(OH))CO(O^-) + O_2 → C(OH)(OH)(OO•)C(OH)(CH(OH)(OH))CO(O^-)		$2.0\ 10^9$			3
CH(OH)(OH)C(OH)(CH(OH)(OH))CO(O^-) + HO• → 0.50 CH(OH)(OH)C(OH)(OO•)CO(O^-) + 0.50 CHO(OH) + 0.50 C(OH)(OH)(OO•)C(OH)(CH(OH)(OH))CO(O^-) + H_2O - O_2	R(812)	$1.6\ 10^9$			12
Pathway 1: CH(OH)(OH)C(OH)(CH(OH)(OH))CO(O^-) + NO_3• → C•(OH)(OH)C(OH)(CH(OH)(OH))CO(O^-) + NO_3^- + H^+		$1.0\ 10^6$			BR: 100%
C•(OH)(OH)C(OH)(CH(OH)(OH))CO(O^-) + O_2 → C(OH)(OH)(OO•)C(OH)(CH(OH)(OH))CO(O^-)		$2.0\ 10^9$			3
CH(OH)(OH)C(OH)(CH(OH)(OH))CO(O^-) + NO_3• → C(OH)(OH)(OO•)C(OH)(CH(OH)(OH))CO(O^-) + NO_3^- + H^+ - O_2	R(813)	$1.0\ 10^6$			= k(CH(OH)(OH)CH(OH)(OH) + NO_3•) - 13
C(OH)(OH)(OO•)C(OH)(CH(OH)(OH))CO(OH) + OH^- → C(OH)(O^-)(OO•)C(OH)(CH(OH)(OH))CO(OH) + H_2O		$4.0\ 10^9$			
C(OH)(O^-)(OO•)C(OH)(CH(OH)(OH))CO(OH) → CO(OH)C(OH)(CH(OH)(OH))CO(OH) + O_2•-					16
C(OH)(OH)(OO•)C(OH)(CH(OH)(OH))CO(OH) + OH^- → CO(OH)C(OH)(CH(OH)(OH))CO(OH) + O_2•- + H_2O	R(814)	$4.0\ 10^9$			= k(CH_3CH(OH)(OO•) + OH^-)
C(OH)(OH)(OO•)C(OH)(CH(OH)(OH))CO(OH) → CO(OH)C(OH)(CH(OH)(OH))CO(OH) + HO_2•	R(815)	$1.0\ 10^6$			17
C(OH)(OH)(OO•)C(OH)(CH(OH)(OH))CO(O^-) + OH^-→C(OH)(O^-)(OO•)C(OH)(CH(OH)(OH))CO(O^-) + H_2O		$4.0\ 10^9$			
C(OH)(O^-)(OO•)C(OH)(CH(OH)(OH))CO(O^-)→ CO(OH)C(OH)(CH(OH)(OH))CO(O^-)+ O_2•-					16
C(OH)(OH)(OO•)C(OH)(CH(OH)(OH))CO(O^-) + OH^- → CO(OH)C(OH)(CH(OH)(OH))CO(O^-) + O_2•- + H_2O	R(816)	$4.0\ 10^9$			= k(CH_3CH(OH)(OO•) + OH^-)
C(OH)(OH)(OO•)C(OH)(CH(OH)(OH))CO(O^-) → CO(OH)C(OH)(CH(OH)(OH))CO(O^-) + HO_2•	R(817)	$1.0\ 10^6$			17
2-(hydroxymethyl)-tartronic acid					102
Pathway 1: CO(OH)C(OH)(CH_2(OH))CO(OH) + HO• → CO(OH)C(OH)(C•H(OH))CO(OH) + H_2O		$3.2\ 10^8$			BR: 78% - 103
CO(OH)C(OH)(C•H(OH))CO(OH) + O_2 → CO(OH)C(OH)(CH(OH)(OO•))CO(OH)		$2.0\ 10^9$			3
Pathway 2: CO(OH)C(OH)(CH_2(OH))CO(OH) + HO• → CO(OH)C(OH)(CH_2(O•))CO(OH) + H_2O		$9.0\ 10^7$			BR: 22% - 103
CO(OH)C(OH)(CH_2(O•))CO(OH) → CH_2O + CO(OH)C•(OH)CO(OH)					4 - 5
CO(OH)C•(OH)CO(OH) + O_2 → CO(OH)C(OH)(OO•)CO(OH)		$2.0\ 10^9$			3
CO(OH)C(OH)(CH_2(OH))CO(OH) + HO• → 0.78 CO(OH)C(OH)(CH(OH)(OO•))CO(OH) + 0.22 CH_2O + 0.22 CO(OH)C(OH)(OO•)CO(OH) + H_2O - O_2	R(818)	$4.1\ 10^8$			12
Pathway 1: CO(OH)C(OH)(CH_2(OH))CO(OH) + NO_3• → CO(OH)C(OH)(C•H(OH))CO(OH) + NO_3^- + H^+		$2.1\ 10^6$			BR: 100%
CO(OH)C(OH)(C•H(OH))CO(OH) + O_2 → CO(OH)C(OH)(CH(OH)(OO•))CO(OH)		$2.0\ 10^9$			3
CO(OH)C(OH)(CH_2(OH))CO(OH) + NO_3• → CO(OH)C(OH)(CH(OH)(OO•))CO(OH) + NO_3^- + H^+ - O_2	R(819)	$2.1{\cdot}10^6$	3248		= k(CH_3CH(OH)CO(OH) + NO_3•) - 13
Pathway 1: CO(OH)C(OH)(CH_2(OH))CO(O^-) + HO• → CO(OH)C(OH)(C•H(OH))CO(O^-) + H_2O		$6.4\ 10^8$			BR: 86% - 104
CO(OH)C(OH)(C•H(OH))CO(O^-) + O_2 → CO(OH)C(OH)(CH(OH)(OO•))CO(O^-)		$2.0\ 10^9$			3
Pathway 2: CO(OH)C(OH)(CH_2(OH))CO(O^-) + HO• → CO(OH)C(OH)(CH_2(O•))CO(O^-) + H_2O		$1.0\ 10^8$			BR: 14% - 104
CO(OH)C(OH)(CH_2(O•))CO(O^-) → CH_2O + CO(OH)C•(OH)CO(O^-)					4 - 5
CO(OH)C•(OH)CO(O^-) + O_2 → CO(OH)C(OH)(OO•)CO(O^-)		$2.0\ 10^9$			3
CO(OH)C(OH)(CH_2(OH))CO(O^-) + HO• → 0.86 CO(OH)C(OH)(CH(OH)(OO•))CO(O^-) + 0.14 CH_2O + 0.14 CO(OH)C(OH)(OO•)CO(O^-) + H_2O - O_2	R(820)	$7.4\ 10^8$			12
Pathway 1: CO(OH)C(OH)(CH_2(OH))CO(O^-) + NO_3• → CO(OH)C(OH)(C•H(OH))CO(O^-) + NO_3^- + H^+		$1.0\ 10^7$			BR: 100%
CO(OH)C(OH)(C•H(OH))CO(O^-) + O_2 → CO(OH)C(OH)(CH(OH)(OO•))CO(O^-)		$2.0\ 10^9$			3
CO(OH)C(OH)(CH_2(OH))CO(O^-) + NO_3• → CO(OH)C(OH)(CH(OH)(OO•))CO(O^-) + NO_3^- + H^+ - O_2	R(821)	$1.0{\cdot}10^7$	2646		= k(CH_3CH(OH)CO(O^-) + NO_3•) - 13
Pathway 1: CO(O^-)C(OH)(CH_2(OH))CO(O^-) + HO• → CO(O^-)C(OH)(C•H(OH))CO(O^-) + H_2O		$1.1\ 10^9$			BR: 79% - 105
CO(O^-)C(OH)(C•H(OH))CO(O^-) + O_2 → CO(O^-)C(OH)(CH(OH)(OO•))CO(O^-)		$2.0\ 10^9$			3
Pathway 2: CO(O^-)C(OH)(CH_2(OH))CO(O^-) + HO• → CO(O^-)C(OH)(CH_2(OH))CO(O•) + OH^-		$3.0\ 10^8$			BR: 21% - 105
CO(O^-)C(OH)(CH_2(OH))CO(O•) → CH_2(OH)C•(OH)CO(O^-) + CO_2					4 - 5
CH_2(OH)C•(OH)CO(O^-) + O_2 → CH_2(OH)C(OH)(OO•)CO(O^-)		$2.0\ 10^9$			3

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CO(O^-)C(OH)(CH_2(OH))CO(O^-) + HO^\bullet \rightarrow 0.79\ CO(O^-)C(OH)(CH(OH)(OO^\bullet))CO(O^-) + 0.21\ CH_2(OH)C(OH)(OO^\bullet)CO(O^-) + 0.21\ CO_2 + 0.21\ OH^- + 0.79\ H_2O - O_2$	R(822)	$1.4\ 10^9$			12
Pathway 1: $CO(O^-)C(OH)(CH_2(OH))CO(O^-) + NO_3^\bullet \rightarrow CO(O^-)C(OH)(C^\bullet H(OH))CO(O^-) + NO_3^- + H^+$		$1.0\ 10^7$			BR: 100%
$CO(O^-)C(OH)(C^\bullet H(OH))CO(O^-) + O_2 \rightarrow CO(O^-)C(OH)(CH(OH)(OO^\bullet))CO(O^-)$		$2.0\ 10^9$			3
$CO(O^-)C(OH)(CH_2(OH))CO(O^-) + NO_3^\bullet \rightarrow CO(O^-)C(OH)(CH(OH)(OO^\bullet))CO(O^-) + NO_3^- + H^+ - O_2$	R(823)	$1.0{\cdot}10^7$	2646		= k($CH_3CH(OH)CO(O^-)$ + $NO_3^\bullet$) - 13
$CO(OH)C(OH)(CH(OH)(OO^\bullet))CO(OH) + OH^- \rightarrow CO(OH)C(OH)(CH(O^-)(OO^\bullet))CO(OH) + H_2O$		$4.0\ 10^9$			
$CO(OH)C(OH)(CH(O^-)(OO^\bullet))CO(OH) \rightarrow CO(OH)C(OH)(CHO)CO(OH) + O_2^{\bullet-}$					16
$CO(OH)C(OH)(CH(OH)(OO^\bullet))CO(OH) + OH^- \rightarrow CO(OH)C(OH)(CHO)CO(OH) + O_2^{\bullet-} + H_2O$	R(824)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^\bullet)$ + OH^-)
$CO(OH)C(OH)(CH(OH)(OO^\bullet))CO(OH) \rightarrow CO(OH)C(OH)(CHO)CO(OH) + HO_2^\bullet$	R(825)	$1.9\ 10^2$			17
$CO(OH)C(OH)(CH(OH)(OO^\bullet))CO(O^-) + OH^- \rightarrow CO(OH)C(OH)(CH(O^-)(OO^\bullet))CO(O^-) + H_2O$		$4.0\ 10^9$			
$CO(OH)C(OH)(CH(O^-)(OO^\bullet))CO(O^-) \rightarrow CO(OH)C(OH)(CHO)CO(O^-) + O_2^{\bullet-}$					16
$CO(OH)C(OH)(CH(OH)(OO^\bullet))CO(O^-) + OH^- \rightarrow CO(OH)C(OH)(CHO)CO(O^-) + O_2^{\bullet-} + H_2O$	R(826)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^\bullet)$ + OH^-)
$CO(OH)C(OH)(CH(OH)(OO^\bullet))CO(O^-) \rightarrow CO(OH)C(OH)(CHO)CO(O^-) + HO_2^\bullet$	R(827)	$1.9\ 10^2$			17
$CO(O^-)C(OH)(CH(OH)(OO^\bullet))CO(O^-) + OH^- \rightarrow CO(O^-)C(OH)(CH(O^-)(OO^\bullet))CO(O^-) + H_2O$		$4.0\ 10^9$			
$CO(O^-)C(OH)(CH(O^-)(OO^\bullet))CO(O^-) \rightarrow CO(O^-)C(OH)(CHO)CO(O^-) + O_2^{\bullet-}$					16
$CO(O^-)C(OH)(CH(OH)(OO^\bullet))CO(O^-) + OH^- \rightarrow CO(O^-)C(OH)(CHO)CO(O^-) + O_2^{\bullet-} + H_2O$	R(828)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^\bullet)$ + OH^-)
$CO(O^-)C(OH)(CH(OH)(OO^\bullet))CO(O^-) \rightarrow CO(O^-)C(OH)(CHO)CO(O^-) + HO_2^\bullet$	R(829)	$1.9\ 10^2$			17
2-(oxomethyl)-tartronic acid					106
Pathway 1: $CO(OH)C(OH)(CH(OH)(OH))CO(OH) + HO^\bullet \rightarrow CO(OH)C(OH)(CH(OH)(O^\bullet))CO(OH) + H_2O$		$3.9\ 10^8$			BR: 72% - 107
$CO(OH)C(OH)(CH(OH)(O^\bullet))CO(OH) \rightarrow CHO(OH) + CO(OH)C^\bullet(OH)CO(OH)$					4 - 5
$CO(OH)C^\bullet(OH)CO(OH) + O_2 \rightarrow CO(OH)C(OH)(OO^\bullet)CO(OH)$		$2.0\ 10^9$			3
Pathway 2: $CO(OH)C(OH)(CH(OH)(OH))CO(OH) + HO^\bullet \rightarrow CO(OH)C(OH)(C^\bullet(OH)(OH))CO(OH) + H_2O$		$1.5\ 10^8$			BR: 28% - 107
$CO(OH)C(OH)(C^\bullet(OH)(OH))CO(OH) + O_2 \rightarrow CO(OH)C(OH)(C(OH)(OH)(OO^\bullet))CO(OH)$		$2.0\ 10^9$			3
$CO(OH)C(OH)(CH(OH)(OH))CO(OH) + HO^\bullet \rightarrow 0.72\ CO(OH)C(OH)(OO^\bullet)CO(OH) + 0.72\ CHO(OH) + 0.28\ CO(OH)C(OH)(C(OH)(OH)(OO^\bullet))CO(OH) + H_2O - O_2$	R(830)	$5.4\ 10^8$			12
Pathway 1: $CO(OH)C(OH)(CH(OH)(OH))CO(OH) + NO_3^\bullet \rightarrow CO(OH)C(OH)(C^\bullet(OH)(OH))CO(OH) + NO_3^- + H^+$		$1.0\ 10^6$			BR: 100%
$CO(OH)C(OH)(C^\bullet(OH)(OH))CO(OH) + O_2 \rightarrow CO(OH)C(OH)(C(OH)(OH)(OO^\bullet))CO(OH)$		$2.0\ 10^9$			3
$CO(OH)C(OH)(CH(OH)(OH))CO(OH) + NO_3^\bullet \rightarrow CO(OH)C(OH)(C(OH)(OH)(OO^\bullet))CO(OH) + NO_3^- + H^+ - O_2$	R(831)	$1.0\ 10^6$			= k(CH(OH)(OH)CH(OH)(OH) + $NO_3^\bullet$) - 13
Pathway 1: $CO(OH)C(OH)(CH(OH)(OH))CO(O^-) + HO^\bullet \rightarrow CO(OH)C(OH)(CH(OH)(O^\bullet))CO(O^-) + H_2O$		$4.4\ 10^8$			BR: 60% - 108
$CO(OH)C(OH)(CH(OH)(O^\bullet))CO(O^-) \rightarrow CHO(OH) + CO(OH)C^\bullet(OH)CO(O^-)$					4 - 5
$CO(OH)C^\bullet(OH)CO(O^-) + O_2 \rightarrow CO(OH)C(OH)(OO^\bullet)CO(O^-)$		$2.0\ 10^9$			3
Pathway 2: $CO(OH)C(OH)(CH(OH)(OH))CO(O^-) + HO^\bullet \rightarrow CO(OH)C(OH)(C^\bullet(OH)(OH))CO(O^-) + H_2O$		$3.0\ 10^8$			BR: 40% - 108
$CO(OH)C(OH)(C^\bullet(OH)(OH))CO(O^-) + O_2 \rightarrow CO(OH)C(OH)(C(OH)(OH)(OO^\bullet))CO(O^-)$		$2.0\ 10^9$			3
$CO(OH)C(OH)(CH(OH)(OH))CO(O^-) + HO^\bullet \rightarrow 0.60\ CO(OH)C(OH)(OO^\bullet)CO(O^-) + 0.60\ CHO(OH) + 0.40\ CO(OH)C(OH)(C(OH)(OH)(OO^\bullet))CO(O^-) + H_2O - O_2$	R(832)	$7.4\ 10^8$			12
Pathway 1: $CO(OH)C(OH)(CH(OH)(OH))CO(O^-) + NO_3^\bullet \rightarrow CO(OH)C(OH)(C^\bullet(OH)(OH))CO(O^-) + NO_3^- + H^+$		$1.0\ 10^6$			BR: 100%
$CO(OH)C(OH)(C^\bullet(OH)(OH))CO(O^-) + O_2 \rightarrow CO(OH)C(OH)(C(OH)(OH)(OO^\bullet))CO(O^-)$		$2.0\ 10^9$			3
$CO(OH)C(OH)(CH(OH)(OH))CO(O^-) + NO_3^\bullet \rightarrow CO(OH)C(OH)(C(OH)(OH)(OO^\bullet))CO(O^-) + NO_3^- + H^+ - O_2$	R(833)	$1.0\ 10^6$			= k(CH(OH)(OH)CH(OH)(OH) + $NO_3^\bullet$) - 13
Pathway 1: $CO(O^-)C(OH)(CH(OH)(OH))CO(O^-) + HO^\bullet \rightarrow CO(O^-)C(OH)(C^\bullet(OH)(OH))CO(O^-) + H_2O$		$4.5\ 10^8$			BR: 41% - 109
$CO(O^-)C(OH)(C^\bullet(OH)(OH))CO(O^-) + O_2 \rightarrow CO(O^-)C(OH)(C(OH)(OH)(OO^\bullet))CO(O^-)$		$2.0\ 10^9$			3
Pathway 2: $CO(O^-)C(OH)(CH(OH)(OH))CO(O^-) + HO^\bullet \rightarrow CO(O^-)C(OH)(CH(OH)(O^\bullet))CO(O^-) + H_2O$		$4.0\ 10^8$			BR:36% -109
$CO(O^-)C(OH)(CH(OH)(O^\bullet))CO(O^-) \rightarrow CHO(OH) + CO(O^-)C^\bullet(OH)CO(O^-)$					4 - 5
$CO(O^-)C^\bullet(OH)CO(O^-) + O_2 \rightarrow CO(O^-)C(OH)(OO^\bullet)CO(O^-)$		$2.0\ 10^9$			3

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
Pathway 3: $CO(O^-)C(OH)(CH(OH)(OH))CO(O^-) + HO^\bullet \rightarrow CO(O^-)C(OH)(CH(OH)(OH))CO(O^\bullet) + HO^-$		2.5 10^8			BR: 23% -109
$CO(O^-)C(OH)(CH(OH)(OH))CO(O^\bullet) \rightarrow CH(OH)(OH)C^\bullet(OH)CO(O^-) + CO_2$					4 - 5
$CH(OH)(OH)C^\bullet(OH)CO(O^-) + O_2 \rightarrow CH(OH)(OH)C(OH)(OO^\bullet)CO(O^-)$		2.0 10^9			3
$CO(O^-)C(OH)(CH(OH)(OH))CO(O^-) + HO^\bullet \rightarrow 0.41\ CO(O^-)C(OH)(C(OH)(OH)(OO^\bullet))CO(O^-) + 0.36\ CHO(OH) + 0.36\ CO(O^-)C(OH)(OO^\bullet)CO(O^-) + 0.23\ CH(OH)(OH)C(OH)(OO^\bullet)CO(O^-) + 0.23\ CO_2 + 0.23\ HO^- + 0.77\ H_2O - O_2$	R(834)	1.1 10^9			12
Pathway 1: $CO(O^-)C(OH)(CH(OH)(OH))CO(O^-) + NO_3^\bullet \rightarrow CO(O^-)C(OH)(C^\bullet(OH)(OH))CO(O^-) + NO_3^- + H^+$		1.0 10^6			BR: 100%
$CO(O^-)C(OH)(C^\bullet(OH)(OH))CO(O^-) + O_2 \rightarrow CO(O^-)C(OH)(C(OH)(OH)(OO^\bullet))CO(O^-)$		2.0 10^9			3
$CO(O^-)C(OH)(CH(OH)(OH))CO(O^-) + NO_3^\bullet \rightarrow CO(O^-)C(OH)(C(OH)(OH)(OO^\bullet))CO(O^-) + NO_3^- + H^+ - O_2$	R(835)	1.0 10^6			= k(CH(OH)(OH)CH(OH)(OH) + $NO_3^\bullet$) - 13
$CO(OH)C(OH)(C(OH)(OH)(OO^\bullet))CO(OH) + OH^- \rightarrow CO(OH)C(OH)(C(OH)(O^-)(OO^\bullet))CO(OH) + H_2O$		4.0 10^9			
$CO(OH)C(OH)(C(OH)(O^-)(OO^\bullet))CO(OH) \rightarrow CO(OH)C(OH)(CO(OH))CO(OH) + O_2^{\bullet-}$					16
$CO(OH)C(OH)(C(OH)(OH)(OO^\bullet))CO(OH) + OH^- \rightarrow CO(OH)C(OH)(CO(OH))CO(OH) + O_2^{\bullet-} + H_2O$	R(836)	4.0 10^9			= k($CH_3CH(OH)(OO^\bullet)$ + OH^-)
$CO(OH)C(OH)(C(OH)(OH)(OO^\bullet))CO(OH) \rightarrow CO(OH)C(OH)(CO(OH))CO(OH) + HO_2^\bullet$	R(837)	1.9 10^2			17
$CO(OH)C(OH)(C(OH)(OH)(OO^\bullet))CO(O^-) + OH^- \rightarrow CO(OH)C(OH)(C(OH)(O^-)(OO^\bullet))CO(O^-) + H_2O$		4.0 10^9			
$CO(OH)C(OH)(C(OH)(O^-)(OO^\bullet))CO(O^-) \rightarrow CO(OH)C(OH)(CO(OH))CO(O^-) + O_2^{\bullet-}$					16
$CO(OH)C(OH)(C(OH)(OH)(OO^\bullet))CO(O^-) + OH^- \rightarrow CO(OH)C(OH)(CO(OH))CO(O^-) + O_2^{\bullet-} + H_2O$	R(838)	4.0 10^9			= k($CH_3CH(OH)(OO^\bullet)$ + OH^-)
$CO(OH)C(OH)(C(OH)(OH)(OO^\bullet))CO(O^-) \rightarrow CO(OH)C(OH)(CO(OH))CO(O^-) + HO_2^\bullet$	R(839)	1.9 10^2			17
$CO(O^-)C(OH)(C(OH)(OH)(OO^\bullet))CO(O^-) + OH^- \rightarrow CO(O^-)C(OH)(C(OH)(O^-)(OO^\bullet))CO(O^-) + H_2O$		4.0 10^9			
$CO(O^-)C(OH)(C(OH)(O^-)(OO^\bullet))CO(O^-) \rightarrow CO(OH)C(OH)(CO(O^-))CO(O^-) + O_2^{\bullet-}$					16
$CO(O^-)C(OH)(C(OH)(OH)(OO^\bullet))CO(O^-) + OH^- \rightarrow CO(O^-)C(OH)(CO(OH))CO(O^-) + O_2^{\bullet-} + H_2O$	R(840)	4.0 10^9			= k($CH_3CH(OH)(OO^\bullet)$ + OH^-)
$CO(O^-)C(OH)(C(OH)(OH)(OO^\bullet))CO(O^-) \rightarrow CO(O^-)C(OH)(CO(OH))CO(O^-) + HO_2^\bullet$	R(841)	1.9 10^2			17
Hydroxymethanetricarboxylic acid					110
Pathway 1: $CO(OH)C(OH)(CO(OH))CO(OH) + HO^\bullet \rightarrow CO(OH)C(O^\bullet)(CO(OH))CO(OH) + H_2O$		2.4 10^7			BR: 100% - 111
$CO(OH)C(O^\bullet)(CO(OH))CO(OH) \rightarrow C^\bullet O(OH) + CO(OH)COCO(OH)$					4 - 5
$C^\bullet O(OH) + O_2 \rightarrow CO(OH)(OO^\bullet)$		2.0 10^9			3
$CO(OH)C(OH)(CO(OH))CO(OH) + HO^\bullet \rightarrow CO(OH)COCO(OH) + CO(OH)(OO^\bullet) + H_2O - O_2$	R(842)	2.4 10^7			12
Pathway 1: $CO(OH)C(OH)(CO(OH))CO(O^-) + HO^\bullet \rightarrow CO(OH)C(OH)(CO(OH))CO(O^\bullet) + OH^-$		4.5 10^7			BR: 52% - 112
$CO(OH)C(OH)(CO(OH))CO(O^\bullet) \rightarrow CO(OH)C^\bullet(OH)CO(OH) + CO_2$					4 -5
$CO(OH)C^\bullet(OH)CO(OH) + O_2 \rightarrow CO(OH)C(OH)(OO^\bullet)CO(OH)$		2.0 10^9			3
Pathway 2: $CO(OH)C(OH)(CO(OH))CO(O^-) + HO^\bullet \rightarrow CO(OH)C(O^\bullet)(CO(OH))CO(O^-) + H_2O$		4.2 10^7			BR: 48% - 112
$CO(OH)C(O^\bullet)(CO(OH))CO(O^-) \rightarrow C^\bullet O(OH) + CO(OH)COCO(O^-)$					4 - 5
$C^\bullet O(OH) + O_2 \rightarrow CO(OH)(OO^\bullet)$		2.0 10^9			3
$CO(OH)C(OH)(CO(OH))CO(O^-) + HO^\bullet \rightarrow 0.52\ CO(OH)C(OH)(OO^\bullet)CO(OH) + 0.52\ CO_2 + 0.48\ CO(OH)COCO(O^-) + 0.48\ CO(OH)(OO^\bullet) + 0.52\ OH^- + 0.48\ H_2O - O_2$	R(843)	8.7 10^7			12
Pathway 1: $CO(OH)C(OH)(CO(O^-))CO(O^-) + HO^\bullet \rightarrow CO(OH)C(OH)(CO(O^-))CO(O^\bullet) + OH^-$		1.6 10^8			BR: 69% - 113
$CO(OH)C(OH)(CO(O^-))CO(O^\bullet) \rightarrow CO(OH)C^\bullet(OH)CO(O^-) + CO_2$					4 - 5
$CO(OH)C^\bullet(OH)CO(O^-) + O_2 \rightarrow CO(OH)C(OH)(OO^\bullet)CO(O^-)$		2.0 10^9			3
Pathway 2: $CO(OH)C(OH)(CO(O^-))CO(O^-) + HO^\bullet \rightarrow CO(OH)C(O^\bullet)(CO(O^-))CO(O^-) + H_2O$		7.0 10^7			BR: 31% - 113
$CO(OH)C(O^\bullet)(CO(O^-))CO(O^-) \rightarrow C^\bullet O(O^-) + CO(OH)COCO(O^-)$					4 - 5
$C^\bullet O(O^-) + O_2 \rightarrow CO(O^-)(OO^\bullet)$		2.0 10^9			3
$CO(OH)C(OH)(CO(O^-))CO(O^-) + HO^\bullet \rightarrow 0.69\ CO(OH)C(OH)(OO^\bullet)CO(O^-) + 0.69\ CO_2 + 0.31\ CO(OH)COCO(O^-) + 0.31\ CO(O^-)(OO^\bullet) + 0.69\ OH^- + 0.31\ H_2O - O_2$	R(844)	2.3 10^8			12
Pathway 1: $CO(O^-)C(OH)(CO(O^-))CO(O^-) + HO^\bullet \rightarrow CO(O^-)C(OH)(CO(O^-))CO(O^\bullet) + OH^-$		5.5 10^8			BR: 100% - 114
$CO(O^-)C(OH)(CO(O^-))CO(O^\bullet) \rightarrow CO(O^-)C^\bullet(OH)CO(O^-) + CO_2$					4 - 5
$CO(O^-)C^\bullet(OH)CO(O^-) + O_2 \rightarrow CO(O^-)C(OH)(OO^\bullet)CO(O^-)$		2.0 10^9			3
$CO(O^-)C(OH)(CO(O^-))CO(O^-) + HO^\bullet \rightarrow CO(O^-)C(OH)(OO^\bullet)CO(O^-) + CO_2 + OH^- - O_2$	R(845)	5.5 10^8			

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
Oxidation of Methacrylic Acid					115
Pathway 1: $CH_2=C(CH_3)CO(OH) + HO^\bullet \rightarrow CH_2(OH)C^\bullet(CH_3)CO(OH)$		9.4 10^9			BR: 100% - 116
$CH_2(OH)C^\bullet(CH_3)CO(OH) + O_2 \rightarrow CH_2(OH)C(OO^\bullet)(CH_3)CO(OH)$		2.0 10^9			3
$CH_2=C(CH_3)CO(OH) + HO^\bullet \rightarrow CH_2(OH)C(OO^\bullet)(CH_3)CO(OH) - O_2$	R(846)	$1.1 \cdot 10^{10}$	1323	Schöne et al., 2014	
Pathway 1: $CH_2=C(CH_3)CO(O^-) + HO^\bullet \rightarrow CH_2(OH)C^\bullet(CH_3)CO(O^-)$		9.4 10^9			BR: 100% - 116
$CH_2(OH)C^\bullet(CH_3)CO(O^-) + O_2 \rightarrow CH_2(OH)C(OO^\bullet)(CH_3)CO(O^-)$		2.0 10^9			3
$CH_2=C(CH_3)CO(O^-) + HO^\bullet \rightarrow CH_2(OH)C(OO^\bullet)(CH_3)CO(O^-) - O_2$	R(847)	$1.1 \cdot 10^{10}$	1924	Schöne et al., 2014	
$2\ CH_2(OH)C(OO^\bullet)(CH_3)CO(OH) \rightarrow 2\ CH_2(OH)C(O^\bullet)(CH_3)CO(OH) + O_2$		7.5 10^7			BR: 100%
$CH_2(OH)C(O^\bullet)(CH_3)CO(OH) \rightarrow CH_3COCH_2(OH) + C^\bullet O(OH)$					4 - 5
$C^\bullet O(OH) + O_2 \rightarrow CO(OH)(OO^\bullet)$		2.0 10^9			3
$2\ CH_2(OH)C(OO^\bullet)(CH_3)CO(OH) \rightarrow 2\ CH_3COCH_2(OH) + 2\ CO(OH)(OO^\bullet) - O_2$	R(848)	$7.5 \cdot 10^7$			= k(2 $CH_2(OO^\bullet)CO(O^-)$) - 6
$2\ CH_2(OH)C(OO^\bullet)(CH_3)CO(O^-) \rightarrow 2\ CH_2(OH)C(O^\bullet)(CH_3)CO(O^-) + O_2$		7.5 10^7			BR: 100%
$CH_2(OH)C(O^\bullet)(CH_3)CO(O^-) \rightarrow CH_3COCH_2(OH) + C^\bullet O(O^-)$					4 - 5
$C^\bullet O(O^-) + O_2 \rightarrow CO(O^-)(OO^\bullet)$		2.0 10^9			3
$2\ CH_2(OH)C(OO^\bullet)(CH_3)CO(O^-) \rightarrow 2\ CH_3COCH_2(OH) + 2\ CO(O^-)(OO^\bullet) - O_2$	R(849)	7.5 10^7			= k(2 $CH_2(OO^\bullet)CO(O^-)$) - 6

1 - MACR is not known to be readily hydrated. Only the non-hydrated form is considered.

2 - For MACR, MVK, HMACR and MVKOH we suppose following Liu et al. (2009) for MACR that the addition on the external double bonded carbon is the main oxidation pathway. The SAR from Minakata et al. (2009) estimates a 97% branching ratio for this external addition on MACR.

3 - 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.

4 - 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.

5 - 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.

6 - 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. (1986)
Others	$CH_3CH_2(OO^\bullet)$	Monod et al. (2007)

7 - As for MACR, only the non-hydrated form of HMACR is considered.

8 - Two equilibriums are possible for MVK: the hydration of the ketone and the keto-enol tautomerism. Even if the enol form can exist in water because of the resonance with the second double bond, we suppose that its proportion is negligible (Smith and March, 2007). Like MACR, only the non-hydrated form is considered.

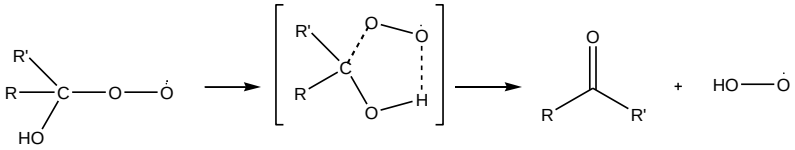
9 - As for MVK, only the non-hydrated form is considered.

10 - Hydroxybutandione can hydrate to three distinct forms : $CH_3C(OH)(OH)COCH_2(OH)$, $CH_3COC(OH)(OH)CH_2(OH)$ and $CH_3C(OH)(OH)C(OH)(OH)CH_2(OH)$. The hydration constants are estimated respectively to 2.28, 5.60 and 3.22, giving contributions of 19%, 46% and 27% to the total species. The non hydrated form is not considered as it contributes only to 8% of the total species.

11 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 44% for OH on C(OH)(OH), 38% on CH_2, 8% on CH_3, 10% for OH on $CH_2(OH)$. The first two pathways are considered corresponding to 82% of the total reactivity. They have been scaled to 54/46%.

12 - Rate constant calculated from Doussin and Monod (2013).

13 - The oxidation by the radicals ($NO_3^{\bullet}$, $SO_4^{\bullet -}$, $Cl^{\bullet}$,$Cl_2^{\bullet -}$, $CO_3^{\bullet -}$) is supposed to produce the same R(OO$^{\bullet}$) as the oxidation by HO$^{\bullet}$ with the same branching ratios. The electron transfer pathways are not considered for these radicals. The H abstraction on an (OH) group by the $NO_3^{\bullet}$ radical is also neglected because this reaction is thermodynamically disfavored.
14 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 45% for OH on C(OH)(OH), 33% on CH_2, 11% on CH_3, 12% for OH on CH_2(OH). The first two pathways are considered corresponding to 78% of the total reactivity. They have been scaled to 58/42%.
15 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 33% for OH on CH_3C(OH)(OH), 31% for (OH) on C(OH)(OH)CH_2(OH), 23% on CH_2(OH), 7% for OH on CH_2(OH), 6% for CH_3. The first three pathways are considered corresponding to 87% of the total reactivity. They have been scaled to 38/36/26%.
16 - Non-limiting reaction following Bothe et al. (1978).
17 - The $HO_2^{\bullet}$ 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}.
18 - 3,4-hydroxybutan-2-one hydration is estimated to K^h = 0.13. The proportion of the hydrate is 12%. Its oxidation is therefore neglected.
19 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 61% on CH_2, 14% on CH, 9% for OH on CH_2(OH). 8% on CH_3 and 8% for OH on CH(OH). The first two pathways are considered corresponding to 75% of the total reactivity. They have been scaled to 81/19%.
20 - 1,4-dihydroxybutanedione has 2 hydrates: the monohydrate CH_2(OH)COC(OH)(OH)CH_2(OH) and the di-hydrate CH_2(OH)C(OH)(OH)C(OH)(OH)CH_2(OH) with hydratation constant estimated respectively to K_h = 20.4 and K_h = 52.5. The mono-hydrate and di-hydrate represent 28% and 70% of the total species. Therefore, only the reactivity of the di-hydrate is considered.
21 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 51% for OH on C(OH), 37% for CH_2 on CH_2(OH), 12% for OH on CH_2(OH). The first two pathways are considered corresponding to 88% of the total reactivity. They have been scaled to 58/42%.
22 - 1,3,4-trihydroxybutanone has one hydrate. The hydration constant leading to CH_2(OH)C(OH)(OH)CH(OH)CH_2(OH) is estimated to K_h = 0.57 and represents 64% of the total species. Only the reactivity of the non-hydrated form is considered.
23 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 47% for CH_2 on CH(OH)CH_2(OH), 24% for CH_2 on COCH_2(OH), 10% for CH on CH(OH), 7% for OH of CH_2(OH) on CH(OH)CH_2(OH), 6% for OH on CH(OH) and 6% for OH on COCH(OH). The three first pathways are considered corresponding to 82% of the total reactivity. They have been scaled to 58/30/12%.
24 - 2,4-dihydroxy-3-oxobutanal has three distinct hydrates. The hydration to CH_2(OH)COCH(OH)CH(OH)(OH), CH_2(OH)C(OH)(OH)CH(OH)CHO and CH_2(OH)C(OH)(OH)CH(OH)CH(OH)(OH) are estimated respectively to K_h = 44.9, K_h = 2.5 and K_h = 112.3. The first mono-hydrate represents 28% of the total species, the second mono-hydrate 2% and the di-hydrate 70%. Therefore, the reactivity of the first mono-hydrate and the di-hydrate was considered.
25 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 32% for OH on CH(OH)(OH), 27% for CH_2 on CH_2(OH), 24% for CH on CH(OH)(OH), 6% for OH on CH_2OH, 6% for OH on CH(OH) and 4% for CH on CH(OH). The three first pathways are considered corresponding to 83% of the total reactivity. They have been scaled to 38/33/29%.
26 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 24% for OH on CH(OH)(OH), 24% for OH on C(OH)(OH), 20% for CH on CH(OH)(OH), 18% for CH_2 on CH_2(OH), 5% for OH on CH_2(OH), 5% for OH on CH(OH) and 3% for CH on CH(OH). The four first pathways are considered corresponding to 86% of the total reactivity. They have been scaled to 28/28/23/21%.
27- Von Sonntag (1987) et Schuchmann & Von Sonntag (1988) have shown that the $HO_2^{\bullet}$ elimination for RC(OH)(OH)(OO$^{\bullet}$) species is fast. This is confirmed by McElroy and Waygood (1991) for hydrated formaldehyde. We supposed a kinetic constant equal to 1.0 10^6 s^{-1}.

28 - 2-oxo-3,4-dihidroxybutanal has three distinct hydrates. The hydration to $CH_2(OH)CH(OH)COCH(OH)(OH)$, $CH_2(OH)CH(OH)C(OH)(OH)CHO$ and $CH_2(OH)CH(OH)C(OH)(OH)CH(OH)(OH)$ are estimated respectively to K_h = 252.4, K_h = 23.2 and K_h = 2126.6. The first mono-hydrate represents 11% of the total species, the second mono-hydrate 1% and the di-hydrate 88%. Therefore, only the reactivity of the di-hydrate is considered.
29 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 37% for CH_2 on $CH_2(OH)$, 20% for OH on CH(OH)(OH), 20% for OH on C(OH)(OH), 7% for CH on CH(OH)(OH), 6% for CH on CH(OH), 5% for OH on CH_2OH, 5% for OH on CH(OH). The three first pathways are considered corresponding to 77% of the total reactivity. They have been scaled to 48/26/26%.
30 - 2-oxo-3-hidroxybutanedial has seven different hydrates. The tri-hydrated form represents 95% of the total species ($K_h = 1.46\ 10^6$). Therefore, only the reactivity of the tri-hydrate is considered.
31 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 23% for OH of CH(OH)(OH) on CH(OH)(OH)CH(OH), 22% for OH of CH(OH)(OH) on C(OH)(OH)CH(OH)(OH), 21% for OH of C(OH)(OH), 19% for CH of CH(OH)(OH) on CH(OH)(OH)CH(OH), 8% for CH of CH(OH)(OH) on C(OH)(OH)CH(OH)(OH), 5% for OH on CH(OH), 2% for CH on CH(OH). The first four pathways are considered corresponding to 86% of the total reactivity. They have been scaled to 27/26/25/22%.
32 - 2,4-dioxo-3-hydroxybutanoic acid has three hydrates. The hydration to $CO(OH)COCH(OH)CH(OH)(OH)$, $CO(OH)C(OH)(OH)CH(OH)CHO$ and $CO(OH)C(OH)(OH)CH(OH)CH(OH)(OH)$ are estimated respectively to K_h = 79, K_h = 86.1 and K_h = 6740.8. The di-hydrated form represents 98% of the total species.Therefore, only the reactivity of the di-hydrated form is considered. For the monanion, the hydration to $CO(O^-)COCH(OH)CH(OH)(OH)$, $CO(O^-)C(OH)(OH)CH(OH)CHO$ and $CO(O^-)C(OH)(OH)CH(OH)CH(OH)(OH)$ are estimated respectively to K_h = 35.3, K_h = 0.56 and K_h = 19.7. The first hydrate represents 63% of the total species. Therefore, onlythe reactivity of this mono-hydrate form is considered.
33 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 36% for OH on CH(OH)(OH), 30% for CH on CH(OH)(OH), 23% for OH on C(OH)(OH), 8% for OH on CH(OH), 3% for CH on CH(OH). The three first pathways are considered corresponding to 89% of the total reactivity. They have been scaled to 41/33/26%.
34 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 45% for OH on CH(OH)(OH), 33% for CH on CH(OH)(OH), 9% for OH on CH(OH), 7% for CH on CH(OH), 6% for for the electron transfer on $CO(O^-)$. The two first pathways are considered corresponding to 78% of the total reactivity. They have been scaled to 58/42%.
35 - 2,3-dioxobutanal has seven distinct hydrates. The hydration to $CH_3C(OH)(OH)C(OH)(OH)CH(OH)(OH)$ and $CH_3COC(OH)(OH)CH(OH)(OH)$ are estimated respectively to $K_h = 1.97\ 10^5$ and $K_h = 5.15\ 10^4$ and represent 77% and 20% of the total species. Therefore, only the reactivity of these two hydrates is considered.
36 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 42% for OH on CH(OH)(OH), 36% for OH on C(OH)(OH), 13% for CH on CH(OH)(OH). 9% on CH_3. The first two pathways are considered corresponding to 78% of the total reactivity. They have been scaled to 54/46%.
37 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 30% for OH on $CH_3C(OH)(OH)$, 28% for OH on CH(OH)(OH), 27% for OH on the other C(OH)(OH), 10% for CH on C(OH)(OH) and 5% on CH_3. The first three pathways are considered corresponding to 85% of the total reactivity. They have been scaled to 35/33/32%.
38 - 2-hydroxy,3-oxobutanal has three distinct hydrates. The hydration to $CH_3COCH(OH)CH(OH)(OH)$ is estimated to $K_h = 3.5\ 10^1$. This hydrate represents 64% of the total species, therefore only its reactivity is considered.
39 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 44% for OH on CH(OH)(OH), 32% for CH on CH(OH)(OH), 9% CH_3. 8% for OH on CH(OH) and 6% for CH on CH(OH). The first two pathways are considered corresponding to 76% of the total reactivity. They have been scaled to 58/42%.
40 - 2-hydroxy, 3-oxobutanoïc acid hydration is estimated to K_h = 0.53. The hydrate represents 35% of the total species. Therefore the reactivity of both the hydrated and non-hydrated species are considered. 2-hydroxy, 3-oxobutanoate ion is estimated to K_h = 0.07. The hydrate represents 7% of the total species. Therefore only the reactivity of non hydrated ion is considered.
41 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 55% on CH_3, 33% for OH on CH(OH) and 12% for CH on CH(OH). The first two pathways are considered corresponding to 88% of the total reactivity. They have been scaled to 63/37%.
42 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 74% for OH on C(OH)(OH), 13% on CH_3, 10% for OH on CH(OH) and 3% for CH on CH(OH). The first two pathways are considered corresponding to 87% of the total reactivity. They have been scaled to 85/15%.
43 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 29% for the electron transfer on $CO(O^-)$, 27% for OH on CH(OH), 25% on CH_3 and 19% for CH on CH(OH). The first three pathways are considered corresponding to 81% of the total reactivity. They have been scaled to 36/33/31%.
44 - 2,4-dihidroxy-3-oxobutanoic acid has one hydrate $CH_2(OH)C(OH)(OH)CH(OH)CO(OH)$ with K_h = 2.36. The hydrated form represents 70% of the total species. Therefore, only the reactivity of the hydrate is considered. For the monoanion, the hydrated form represents only 24% of the total species (K_h = 0.31). Therefore, only the reactivity of the non-hydrated form is considered.
45 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 47% for OH on C(OH)(OH) 34% for CH_2 on $CH_2(OH)$, 10% for OH on $CH_2(OH)$, 7% for OH on CH(OH) and 2% for CH on CH(OH). The two first pathways are considered corresponding to 81% of the total reactivity. They have been scaled to 58/42%.
46 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 50% for CH_2 on $CH_2(OH)$, 15% for the electron transfer on $CO(O^-)$, 14% for OH on CH(OH), 12% for OH on $CH_2(OH)$, 9% for CH on CH(OH). The three first pathways are considered corresponding to 79% of the total reactivity. They have been scaled to 63/19/18%.
47 - 2-hydroxy, 3,4-dioxobutanoic acid di-hydration is estimated to $K_h = 1.5\ 10^4$. The dihydrate represents 96% of the total species. Therefore only the reactivity of the dihydrate is considered. 2-hydroxy, 3,4-dioxobutanoate ion is estimated to $K_h = 9.2\ 10^2$. The dihydrate and the monohydrate (on the aldehyde function) represent respectively 81% and 18% of the total species. Therefore the reactivity of these two hydrates is considered.
48 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 39% for OH on CH(OH)(OH), 39% for OH on C(OH)(OH), 14% for CH on CH(OH)(OH), 6% for OH on CH(OH) and 2% for CH on CH(OH). The first two pathways are considered corresponding to 78% of the total reactivity. They have been scaled to 50/50%.
49 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 46% for OH on CH(OH)(OH), 21% for CH on CH(OH)(OH), 13% for the electron transfer on $CO(O^-)$, 12% for OH on CH(OH), 8% for CH on CH(OH). The first three pathways are considered corresponding to 80% of the total reactivity. They have been scaled to 58/26/16%.
50 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 33% for OH on CH(OH)(OH), 33% for OH on C(OH)(OH), 12% CH on CH(OH)(OH), 9% for the electron transfer on $CO(O^-)$, 9% for OH on CH(OH), 4% for CH on CH(OH). The first three pathways are considered corresponding to 78% of the total reactivity. They have been scaled to 42/42/16%.

51 - 2-oxomalic acid hydration is estimated to K_h = 80. The hydrate represents 99% of the total species. Therefore only the reactivity of the hydrate is considered. The first 2-oxomalate monoanion ($CO(OH)CH(OH)COCO(O^-)$) hydration is estimated to K_h = 0.52. The hydrate represents 34% of the total species. Therefore the reactivity of both hydrated and non hydrated ions is considered. The second 2-oxomalate monoanion ($CO(O^-)CH(OH)COCO(OH)$) hydration is estimated to K_h = 10.8. The hydrate represents 92% of the total species. Therefore only the reactivity of the hydrate is considered. The 2-oxomalate dianion hydration is estimated to K_h = 0.07. The hydrate represents 7% of the total species. Therefore only the reactivity of the non hydrated form is considered.
52 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 79% for OH on C(OH)(OH), 18% for OH on CH(OH), 3% for CH on CH(OH). The first pathway is considered corresponding to 79% of the total reactivity. It has been scaled to 100%.
53 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 42% for the electron transfer on $CO(O^-)$, 42% for OH on CH(OH), 16% for CH on CH(OH). The first two pathways are considered corresponding to 84% of the total reactivity. They have been scaled to 50/50%.
54 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 79% for OH on C(OH)(OH), 10% for OH on CH(OH), 8% for the electron transfer on $CO(O^-)$, 3% for CH on CH(OH). The first pathway is considered corresponding to 79% of the total reactivity. It has been scaled to 100%.
55 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 51% for OH on C(OH)(OH), 22% for the electron transfer on $CO(O^-)$, 20% for OH on CH(OH), 7% for CH on CH(OH). The first three pathways are considered corresponding to 93% of the total reactivity. They have been scaled to 55/24/21%.
56 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 32% for the electron transfer on $CO(O^-)CH(OH)$, 29% for OH on CH(OH), 22% for CH on CH(OH). 17% for the electron transfer on $COCO(O^-)$. The first three pathways are considered corresponding to 83% of the total reactivity. They have been scaled to 39/35/26%.
57 - Dioxosuccinic acid di-hydration is estimated to $1.0\ 10^6$. The dihydrate represents 99% of the total species. Therefore only the reactivity of the dihydrate is considered. Dioxosuccinate monoanion di-hydration is estimated to $1.1\ 10^3$. The dihydrate and the monohydrate represent 81% and 17% of the total species. Therefore only the reactivity of the dihydrate and the monohydrate is considered. Dioxosuccinate dianion hydration is estimated to 3.3. The monohydrate and the non-hydrated form represent 58% and 23% of the total species respectively. Therefore only the reactivity of the monohydrate and the non-hydrated form is considered.
58 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 100% for OH on C(OH)(OH).
59 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 82% for OH on C(OH)(OH), 18% for the electron transfer on $CO(O^-)$. The first pathway is considered corresponding to 82% of the total reactivity. It has been scaled to 100%.
60 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 60% for OH on $C(OH)(OH)CO(O^-)$, 34% for OH on CO(OH)C(OH)(OH), 6% for the electron transfer on $CO(O^-)$. The first two pathways are considered corresponding to 94% of the total reactivity. They have been scaled to 64/36%
61 - Branching ratios are calculated by the SAR from Doussin and Monod (2013): 100% for the electron transfer on $CO(O^-)$.
62 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 82% for OH on C(OH)(OH), 10% for the electron transfer on $COCO(O^-)$, 8% for the electron transfer on $C(OH)(OH)CO(O^-)$. The first pathway is considered corresponding to 82% of the total reactivity. It has been scaled to 100%.
63 - 2,3-dioxobutanedial tri-hydration is estimated to $2.58\ 10^{11}$. The dihydrate represents 98% of the total species. Therefore only the reactivity of the trihydrate is considered.
64 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 44% for OH on CH(OH)(OH), 41% for OH C(OH)(OH), 15% for H on CH(OH)(OH). The two first pathways are considered corresponding to 85% of the total reactivity. It has been scaled to 52/48%.
65 - 2,3-dioxobutanoic acid di-hydration is estimated to $1.1\ 10^3$. The dihydrate represents 82% of the total species. Therefore only the reactivity of the dihydrate is considered. For the first mono-hydrate $CH_3C(OH)(OH)COCO(O-)$, K_h = 1.25 and for the second mono-hydrate, K_h = 1.25. For the di-hydrate, K_h = 0.78. The two hydrates represent 29% and 29% of the total species. The di-hydrate represents only 18% of the total species. Therefore the reactivity of the two mono-hydrates and the non-hydrated form is considered.
66 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 56% for OH of C(OH)(OH) on $CH_3C(OH)(OH)$, 34% for OH of C(OH)(OH) on C(OH)(OH)CO(OH), 10% for CH_3. The two first pathways are considered corresponding to 90% of the total reactivity. It has been scaled to 62/38%.
67 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 63% for CH_3, 37% for the electron transfer on $COCO(O^-)$. The two pathways are considered corresponding to 100% of the total reactivity.
68 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 76% for OH on C(OH)(OH), 14% for CH_3 and 10% for the electron transfer on $COCO(O^-)$. The first pathway is considered corresponding to 76% of the total reactivity. It has been scaled to 100%.
69 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 76% for OH on C(OH)(OH), 16% for CH_3 and 10% for the electron transfer on $COCO(O^-)$. The first pathway is considered corresponding to 76% of the total reactivity. It has been scaled to 100%.
70 - 2,3-dioxo-4-hydroxybutanal tri-hydration is estimated to $2.0\ 10^6$. The tri-hydrate represents 93% of the total species. Therefore only the reactivity of the trihydrate is considered.
71 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 24% for OH on CH(OH)(OH), 24% for OH of C(OH)(OH) on $CH_2(OH)C(OH)(OH)$, 22% for OH of C(OH)(OH) on C(OH)(OH)CH(OH)(OH), 17% for CH_2, 8% for CH on CH(OH)(OH), 5% for OH on $CH_2(OH)$. The 4 first pathways are considered corresponding to 87% of the total reactivity. It has been scaled to 28/27/25/20%.
72 - 2,3-dioxo-4-hydroxybutanoic acid dihydration is estimated to $7.3\ 10^3$. The dihydrate represents 95% of the total species. Therefore only the reactivity of the dihydrate is considered. The K_h for the monohydrates $CH_2(OH)C(OH)(OH)COCO(O^-)$ and $CH_2(OH)COC(OH)(OH)CO(O^-)$ are respectively estimated to 5.6 and 2.3; for the di-hydrate, K_h = 6.4. Therefore, only the reactivity of $CH_2(OH)C(OH)(OH)COCO(O^-)$ and of the di-hydrate is considered.
73 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 38% for OH of C(OH)(OH) on $CH_2(OH)C(OH)(OH)$, 28% for CH_2, 24% for OH of C(OH)(OH) on C(OH)(OH)CO(OH), 9% for OH on $CH_2(OH)$. The three first pathways are considered corresponding to 90% of the total reactivity. It has been scaled to 42/31/27%.

74 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) :48% for OH on C(OH)(OH), 34% for CH_2, 12% for OH on CH_2(OH), 7% for the electron transfer on $CO(O^-)$. The two first pathways are considered corresponding to 82% of the total reactivity. It has been scaled to 58/42%.

75 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 35% for OH of C(OH)(OH) on C(OH)(OH)$CO(O^-)$, 31% for OH of C(OH)(OH) on CH_2(OH)C(OH)(OH), 23% for CH2, 7% for OH on CH_2(OH), 3% for the electron transfer on $CO(O^-)$. The three first pathways are considered corresponding to 89% of the total reactivity. It has been scaled to 39/35/26%.

76 - 2,3,4-trioxobutanoic acid tri-hydration is estimated to 5.08 10^8. The trihydrate represents 99% of the total species. Therefore only the reactivity of the trihydrate is considered. The monoanion tri-hydration is estimated to 1.97 10^5. The trihydrate and the dihydrate CH(OH)(OH)C(OH)(OH)$COCO(O^-)$ represent 76% and 20% of the total species. Therefore only the reactivity of the trihydrate and this dihydrate is considered.

77 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 34% for OH on CH(OH)(OH), 32% for OH of C(OH)(OH) on CH(OH)(OH)C(OH)(OH), 22% for OH on C(OH)(OH) on C(OH)(OH)CO(OH), 12% for CH on CH(OH)(OH). The three first pathways are considered corresponding to 88% of the total reactivity. It has been scaled to 39/36/25%.

78 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 44% for OH on CH(OH)(OH), 37% for OH on C(OH)(OH), 13% for CH on CH(OH)(OH), 6% for the electron transfer on $CO(O^-)$. The two first pathways are considered corresponding to 81% of the total reactivity. It has been scaled to 54/46%.

79 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 32% for OH of C(OH)(OH) on C(OH)(OH)CO(O-), 29% for OH on CH(OH)(OH), 27% for OH of C(OH)(OH) on CH(OH)(OH)C(OH)(OH), 10% for CH of CH(OH)(OH), 3% for for the electron transfer on $CO(O^-)$.The three first pathways are considered corresponding to 88% of the total reactivity. It has been scaled to 36/33/31%.

80 - Methacrylic acid epoxide is supposed to be quickly hydrolysed. The pH dependence of this hydrolysis has been studied by Birdsall et al. (2014) and is considered for this species.

81 - Hydroxymethyl-methyl-α-lactone is supposed to be quickly hydrolysed like methacrylic acid. The same hypothesis can be found in Kjaergaard et al. (2012). We do not consider here the potential reactions with nitric acid proposed by Kjaergaard et al. (2012).

82 - The hydrolysis kinetics for HMML is unknown. An arbitrarily fast value ($k = 10^6\ s^{-1}$) is therefore applied here.

83 - 2-Methylglyceric acid can be protonated. The acidic form and the anionic form are considered.

84 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 65% for CH_2(OH), 16% for CH_3, 11% for OH on CH_2(OH) and 8% for OH on C(OH). The first two pathways are considered corresponding to 81% of the total reactivity. They have been scaled to 80/20%.

85 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 62% for CH_2(OH), 15% for CH_3, 9% for the electron transfer, 8% for OH on C(OH) and 6% for OH on CH_2(OH). The first two pathways are considered corresponding to 77% of the total reactivity. They have been scaled to 81/19%.

86 - 2-hydroxy,3-(oxomethyl)-propanoic acid hydration is estimated to 46. The hydrate represents 98% of the total species. Therefore only the reactivity of the hydrate is considered. 2-hydroxy,3-(oxomethyl)-propanoate anion hydration is estimated to 6.1. The monohydrate represents 86% of the total species. Therefore only the reactivity the hydrate is considered.

87 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 47% for OH on CH(OH)(OH), 30% for CH(OH)(OH), 15% for CH_3 and 8% for OH on C(OH). The first two pathways are considered corresponding to 77% of the total reactivity. They have been scaled to 61/39%.

88 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 34% for CH(OH)(OH), 31% for OH on CH(OH)(OH), 17% for CH_3, 9% for the electron transfer and 9% for OH on C(OH). The first three pathways are considered corresponding to 82% of the total reactivity. They have been scaled to 41/38/21%.

89 - 2-hydroxy-2-(hydroxymethyl)-3-oxopropanoic acid hydration is estimated to 84. The hydrate represents 99% of the total species. Therefore only the reactivity of the hydrate is considered. 2-hydroxy-2-(hydroxymethyl)-3-oxopropanoate anion hydration is estimated to 11. The monohydrate represents 92% of the total species. Therefore only the reactivity the hydrate is considered.

90 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 38% for CH_2(OH), 31% for OH on CH(OH)(OH), 19% for CH on CH(OH)(OH), 7% for OH on CH_2(OH) and 5% for OH on C(OH). The first three pathways are considered corresponding to 88% of the total reactivity. They have been scaled to 43/35/22%.

91 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 43% for CH_2(OH), 21% for CH(OH)(OH), 20% for OH on CH(OH)(OH), 6% for the electron transfer, 5% for OH on C(OH) and 5% forOH on CH_2(OH). The first three pathways are considered corresponding to 84% of the total reactivity. They have been scaled to 51/25/24%.

92 - 2,3-hydroxy-2-(hydroxymethyl)-propanoic acid can be protonated. The acidic form and the anionic form are considered.

93 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 80% for CH_2(OH), 15% for OH on CH_2(OH), 5% forOH on C(OH). The first pathway is considered corresponding to 80% of the total reactivity. It has been scaled to 100%.

94 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 81% for CH_2(OH), 8% for OH on CH_2(OH), 6% for the electron transfer and 5% forOH on C(OH). The first pathway is considered corresponding to 81% of the total reactivity. It has been scaled to 100%.

95 - Methyltartronic acid can be protonated two times. The acidic form and the two anionic forms are considered.

96 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 66% for CH_3 and 34% for OH on C(OH). The first two pathways are considered corresponding to 100% of the total reactivity.

97 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 48% for CH_3, 27% for electron transfer, and 25% forOH on C(OH). The first two pathways are considered corresponding to 75% of the total reactivity. They have been scaled to 64/36%.

98 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 43% for electron transfer, 38% for CH_3, and 19% forOH on C(OH). The first two pathways are considered corresponding to 80% of the total reactivity. They have been scaled to 53/47%.

99 - 2-hydroxy-2-(oxomethyl)-3-oxopropanoic acid hydration is estimated to 1.1 10^5. The dihydrate represents 99% of the total species. Therefore only the reactivity of the dihydrate is considered. 2-hydroxy-2-(oxomethyl)-3-oxopropanoic anion hydration is estimated to 2 10^3. The dihydrate represents 95% of the total species. Therefore only the reactivity of the dihydrate is considered.

100 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 61% for OH on CH(OH)(OH), 35% for CH(OH)(OH), and 4% forOH on C(OH). The first two pathways are considered corresponding to 96% of the total reactivity. They have been scaled to 64/36%.

101 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 44% for CH on CH(OH)(OH), 44% for OH on CH(OH)(OH), 6% for the electron transfer and 6% forOH on C(OH). The first two pathways are considered corresponding to 88% of the total reactivity. They have been scaled to 50/50%.

102 -2-(hydroxymethyl)-tartronic acid can be protonated two times. The acidic form and the two anionic forms are considered.

103 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 71% for CH_2(OH), 20% for OH on CH_2(OH), 9% for the electron transfer and 9% forOH on C(OH). The first two pathways are considered corresponding to 91% of the total reactivity. They have been scaled to 78/22%.

104 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 70% for CH_2(OH), 11% for OH on CH_2(OH), 10% for the electron transfer and 9% forOH on C(OH). The first two pathways are considered corresponding to 81% of the total reactivity. They have been scaled to 86/14%.

105 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 67% for CH_2(OH), 18% for the electron transfer, 9% forOH on C(OH) and 6% for OH on CH_2(OH). The first two pathways are considered corresponding to 85% of the total reactivity. They have been scaled to 79/21%.

106 - 2-(oxomethyl)-tartronic acid hydration is estimated to 343. The hydrate represents 99.7% of the total species. Therefore only the reactivity of the hydrate is considered. 2-(oxomethyl)-tartronate monoanion hydration is estimated to 46. The hydrate represents 98% of the total species. Therefore only the reactivity of the hydrate is considered. 2-(oxomethyl)-tartronate dianion hydration is estimated to 6.1. The hydrate represents 86% of the total species. Therefore only the reactivity of the hydrate is considered.

107 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 68% for OH on CH(OH)(OH), 26% for CH on CH(OH)(OH) and 6% fo OH on C(OH). The first two pathways are considered corresponding to 94% of the total reactivity. They have been scaled to 72/28%.

108 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 49% for OH on CH(OH)(OH), 33% for CH on CH(OH)(OH), 9% for the electron transfer and 9% fo OH on C(OH). The first two pathways are considered corresponding to 82% of the total reactivity. They have been scaled to 60/40%.

109 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 37% for CH on CH(OH)(OH), 32% for OH on CH(OH)(OH), 21% for the electron transfer and 10% fo OH on C(OH). The first three pathways are considered corresponding to 90% of the total reactivity. They have been scaled to 41/36/23%.

110 - Hydroxymethanetricarboxylic acid can be protonated three times. The acidic form and the three anionic forms are considered.

111 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 100% for OH on C(OH).

112 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 52% for the electron transfer, 48% for OH on C(OH). Both pathways are considered corresponding to 100% of the total reactivity.

113 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 69% for the electron transfer, 31% for OH on C(OH). Both pathways are considered corresponding to 100% of the total reactivity.

114 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 77% for the electron transfer, 23% for OH on C(OH). The first pathway is considered corresponding to 77% of the total reactivity. It has been scaled to 100%.

115 - Methacrylic acid can be protonated. The acidic form and the anionic form are considered.

116 - For Methacrylic acid and Methacrylate, we suppose that the addition on the external double bonded carbon is the main oxidation pathway. This is corroborated by RPE measurements carried out by J.-L. Clément (pers. comm.).

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Species		K_a or K_h	-ΔH/R (K)	References	Notes
C4 compounds					
Hydroxybutanedione					
$CH_3COCOCH_2(OH) + H_2O \leftrightarrow CH_3C(OH)(OH)COCH_2(OH)$	T(163)	2.3		Estimated with GROMHE	
$CH_3COCOCH_2(OH) + H_2O \leftrightarrow CH_3COC(OH)(OH)CH_2(OH)$	T(164)	5.6		Estimated with GROMHE	
$CH_3COCOCH_2(OH) + 2\ H_2O \leftrightarrow CH_3C(OH)(OH)C(OH)(OH)CH_2(OH)$	T(165)	6.4		Estimated with GROMHE	
$CH_3COCOCH(OH)(OO^\bullet) + H_2O \leftrightarrow CH_3C(OH)(OH)COCH(OH)(OO^\bullet)$	T(166)	2.3			1 = $K_h(CH_3COCOCH_2(OH)/CH_3C(OH)(OH)COCH_2(OH))$
$CH_3COCOCH(OH)(OO^\bullet) + H_2O \leftrightarrow CH_3COC(OH)(OH)CH(OH)(OO^\bullet)$	T(167)	5.6			1 = $K_h(CH_3COCOCH_2(OH)/CH_3COC(OH)(OH)CH_2(OH))$
$CH_3COCOCH(OH)(OO^\bullet) + 2\ H_2O \leftrightarrow CH_3C(OH)(OH)C(OH)(OH)CH(OH)(OO^\bullet)$	T(168)	6.4			1 = $K_h(CH_3COCOCH_2(OH)/CH_3C(OH)(OH)C(OH)(OH)CH_2(OH))$
3,4-dihydroxybutan-2-one					
$CH_2(OH)CH(OH)COCH_3 + H_2O \leftrightarrow CH_2(OH)CH(OH)C(OH)(OH)CH_3$	T(169)	$1.3\ 10^{-1}$		Estimated with GROMHE	
$CH(OH)(OO^\bullet)CH(OH)COCH_3 + H_2O \leftrightarrow CH(OH)(OO^\bullet)CH(OH)C(OH)(OH)CH_3$	T(170)	$1.3\ 10^{-1}$			1 = $K_h(CH_2(OH)CH(OH)COCH_3/CH_2(OH)CH(OH)C(OH)(OH)CH_3)$
$CH_2(OH)C(OH)(OO^\bullet)COCH_3 + H_2O \leftrightarrow CH_2(OH)C(OH)(OO^\bullet)C(OH)(OH)CH_3$	T(171)	$1.3\ 10^{-1}$			1 = $K_h(CH_2(OH)CH(OH)COCH_3/CH_2(OH)CH(OH)C(OH)(OH)CH_3)$
1,4-dihydroxybutanedione					
$CH_2(OH)COCOCH_2(OH) + H_2O \leftrightarrow CH_2(OH)C(OH)(OH)COCH_2(OH)$	T(172)	$2.0\ 10^{1}$		Estimated with GROMHE	
$CH_2(OH)COCOCH_2(OH) + 2\ H_2O \leftrightarrow CH_2(OH)C(OH)(OH)C(OH)(OH)CH_2(OH)$	T(173)	$5.3\ 10^{1}$		Estimated with GROMHE	
$CH_2(OH)COCOCH(OH)(OO^\bullet) + H_2O \leftrightarrow CH_2(OH)C(OH)(OH)COCH(OH)(OO^\bullet)$	T(174)	$2.0\ 10^{1}$			1 = $K_h(CH_2(OH)COCOCH_2(OH)/CH_2(OH)C(OH)(OH)COCH_2(OH))$
$CH_2(OH)COCOCH(OH)(OO^\bullet) + 2\ H_2O \leftrightarrow CH_2(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OO^\bullet)$	T(175)	$5.3\ 10^{1}$			1 = $K_h(CH_2(OH)COCOCH_2(OH)/CH_2(OH)C(OH)(OH)C(OH)(OH)CH_2(OH))$
1,3,4-trihydroxybutanone					
$CH_2(OH)COCH(OH)CH_2(OH) + H_2O \leftrightarrow CH_2(OH)C(OH)(OH)CH(OH)CH_2(OH)$	T(176)	$5.7\ 10^{-1}$		Estimated with GROMHE	
$CH_2(OH)COCH(OH)CH(OH)(OO^\bullet) + H_2O \leftrightarrow CH_2(OH)C(OH)(OH)CH(OH)CH(OH)(OO^\bullet)$	T(177)	$5.7\ 10^{-1}$			1 =$K_h(CH_2(OH)COCH(OH)CH_2(OH)/CH_2(OH)C(OH)(OH)CH(OH)CH_2(OH)$
$CH_2(OH)CH(OH)COCH(OH)(OO^\bullet) + H_2O \leftrightarrow CH_2(OH)CH(OH)C(OH)(OH)CH(OH)(OO^\bullet)$	T(178)	$5.7\ 10^{-1}$			1 = $K_h(CH_2(OH)COCH(OH)CH_2(OH)/CH_2(OH)C(OH)(OH)CH(OH)CH_2(OH)$
$CH_2(OH)COC(OH)(OO^\bullet)CH_2(OH) + H_2O \leftrightarrow CH_2(OH)C(OH)(OH)C(OH)(OO^\bullet)CH_2(OH)$	T(179)	$5.7\ 10^{-1}$			1

Species		K_a or K_h	-ΔH/R (K)	References	Notes
					= $K_h(CH_2(OH)COCH(OH)CH_2(OH)/CH_2(OH)C(OH)(OH)CH(OH)CH_2(OH)$
2,4-dihydroxy-3-oxobutanal					
$CH_2(OH)COCH(OH)CHO + H_2O \leftrightarrow CH_2(OH)COCH(OH)CH(OH)(OH)$	T(180)	$4.5\ 10^1$		Estimated with GROMHE	
$CH_2(OH)COCH(OH)CHO + H_2O \leftrightarrow CH_2(OH)C(OH)(OH)CH(OH)CHO$	T(181)	2.5		Estimated with GROMHE	
$CH_2(OH)COCH(OH)CHO + 2\ H_2O \leftrightarrow CH_2(OH)C(OH)(OH)CH(OH)CH(OH)(OH)$	T(182)	$1.1\ 10^2$		Estimated with GROMHE	
$CHOCH(OH)COCH(OH)(OO^\bullet) + H_2O \leftrightarrow CH(OH)(OH)CH(OH)COCH(OH)(OO^\bullet)$	T(183)	$4.5\ 10^1$			1 = $K_h(CH_2(OH)COCH(OH)CHO/CH_2(OH)COCH(OH)CH(OH)(OH)$
$CHOCH(OH)COCH(OH)(OO^\bullet) + H_2O \leftrightarrow CHOCH(OH)C(OH)(OH)CH(OH)(OO^\bullet)$	T(184)	2.5			1 = $K_h(CH_2(OH)COCH(OH)CHO/CH_2(OH)C(OH)(OH)CH(OH)CHO)$
$CHOCH(OH)COCH(OH)(OO^\bullet) + 2\ H_2O \leftrightarrow$ $CH(OH)(OH)CH(OH)C(OH)(OH)CH(OH)(OO^\bullet)$	T(185)	$1.1\ 10^2$			1 = $K_h(CH_2(OH)COCH(OH)CHO/CH_2(OH)C(OH)(OH)CH(OH)CH(OH)(OH))$
$CH_2(OH)COCH(OH)CO(OO^\bullet) + H_2O \leftrightarrow CH_2(OH)COCH(OH)C(OH)(OH)(OO^\bullet)$	T(186)	$1.0\ 10^{-3}$			2
$CH_2(OH)COCH(OH)CO(OO^\bullet) + H_2O \leftrightarrow CH_2(OH)C(OH)(OH)CH(OH)CO(OO^\bullet)$	T(187)	2.5			1 = $K_h(CH_2(OH)COCH(OH)CHO/CH_2(OH)C(OH)(OH)CH(OH)CHO)$
$CH_2(OH)COCH(OH)CO(OO^\bullet) + 2\ H_2O \leftrightarrow CH_2(OH)C(OH)(OH)CH(OH)C(OH)(OH)(OO^\bullet)$	T(188)	$1.1\ 10^2$			1 = $K_h(CH_2(OH)COCH(OH)CHO/CH_2(OH)C(OH)(OH)CH(OH)CH(OH)(OH))$
2-oxo-3,4-dihydroxybutanal					
$CH_2(OH)CH(OH)COCHO + H_2O \leftrightarrow CH_2(OH)CH(OH)COCH(OH)(OH)$	T(189)	$2.5\ 10^2$		Estimated with GROMHE	
$CH_2(OH)CH(OH)COCHO + H_2O \leftrightarrow CH_2(OH)CH(OH)C(OH)(OH)CHO$	T(190)	$2.3\ 10^1$		Estimated with GROMHE	
$CH_2(OH)CH(OH)COCHO + 2\ H_2O \leftrightarrow CH_2(OH)CH(OH)C(OH)(OH)CH(OH)(OH)$	T(191)	$2.1\ 10^3$		Estimated with GROMHE	
$CHOCOCH(OH)CH(OH)(OO^\bullet) + H_2O \leftrightarrow CH(OH)(OH)COCH(OH)CH(OH)(OO^\bullet)$	T(192)	$2.5\ 10^2$			1 = $K_h(CH_2(OH)CH(OH)COCHO/CH_2(OH)CH(OH)COCH(OH)(OH))$
$CHOCOCH(OH)CH(OH)(OO^\bullet) + H_2O \leftrightarrow CHOC(OH)(OH)CH(OH)CH(OH)(OO^\bullet)$	T(193)	$2.3\ 10^1$			1 = $K_h(CH_2(OH)CH(OH)COCHO/CH_2(OH)CH(OH)C(OH)(OH)CHO)$
$CHOCOCH(OH)CH(OH)(OO^\bullet) + 2\ H_2O \leftrightarrow$ $CH(OH)(OH)C(OH)(OH)CH(OH)CH(OH)(OO^\bullet)$	T(194)	$2.1\ 10^3$			1 = $K_h(CH_2(OH)CH(OH)COCHO/CH_2(OH)CH(OH)C(OH)(OH)CH(OH)(OH))$
2-oxo-3-hydroxybutanedial					
$CHOCH(OH)COCHO + H_2O \leftrightarrow CH(OH)(OH)CH(OH)COCHO$	T(195)	$8.1\ 10^1$		Estimated with GROMHE	
$CHOCH(OH)COCHO + H_2O \leftrightarrow CHOCH(OH)COCH(OH)(OH)$	T(196)	$4.6\ 10^2$		Estimated with GROMHE	

Species		K_a or K_h	-ΔH/R (K)	References	Notes
CHOCH(OH)COCHO + H_2O ↔ CHOCH(OH)C(OH)(OH)CHO	T(197)	$1.0\ 10^{2}$		Estimated with GROMHE	
CHOCH(OH)COCHO +2 H_2O ↔ CH(OH)(OH)CH(OH)COCH(OH)(OH)	T(198)	$5.2\ 10^{4}$		Estimated with GROMHE	
CHOCH(OH)COCHO + 2 H_2O ↔ CH(OH)(OH)CH(OH)C(OH)(OH)CHO	T(199)	$8.2\ 10^{3}$		Estimated with GROMHE	
CHOCH(OH)COCHO + 2 H_2O ↔ CHOCH(OH)C(OH)(OH)CH(OH)(OH)	T(200)	$1.7\ 10^{4}$		Estimated with GROMHE	
CHOCH(OH)COCHO + 3 H_2O ↔ CH(OH)(OH)CH(OH)C(OH)(OH)CH(OH)(OH)	T(201)	$1.4\ 10^{6}$		Estimated with GROMHE	
CHOCOCH(OH)CO($OO^{\bullet}$) + H_2O ↔ CHOCOCH(OH)C(OH)(OH)($OO^{\bullet}$)	T(202)	$1.0\ 10^{-3}$			2
CHOCOCH(OH)CO($OO^{\bullet}$) + H_2O ↔ CH(OH)(OH)COCH(OH)CO($OO^{\bullet}$)	T(203)	$4.6\ 10^{2}$			1 = K_h(CHOCH(OH)COCHO/CHOCH(OH)COCH(OH)(OH))
CHOCOCH(OH)CO($OO^{\bullet}$) + H_2O ↔ CHOC(OH)(OH)CH(OH)CO($OO^{\bullet}$)	T(204)	$1.0\ 10^{2}$			1 = K_h(CHOCH(OH)COCHO/CHOCH(OH)C(OH)(OH)CHO)
CHOCOCH(OH)CO($OO^{\bullet}$) + 2 H_2O ↔ CH(OH)(OH)COCH(OH)C(OH)(OH)($OO^{\bullet}$)	T(205)	$5.2\ 10^{4}$			1 = K_h(CHOCH(OH)COCHO/CH(OH)(OH)CH(OH)COCH(OH)(OH))
CHOCOCH(OH)CO($OO^{\bullet}$) + 2 H_2O ↔ CHOC(OH)(OH)CH(OH)C(OH)(OH)($OO^{\bullet}$)	T(206)	$8.2\ 10^{3}$			1 = K_h(CHOCH(OH)COCHO/CH(OH)(OH)CH(OH)C(OH)(OH)CHO)
CHOCOCH(OH)CO($OO^{\bullet}$) + 2 H_2O ↔ CH(OH)(OH)C(OH)(OH)CH(OH)CO($OO^{\bullet}$)	T(207)	$1.7\ 10^{4}$			1 = K_h(CHOCH(OH)COCHO/CHOCH(OH)C(OH)(OH)CH(OH)(OH))
CHOCOCH(OH)CO($OO^{\bullet}$) + 3 H_2O ↔ CH(OH)(OH)C(OH)(OH)CH(OH)C(OH)(OH)($OO^{\bullet}$)	T(208)	$1.4\ 10^{6}$			1 = K_h(CHOCH(OH)COCHO/CH(OH)(OH)CH(OH)C(OH)(OH)CH(OH)(OH))
CHOCH(OH)COCO($OO^{\bullet}$) + H_2O ↔ CH(OH)(OH)CH(OH)COCO($OO^{\bullet}$)	T(209)	$8.1\ 10^{1}$			1 = K_h(CHOCH(OH)COCHO/CH(OH)(OH)CH(OH)COCHO)
CHOCH(OH)COCO($OO^{\bullet}$) + H_2O ↔ CHOCH(OH)COC(OH)(OH)($OO^{\bullet}$)	T(210)	$1.0\ 10^{-3}$			2
CHOCH(OH)COCO($OO^{\bullet}$) + H_2O ↔ CHOCH(OH)C(OH)(OH)CO($OO^{\bullet}$)	T(211)	$1.0\ 10^{2}$			1 = K_h(CHOCH(OH)COCHO/CHOCH(OH)C(OH)(OH)CHO)
CHOCH(OH)COCO($OO^{\bullet}$) + 2 H_2O ↔ CH(OH)(OH)CH(OH)COC(OH)(OH)($OO^{\bullet}$)	T(212)	$5.2\ 10^{4}$			1 = K_h(CHOCH(OH)COCHO/CH(OH)(OH)CH(OH)COCH(OH)(OH))
CHOCH(OH)COCO($OO^{\bullet}$) + 2 H_2O ↔ CH(OH)(OH)CH(OH)C(OH)(OH)CO($OO^{\bullet}$)	T(213)	$8.2\ 10^{3}$			1 = K_h(CHOCH(OH)COCHO/CH(OH)(OH)CH(OH)C(OH)(OH)CHO)
CHOCH(OH)COCO($OO^{\bullet}$) + 2 H_2O ↔ CHOCH(OH)C(OH)(OH)C(OH)(OH)($OO^{\bullet}$)	T(214)	$1.7\ 10^{4}$			1 = K_h(CHOCH(OH)COCHO/CHOCH(OH)C(OH)(OH)CH(OH)(OH))
CHOCH(OH)COCO($OO^{\bullet}$) + 3 H_2O ↔ CH(OH)(OH)CH(OH)C(OH)(OH)C(OH)(OH)($OO^{\bullet}$)	T(215)	$1.4\ 10^{6}$			1 = K_h(CHOCH(OH)COCHO/CH(OH)(OH)CH(OH)C(OH)(OH)CH(OH)(OH))
2,4-dioxo-3-hydroxybutanoic acid					
CO(OH)COCH(OH)CHO ↔ CO(O^{-})COCH(OH)CHO + H^{+}	T(216)	$4.1\ 10^{-3}$			= K_a($CH_3COCO(OH)/CH_3COCO(O^{-})$)
CO(OH)COCH(OH)CHO + H_2O ↔ CO(OH)COCH(OH)CH(OH)(OH)	T(217)	$7.9\ 10^{1}$		Estimated with GROMHE	

Species		K_a or K_h	-ΔH/R (K)	References	Notes
$CO(OH)COCH(OH)CHO + H_2O \leftrightarrow CO(OH)C(OH)(OH)CH(OH)CHO$	T(218)	$8.6\ 10^{1}$		Estimated with GROMHE	
$CO(OH)COCH(OH)CHO + 2\ H_2O \leftrightarrow CO(OH)C(OH)(OH)CH(OH)CH(OH)(OH)$	T(219)	$6.7\ 10^{3}$		Estimated with GROMHE	
$CO(O^-)COCH(OH)CHO + H_2O \leftrightarrow CO(O^-)COCH(OH)CH(OH)(OH)$	T(220)	$3.5\ 10^{1}$		Estimated with GROMHE	
$CO(O^-)COCH(OH)CHO + H_2O \leftrightarrow CO(O^-)C(OH)(OH)CH(OH)CHO$	T(221)	$5.6\ 10^{-1}$		Estimated with GROMHE	
$CO(O^-)COCH(OH)CHO + 2\ H_2O \leftrightarrow CO(O^-)C(OH)(OH)CH(OH)CH(OH)(OH)$	T(222)	19.7		Estimated with GROMHE	
$CO(OO^\bullet)CH(OH)COCO(OH) \leftrightarrow CO(OO^\bullet)CH(OH)COCO(O^-) + H^+$	T(223)	$4.1\ 10^{-3}$			3 = K_a(CO(OH)COCH(OH)CHO/CO(O⁻)COCH(OH)CHO)
$CO(OO^\bullet)CH(OH)COCO(OH) + H_2O \leftrightarrow C(OH)(OH)(OO^\bullet)CH(OH)COCO(OH)$	T(224)	$1.0\ 10^{-3}$			2
$CO(OO^\bullet)CH(OH)COCO(OH) + H_2O \leftrightarrow CO(OO^\bullet)CH(OH)C(OH)(OH)CO(OH)$	T(225)	$8.6\ 10^{1}$			1 = K_h(CO(OH)COCH(OH)CHO/CO(OH)C(OH)(OH)CH(OH)CHO)
$CO(OO^\bullet)CH(OH)COCO(OH) + 2\ H_2O \leftrightarrow C(OH)(OH)(OO^\bullet)CH(OH)C(OH)(OH)CO(OH)$	T(226)	$6.7\ 10^{3}$			1 = K_h(CO(OH)COCH(OH)CHO/CO(OH)C(OH)(OH)CH(OH)CH(OH)(OH))
$CO(OO^\bullet)CH(OH)COCO(O^-) + H_2O \leftrightarrow C(OH)(OH)(OO^\bullet)CH(OH)COCO(O^-)$	T(227)	$1.0\ 10^{-3}$			2
$CO(OO^\bullet)CH(OH)COCO(O^-) + H_2O \leftrightarrow CO(OO^\bullet)CH(OH)C(OH)(OH)CO(O^-)$	T(228)	$5.6\ 10^{-1}$			1 = K_h(CO(O⁻)COCH(OH)CHO/CO(O⁻)C(OH)(OH)CH(OH)CHO)
$CO(OO^\bullet)CH(OH)COCO(O^-) + 2\ H_2O \leftrightarrow C(OH)(OH)(OO^\bullet)CH(OH)C(OH)(OH)CO(O^-)$	T(229)	19.7			1 = K_h(CO(O⁻)COCH(OH)CHO/CO(O⁻)C(OH)(OH)CH(OH)CH(OH)(OH))
2,3-dioxobutanal					
$CH_3COCOCHO + H_2O \leftrightarrow CH_3COCOCH(OH)(OH)$	T(230)	$6.3\ 10^{2}$		Estimated with GROMHE	
$CH_3COCOCHO + H_2O \leftrightarrow CH_3C(OH)(OH)COCHO$	T(231)	$1.0\ 10^{1}$		Estimated with GROMHE	
$CH_3COCOCHO + H_2O \leftrightarrow CH_3COC(OH)(OH)CHO$	T(232)	$2.3\ 10^{2}$		Estimated with GROMHE	
$CH_3COCOCHO + 2\ H_2O \leftrightarrow CH_3C(OH)(OH)COCH(OH)(OH)$	T(233)	$3.1\ 10^{3}$		Estimated with GROMHE	
$CH_3COCOCHO + 2\ H_2O \leftrightarrow CH_3COC(OH)(OH)CH(OH)(OH)$	T(234)	$2.4\ 10^{4}$		Estimated with GROMHE	
$CH_3COCOCHO + 2\ H_2O \leftrightarrow CH_3C(OH)(OH)C(OH)(OH)CHO$	T(235)	$5.7\ 10^{2}$		Estimated with GROMHE	
$CH_3COCOCHO + 3\ H_2O \leftrightarrow CH_3C(OH)(OH)C(OH)(OH)CH(OH)(OH)$	T(236)	$2.9\ 10^{4}$		Estimated with GROMHE	
$CH_3COCOCO(OO^\bullet) + H_2O \leftrightarrow CH_3COCOC(OH)(OH)(OO^\bullet)$	T(237)	$1.0\ 10^{-3}$			2
$CH_3COCOCO(OO^\bullet) + H_2O \leftrightarrow CH_3C(OH)(OH)COCO(OO^\bullet)$	T(238)	$1.0\ 10^{1}$			1 = K_h($CH_3COCOCHO/CH_3C(OH)(OH)COCHO$)
$CH_3COCOCO(OO^\bullet) + H_2O \leftrightarrow CH_3COC(OH)(OH)CO(OO^\bullet)$	T(239)	$2.3\ 10^{2}$			1 = K_h($CH_3COCOCHO/CH_3COC(OH)(OH)CHO$)

Species		K_a or K_h	-ΔH/R (K)	References	Notes
$CH_3COCOCO(OO^\bullet)$ + 2 H_2O ↔ $CH_3C(OH)(OH)COC(OH)(OH)(OO^\bullet)$	T(240)	$3.1\ 10^3$			1 = $K_h(CH_3COCOCHO/CH_3C(OH)(OH)COCH(OH)(OH))$
$CH_3COCOCO(OO^\bullet)$ + 2 H_2O ↔ $CH_3COC(OH)(OH)C(OH)(OH)(OO^\bullet)$	T(241)	$2.4\ 10^4$			1 = $K_h(CH_3COCOCHO/CH_3COC(OH)(OH)CH(OH)(OH))$
$CH_3COCOCO(OO^\bullet)$ + 2 H_2O ↔ $CH_3C(OH)(OH)C(OH)(OH)CO(OO^\bullet)$	T(242)	$5.7\ 10^2$			1 = $K_h(CH_3COCOCHO/CH_3C(OH)(OH)C(OH)(OH)CHO)$
$CH_3COCOCO(OO^\bullet)$ + 3 H_2O ↔ $CH_3C(OH)(OH)C(OH)(OH)C(OH)(OH)(OO^\bullet)$	T(243)	$2.9\ 10^4$			1 = $K_h(CH_3COCOCHO/CH_3C(OH)(OH)C(OH)(OH)CH(OH)(OH))$
$CH_2(OO^\bullet)COCOCHO$ + H_2O ↔$CH_2(OO^\bullet)COCOCH(OH)(OH)$	T(244)	$6.3\ 10^2$			1 = $K_h(CH_3COCOCHO/CH_3COCOCH(OH)(OH))$
$CH_2(OO^\bullet)COCOCHO$ + H_2O ↔ $CH_2(OO^\bullet)C(OH)(OH)COCHO$	T(245)	$1.0\ 10^1$			1 = $K_h(CH_3COCOCHO/CH_3C(OH)(OH)COCHO)$
$CH_2(OO^\bullet)COCOCHO$ + H_2O ↔ $CH_2(OO^\bullet)COC(OH)(OH)CHO$	T(246)	$2.3\ 10^2$			1 = $K_h(CH_3COCOCHO/CH_3COC(OH)(OH)CHO)$
$CH_2(OO^\bullet)COCOCHO$ + 2 H_2O ↔ $CH_2(OO^\bullet)C(OH)(OH)COCH(OH)(OH)$	T(247)	$3.1\ 10^3$			1 = $K_h(CH_3COCOCHO/CH_3C(OH)(OH)COCH(OH)(OH))$
$CH_2(OO^\bullet)COCOCHO$ + 2 H_2O ↔ $CH_2(OO^\bullet)COC(OH)(OH)CH(OH)(OH)$	T(248)	$2.4\ 10^4$			1 = $K_h(CH_3COCOCHO/CH_3COC(OH)(OH)CH(OH)(OH))$
$CH_2(OO^\bullet)COCOCHO$ + 2 H_2O ↔ $CH_2(OO^\bullet)C(OH)(OH)C(OH)(OH)CHO$	T(249)	$5.7\ 10^2$			1 = $K_h(CH_3COCOCHO/CH_3C(OH)(OH)C(OH)(OH)CHO)$
$CH_2(OO^\bullet)COCOCHO$ + 3 H_2O ↔ $CH_2(OO^\bullet)C(OH)(OH)C(OH)(OH)CH(OH)(OH)$	T(250)	$2.9\ 10^4$			1 = $K_h(CH_3COCOCHO/CH_3C(OH)(OH)C(OH)(OH)CH(OH)(OH))$
2-hydroxy, 3-oxobutanal					
$CH_3COCH(OH)CHO$ + H_2O ↔ $CH_3COCH(OH)CH(OH)(OH)$	T(251)	$3.5\ 10^1$		Estimated with GROMHE	
$CH_3COCH(OH)CHO$ + H_2O ↔ $CH_3C(OH)(OH)CH(OH)CHO$	T(252)	$5.6\ 10^{-1}$		Estimated with GROMHE	
$CH_3COCH(OH)CHO$ + 2 H_2O ↔ $CH_3C(OH)(OH)CH(OH)CH(OH)(OH)$	T(253)	9.7		Estimated with GROMHE	
$CH_3COCH(OH)CO(OO^\bullet)$ + H_2O ↔ $CH_3COCH(OH)C(OH)(OH)(OO^\bullet)$	T(254)	10^{-3}			2
$CH_3COCH(OH)CO(OO^\bullet)$ + H_2O ↔ $CH_3C(OH)(OH)CH(OH)CO(OO^\bullet)$	T(255)	$5.6\ 10^{-1}$			1 = $K_h(CH_3COCH(OH)CHO/CH_3C(OH)(OH)CH(OH)CHO)$
$CH_3COCH(OH)CO(OO^\bullet)$ + 2 H_2O ↔ $CH_3C(OH)(OH)CH(OH)C(OH)(OH)(OO^\bullet)$	T(256)	9.7			1 = $K_h(CH_3COCH(OH)CHO/CH_3C(OH)(OH)CH(OH)CH(OH)(OH))$
$CH_2(OO^\bullet)COCH(OH)CHO$ + H_2O ↔ $CH_2(OO^\bullet)COCH(OH)CH(OH)(OH)$	T(257)	$3.5\ 10^1$			1 = $K_h(CH_3COCH(OH)CHO/CH_3COCH(OH)CH(OH)(OH))$
$CH_2(OO^\bullet)COCH(OH)CHO$ + H_2O ↔$CH_2(OO^\bullet)C(OH)(OH)CH(OH)CHO$	T(258)	$5.6\ 10^{-1}$			1 = $K_h(CH_3COCH(OH)CHO/CH_3C(OH)(OH)CH(OH)CHO)$
$CH_2(OO^\bullet)COCH(OH)CHO$ + 2 H_2O ↔$CH_2(OO^\bullet)C(OH)(OH)CH(OH)CH(OH)(OH)$	T(259)	9.7			1 = $K_h(CH_3COCH(OH)CHO/CH_3C(OH)(OH)CH(OH)CH(OH)(OH))$
2-hydroxy, 3-oxobutanoïc acid					
$CH_3COCH(OH)CO(OH)$ ↔ $CH_3COCH(OH)CO(O^-)$ + H^+	T(260)	$3.0\ 10^{-4}$			= $K_a(CH_2(OH)CH(OH)CO(OH)/CH_2(OH)CH(OH)CO(O^-))$

Species		K_a or K_h	-ΔH/R (K)	References	Notes
$CH_3COCH(OH)CO(OH) + H_2O \leftrightarrow CH_3C(OH)(OH)CH(OH)CO(OH)$	T(261)	$5.3\ 10^{-1}$		Estimated with GROMHE	
$CH_3COCH(OH)CO(O^-) + H_2O \leftrightarrow CH_3C(OH)(OH)CH(OH)CO(O^-)$	T(262)	$7.0\ 10^{-2}$		Estimated with GROMHE	
$CO(OH)CH(OH)COCH_2(OO^\bullet) \leftrightarrow CO(O^-)CH(OH)COCH_2(OO^\bullet) + H^+$	T(263)	$3.0\ 10^{-4}$			3 = $K_a(CH_3COCH(OH)CO(OH)/CH_3COCH(OH)CO(O^-))$
$CO(OH)CH(OH)COCH_2(OO^\bullet) + H_2O \leftrightarrow CO(OH)CH(OH)C(OH)(OH)CH_2(OO^\bullet)$	T(264)	$5.3\ 10^{-1}$			1 = $K_h(CH_3COCH(OH)CO(OH)/CH_3C(OH)(OH)CH(OH)CO(OH))$
$CO(O^-)CH(OH)COCH_2(OO^\bullet) + H_2O \leftrightarrow CO(O^-)CH(OH)C(OH)(OH)CH_2(OO^\bullet)$	T(265)	$7.0\ 10^{-2}$			1 = $K_h(CH_3COCH(OH)CO(O^-)/CH_3C(OH)(OH)CH(OH)CO(O^-))$
$CH_3COC(OH)(OO^\bullet)CO(OH) \leftrightarrow CH_3COC(OH)(OO^\bullet)CO(O^-) + H^+$	T(266)	$3.0\ 10^{-4}$			= $K_a(CH_2(OH)CH(OH)CO(OH)/CH_2(OH)CH(OH)CO(O^-))$
$CH_3COC(OH)(OO^\bullet)CO(OH) + H_2O \leftrightarrow CH_3C(OH)(OH)C(OH)(OO^\bullet)CO(OH)$	T(267)	$5.3\ 10^{-1}$		Estimated with GROMHE	
$CH_3COC(OH)(OO^\bullet)CO(O^-) + H_2O \leftrightarrow CH_3C(OH)(OH)C(OH)(OO^\bullet)CO(O^-)$	T(268)	$7.0\ 10^{-2}$		Estimated with GROMHE	
2,4-dihydroxy, 3-oxobutanoic acid					
$CO(OH)CH(OH)COCH_2(OH) \leftrightarrow CO(O^-)CH(OH)COCH_2(OH) + H^+$	T(269)	$3.0\ 10^{-4}$			= $K_a(CH_2(OH)CH(OH)CO(OH)/CH_2(OH)CH(OH)CO(O^-))$
$CO(OH)CH(OH)COCH_2(OH) + H_2O \leftrightarrow CO(OH)CH(OH)C(OH)(OH)CH_2(OH)$	T(270)	2.4		Estimated with GROMHE	
$CO(O^-)CH(OH)COCH_2(OH) + H_2O \leftrightarrow CO(O^-)CH(OH)C(OH)(OH)CH_2(OH)$	T(271)	$3.2\ 10^{-1}$		Estimated with GROMHE	
$CO(OH)CH(OH)COCH(OH)(OO^\bullet) \leftrightarrow CO(O^-)CH(OH)COCH(OH)(OO^\bullet) + H^+$	T(272)	$3.0\ 10^{-4}$			3 = $K_a(CO(OH)CH(OH)COCH_2(OH)/CO(O^-)CH(OH)COCH_2(OH))$
$CO(OH)CH(OH)COCH(OH)(OO^\bullet) + H_2O \leftrightarrow CO(OH)CH(OH)C(OH)(OH)CH(OH)(OO^\bullet)$	T(273)	2.4			1 = $K_h(CO(OH)CH(OH)COCH_2(OH)/CO(OH)CH(OH)C(OH)(OH)CH_2(OH))$
$CO(O^-)CH(OH)COCH(OH)(OO^\bullet) + H_2O \leftrightarrow CO(O^-)CH(OH)C(OH)(OH)CH(OH)(OO^\bullet)$	T(274)	$3.2\ 10^{-1}$			1 = $K_h(CO(O^-)CH(OH)COCH_2(OH)/CO(O^-)CH(OH)C(OH)(OH)CH_2(OH))$
2-hydroxy, 3,4-dioxobutanoic acid					
$CO(OH)CH(OH)COCHO \leftrightarrow CO(O^-)CH(OH)COCHO + H^+$	T(275)	$3.0\ 10^{-4}$			= $K_a(CH_2(OH)CH(OH)CO(OH)/CH_2(OH)CH(OH)CO(O^-))$
$CO(OH)CH(OH)COCHO + H_2O \leftrightarrow CO(OH)CH(OH)COCH(OH)(OH)$	T(276)	$4.4\ 10^{2}$		Estimated with GROMHE	
$CO(OH)CH(OH)COCHO + H_2O \leftrightarrow CO(OH)CH(OH)C(OH)(OH)CHO$	T(277)	$9.5\ 10^{1}$		Estimated with GROMHE	
$CO(OH)CH(OH)COCHO + 2\ H_2O \leftrightarrow CO(OH)CH(OH)C(OH)(OH)CH(OH)(OH)$	T(278)	$7.1\ 10^{3}$		Estimated with GROMHE	
$CO(O^-)CH(OH)COCHO + H_2O \leftrightarrow CO(O^-)CH(OH)COCH(OH)(OH)$	T(279)	$2.0\ 10^{2}$		Estimated with GROMHE	
$CO(O^-)CH(OH)COCHO + H_2O \leftrightarrow CO(O^-)CH(OH)C(OH)(OH)CHO$	T(280)	$1.3\ 10^{1}$		Estimated with GROMHE	
$CO(O^-)CH(OH)COCHO + 2\ H_2O \leftrightarrow CO(O^-)CH(OH)C(OH)(OH)CH(OH)(OH)$	T(281)	$4.2\ 10^{2}$		Estimated with GROMHE	
$CO(OH)CH(OH)COCO(OO^\bullet) \leftrightarrow CO(O^-)CH(OH)COCO(OO^\bullet) + H^+$	T(282)	$3.0\ 10^{-4}$			3

Species		K_a or K_h	-ΔH/R (K)	References	Notes
					= K_a(CO(OH)CH(OH)COCHO/CO(O$^-$)CH(OH)COCHO)
CO(OH)CH(OH)COCO(OO$^\bullet$) + H_2O ↔ CO(OH)CH(OH)COC(OH)(OH)(OO$^\bullet$)	T(283)	1.0 10^{-3}			2
CO(OH)CH(OH)COCO(OO$^\bullet$) + H_2O ↔ CO(OH)CH(OH)C(OH)(OH)CO(OO$^\bullet$)	T(284)	9.5 10^{1}			1
					= K_h(CO(OH)CH(OH)COCHO/CO(OH)CH(OH)C(OH)(OH)CHO)
CO(OH)CH(OH)COCO(OO$^\bullet$) + 2 H_2O ↔ CO(OH)CH(OH)C(OH)(OH)C(OH)(OH)(OO$^\bullet$)	T(285)	7.1 10^{3}			1
					= K_h(CO(OH)CH(OH)COCHO/CO(OH)CH(OH)C(OH)(OH)CH(OH)(OH))
CO(O$^-$)CH(OH)COCO(OO$^\bullet$) + H_2O ↔ CO(O$^-$)CH(OH)COC(OH)(OH)(OO$^\bullet$)	T(286)	1.0 10^{-3}			2
CO(O$^-$)CH(OH)COCO(OO$^\bullet$) + H_2O ↔ CO(O$^-$)CH(OH)C(OH)(OH)CO(OO$^\bullet$)	T(287)	1.3 10^{1}			1
					= K_h(CO(O$^-$)CH(OH)COCHO/CO(O$^-$)CH(OH)C(OH)(OH)CHO)
CO(O$^-$)CH(OH)COCO(OO$^\bullet$) + 2 H_2O ↔ CO(O$^-$)CH(OH)C(OH)(OH)C(OH)(OH)(OO$^\bullet$)	T(288)	4.2 10^{2}			1
					= K_h(CO(O$^-$)CH(OH)COCHO/CO(O$^-$)CH(OH)C(OH)(OH)CH(OH)(OH))
CO(OH)C(OH)(OO$^\bullet$)COCHO↔ CO(O$^-$)C(OH)(OO$^\bullet$)COCHO + H^+	T(289)	3.0 10^{-4}			3
					= K_a(CO(OH)CH(OH)COCHO/CO(O$^-$)CH(OH)COCHO)
CO(OH)C(OH)(OO$^\bullet$)COCHO + H_2O ↔ CO(OH)C(OH)(OO$^\bullet$)COCH(OH)(OH)	T(290)	4.4 10^{2}			1
					= K_h(CO(OH)CH(OH)COCHO/CO(OH)CH(OH)COCH(OH)(OH))
CO(OH)C(OH)(OO$^\bullet$)COCHO + H_2O ↔ CO(OH)C(OH)(OO$^\bullet$)C(OH)(OH)CHO	T(291)	9.5 10^{1}			1
					= K_h(CO(OH)CH(OH)COCHO/CO(OH)CH(OH)C(OH)(OH)CHO)
CO(OH)C(OH)(OO$^\bullet$)COCHO + 2 H_2O ↔ CO(OH)C(OH)(OO$^\bullet$)C(OH)(OH)CH(OH)(OH)	T(292)	7.1 10^{3}			1
					= K_h(CO(OH)CH(OH)COCHO/CO(OH)CH(OH)C(OH)(OH)CH(OH)(OH))
CO(O$^-$)C(OH)(OO$^\bullet$)COCHO + H_2O ↔ CO(O$^-$)C(OH)(OO$^\bullet$)COCH(OH)(OH)	T(293)	2.0 10^{2}			1
					= K_h(CO(O$^-$)CH(OH)COCHO/CO(O$^-$)CH(OH)COCH(OH)(OH))
CO(O$^-$)C(OH)(OO$^\bullet$)COCHO + H_2O ↔ CO(O$^-$)C(OH)(OO$^\bullet$)C(OH)(OH)CHO	T(294)	1.3 10^{1}			1
					= K_h(CO(O$^-$)CH(OH)COCHO/CO(O$^-$)CH(OH)C(OH)(OH)CHO)
CO(O$^-$)C(OH)(OO$^\bullet$)COCHO + 2 H_2O ↔ CO(O$^-$)C(OH)(OO$^\bullet$)C(OH)(OH)CH(OH)(OH)	T(295)	4.2 10^{2}			1
					= K_h(CO(O$^-$)CH(OH)COCHO/CO(O$^-$)CH(OH)C(OH)(OH)CH(OH)(OH))
2-oxomalic acid					
CO(OH)CH(OH)COCO(OH) ↔ CO(OH)CH(OH)COCO(O$^-$) + H^+	T(296)	3.2 10^{-3}			= K_a(CO(OH)COCO(OH)/CO(OH)COCO(O$^-$))
CO(OH)CH(OH)COCO(OH) ↔ CO(O$^-$)CH(OH)COCO(OH) + H^+	T(297)	3.8 10^{-3}			= K_a(CO(OH)CH(OH)CO(OH)/CO(OH)CH(OH)CO(O$^-$))
CO(OH)CH(OH)COCO(O$^-$) ↔ CO(O$^-$)CH(OH)COCO(O$^-$) + H^+	T(298)	1.3 10^{-4}			= K_a(CO(OH)COCO(O$^-$)/CO(O$^-$)COCO(O$^-$))
CO(OH)CH(OH)COCO(OH) + H_2O ↔ CO(OH)CH(OH)C(OH)(OH)CO(OH)	T(299)	8.0 10^{1}		Estimated with GROMHE	
CO(OH)CH(OH)COCO(O$^-$) + H_2O ↔ CO(OH)CH(OH)C(OH)(OH)CO(O$^-$)	T(300)	5.3 10^{-1}		Estimated with GROMHE	
CO(O$^-$)CH(OH)COCO(OH) + H_2O ↔ CO(O$^-$)CH(OH)C(OH)(OH)CO(OH)	T(301)	1.1 10^{1}		Estimated with GROMHE	
CO(O$^-$)CH(OH)COCO(O$^-$) + H_2O ↔ CO(O$^-$)CH(OH)C(OH)(OH)CO(O$^-$)	T(302)	7.0 10^{-2}		Estimated with GROMHE	
CO(OH)C(OH)(OO$^\bullet$)COCO(OH) ↔ CO(OH)C(OH)(OO$^\bullet$)COCO(O$^-$) + H^+	T(303)	3.2 10^{-3}			3
					= K_a(CO(OH)CH(OH)COCO(OH)/CO(OH)CH(OH)COCO(O$^-$))
CO(OH)C(OH)(OO$^\bullet$)COCO(OH) ↔ CO(O$^-$)C(OH)(OO$^\bullet$)COCO(OH) + H^+	T(304)	3.8 10^{-3}			3
					= K_a(CO(OH)CH(OH)COCO(OH)/CO(O$^-$)CH(OH)COCO(OH))
CO(OH)C(OH)(OO$^\bullet$)COCO(O$^-$) ↔ CO(O$^-$)C(OH)(OO$^\bullet$)COCO(O$^-$) + H^+	T(305)	1.3 10^{-4}			3

Species		K_a or K_h	-ΔH/R (K)	References	Notes
					$= K_a(CO(OH)CH(OH)COCO(O^-)/CO(O^-)CH(OH)COCO(O^-))$
$CO(OH)C(OH)(OO^\bullet)COCO(OH) + H_2O \leftrightarrow CO(OH)C(OH)(OO^\bullet)C(OH)(OH)CO(OH)$	T(306)	$8.0\ 10^1$			1
					$= K_h(CO(OH)CH(OH)COCO(OH)/CO(OH)CH(OH)C(OH)(OH)CO(OH))$
$CO(OH)C(OH)(OO^\bullet)COCO(O^-) + H_2O \leftrightarrow CO(OH)C(OH)(OO^\bullet)C(OH)(OH)CO(O^-)$	T(307)	$5.3\ 10^{-1}$			1
					$= K_h(CO(OH)CH(OH)COCO(O^-)/CO(OH)CH(OH)C(OH)(OH)CO(O^-))$
$CO(O^-)C(OH)(OO^\bullet)COCO(OH) + H_2O \leftrightarrow CO(O^-)C(OH)(OO^\bullet)C(OH)(OH)CO(OH)$	T(308)	$1.1\ 10^1$			1
					$= K_h(CO(O^-)CH(OH)COCO(OH)/CO(O^-)CH(OH)C(OH)(OH)CO(OH))$
$CO(O^-)C(OH)(OO^\bullet)COCO(O^-) + H_2O \leftrightarrow CO(O^-)C(OH)(OO^\bullet)C(OH)(OH)CO(O^-)$	T(309)	$7.0\ 10^{-2}$			1
					$= K_h(CO(O^-)CH(OH)COCO(O^-)/CO(O^-)CH(OH)C(OH)(OH)CO(O^-))$
Dioxosuccinic acid					
$CO(OH)COCOCO(OH) \leftrightarrow CO(OH)COCOCO(O^-) + H^+$	T(310)	$3.2\ 10^{-3}$			$= K_a(CO(OH)COCO(OH)/CO(OH)COCO(O^-))$
$CO(OH)COCOCO(O^-) \leftrightarrow CO(O^-)COCOCO(O^-) + H^+$	T(311)	$1.3\ 10^{-4}$			$= K_a(CO(OH)COCO(O^-)/CO(O^-)COCO(O^-))$
$CO(OH)COCOCO(OH) + H_2O \leftrightarrow CO(OH)COC(OH)(OH)CO(OH)$	T(312)	$2.9\ 10^3$		Estimated with GROMHE	
$CO(OH)COCOCO(OH) + 2\ H_2O \leftrightarrow CO(OH)C(OH)(OH)C(OH)(OH)CO(OH)$	T(313)	$1.0\ 10^6$		Estimated with GROMHE	
$CO(OH)COCOCO(O^-) + H_2O \leftrightarrow CO(OH)C(OH)(OH)COCO(O^-)$	T(314)	$1.9\ 10^2$		Estimated with GROMHE	
$CO(OH)COCOCO(O^-) + H_2O \leftrightarrow CO(OH)COC(OH)(OH)CO(O^-)$	T(315)	9.4		Estimated with GROMHE	
$CO(OH)COCOCO(O^-) + 2\ H_2O \leftrightarrow CO(OH)C(OH)(OH)C(OH)(OH)CO(O^-)$	T(316)	$4.5\ 10^2$		Estimated with GROMHE	
$CO(O^-)COCOCO(O^-) + H_2O \leftrightarrow CO(O^-)COC(OH)(OH)CO(O^-)$	T(317)	2.5		Estimated with GROMHE	
$CO(O^-)COCOCO(O^-) + 2\ H_2O \leftrightarrow CO(O^-)C(OH)(OH)C(OH)(OH)CO(O^-)$	T(318)	$8.0\ 10^{-1}$		Estimated with GROMHE	
2,3-dioxobutanedial					
$CHOCOCOCHO + H_2O \leftrightarrow CH(OH)(OH)COCOCHO$	T(319)	$2.9\ 10^3$		Estimated with GROMHE	
$CHOCOCOCHO + H_2O \leftrightarrow CHOC(OH)(OH)COCHO$	T(320)	$3.6\ 10^3$		Estimated with GROMHE	
$CHOCOCOCHO + 2\ H_2O \leftrightarrow CH(OH)(OH)COCOCH(OH)(OH)$	T(321)	$2.9\ 10^6$		Estimated with GROMHE	
$CHOCOCOCHO + 2\ H_2O \leftrightarrow CH(OH)(OH)C(OH)(OH)COCHO$	T(322)	$8.7\ 10^5$		Estimated with GROMHE	
$CHOCOCOCHO + 2\ H_2O \leftrightarrow CH(OH)(OH)COC(OH)(OH)CHO$	T(323)	$2.6\ 10^6$		Estimated with GROMHE	
$CHOCOCOCHO + 2\ H_2O \leftrightarrow CHOC(OH)(OH)C(OH)(OH)CHO$	T(324)	$1.7\ 10^6$		Estimated with GROMHE	
$CHOCOCOCHO + 3\ H_2O \leftrightarrow CH(OH)(OH)C(OH)(OH)COCH(OH)(OH)$	T(325)	$5.5\ 10^8$		Estimated with GROMHE	

Species		K_a or K_h	-ΔH/R (K)	References	Notes
CHOCOCOCHO + 3 H_2O ↔ CH(OH)(OH)C(OH)(OH)C(OH)(OH)CHO	T(326)	$2.5\ 10^{8}$		Estimated with GROMHE	
CHOCOCOCHO + 4 H_2O ↔ CH(OH)(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OH)	T(327)	$2.0\ 10^{10}$		Estimated with GROMHE	
CHOCOCOCO($OO^{\bullet}$) + H_2O ↔ CH(OH)(OH)COCOCO($OO^{\bullet}$)	T(328)	$2.9\ 10^{3}$			1 = K_h(CHOCOCOCHO/CH(OH)(OH)COCOCHO)
CHOCOCOCO($OO^{\bullet}$) + H_2O ↔ CHOC(OH)(OH)COCO($OO^{\bullet}$)	T(329)	$3.6\ 10^{3}$			1 = K_h(CHOCOCOCHO/CHOC(OH)(OH)COCHO)
CHOCOCOCO($OO^{\bullet}$) + 2 H_2O ↔ CH(OH)(OH)COCOC(OH)(OH)($OO^{\bullet}$)	T(330)	$2.9\ 10^{6}$			1 = K_h(CHOCOCOCHO/CH(OH)(OH)COCOCH(OH)(OH))
CHOCOCOCO($OO^{\bullet}$) + 2 H_2O ↔ CH(OH)(OH)C(OH)(OH)COCO($OO^{\bullet}$)	T(331)	$8.7\ 10^{5}$			1 = K_h(CHOCOCOCHO/CH(OH)(OH)C(OH)(OH)COCHO)
CHOCOCOCO($OO^{\bullet}$) + 2 H_2O ↔ CH(OH)(OH)COC(OH)(OH)CO($OO^{\bullet}$)	T(332)	$2.6\ 10^{6}$			1 = K_h(CHOCOCOCHO/CH(OH)(OH)COC(OH)(OH)CHO)
CHOCOCOCO($OO^{\bullet}$) + 2 H_2O ↔ CHOC(OH)(OH)C(OH)(OH)CO($OO^{\bullet}$)	T(333)	$1.7\ 10^{6}$			1 = K_h(CHOCOCOCHO/CHOC(OH)(OH)C(OH)(OH)CHO)
CHOCOCOCO($OO^{\bullet}$) + 3 H_2O ↔ CH(OH)(OH)C(OH)(OH)COC(OH)(OH)($OO^{\bullet}$)	T(334)	$5.5\ 10^{8}$			1 = K_h(CHOCOCOCHO/CH(OH)(OH)C(OH)(OH)COCH(OH)(OH))
CHOCOCOCO($OO^{\bullet}$) + 3 H_2O ↔ CH(OH)(OH)C(OH)(OH)C(OH)(OH)CO($OO^{\bullet}$)	T(335)	$2.5\ 10^{8}$			1 = K_h(CHOCOCOCHO/CH(OH)(OH)C(OH)(OH)C(OH)(OH)CHO)
CHOCOCOCO($OO^{\bullet}$) + 4 H_2O ↔ CH(OH)(OH)C(OH)(OH)C(OH)(OH)C(OH)(OH)($OO^{\bullet}$)	T(336)	$2.0\ 10^{10}$			1 = K_h(CHOCOCOCHO/CH(OH)(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OH))
2,3-dioxobutanoic acid					
$CH_3COCOCO(OH)$ ↔ $CH_3COCOCO(O^-)$ + H^+	T(337)	$4.1\ 10^{-3}$			= K_a($CH_3COCO(OH)$/$CH_3COCO(O^-)$)
$CH_3COCOCO(OH)$ + H_2O ↔ $CH_3C(OH)(OH)COCO(OH)$	T(338)	9.4		Estimated with GROMHE	
$CH_3COCOCO(OH)$ + H_2O ↔ $CH_3COC(OH)(OH)CO(OH)$	T(339)	$1.9\ 10^{2}$		Estimated with GROMHE	
$CH_3COCOCO(OH)$ + 2 H_2O ↔ $CH_3C(OH)(OH)C(OH)(OH)CO(OH)$	T(340)	$4.5\ 10^{2}$		Estimated with GROMHE	
$CH_3COCOCO(O^-)$ + H_2O ↔ $CH_3C(OH)(OH)COCO(O^-)$	T(341)	1.3		Estimated with GROMHE	
$CH_3COCOCO(O^-)$ + H_2O ↔ $CH_3COC(OH)(OH)CO(O^-)$	T(342)	1.3		Estimated with GROMHE	
$CH_3COCOCO(O^-)$ + 2 H_2O ↔ $CH_3C(OH)(OH)C(OH)(OH)CO(O^-)$	T(343)	$3.9\ 10^{-1}$		Estimated with GROMHE	
$CH_2(OO^{\bullet})COCOCO(OH)$ ↔ $CH_2(OO^{\bullet})COCOCO(O^-)$ + H^+	T(344)	$4.1\ 10^{-3}$			= K_a($CH_3COCOCO(OH)$/$CH_3COCOCO(O^-)$)
$CH_2(OO^{\bullet})COCOCO(OH)$ + H_2O ↔ $CH_2(OO^{\bullet})C(OH)(OH)COCO(OH)$	T(345)	9.4			1 = K_h($CH_3COCOCO(OH)$/$CH_3C(OH)(OH)COCO(OH)$)
$CH_2(OO^{\bullet})COCOCO(OH)$ + H_2O ↔ $CH_2(OO^{\bullet})COC(OH)(OH)CO(OH)$	T(346)	$1.9\ 10^{2}$			1 = K_h($CH_3COCOCO(OH)$/$CH_3COC(OH)(OH)CO(OH)$)
$CH_2(OO^{\bullet})COCOCO(OH)$ + 2 H_2O ↔ $CH_2(OO^{\bullet})C(OH)(OH)C(OH)(OH)CO(OH)$	T(347)	$4.5\ 10^{2}$			1

Species		K_a or K_h	-ΔH/R (K)	References	Notes
					= $K_h(CH_3COCOCO(OH)/CH_3C(OH)(OH)C(OH)(OH)CO(OH))$
$CH_2(OO^\bullet)COCOCO(O^-) + H_2O \leftrightarrow CH_2(OO^\bullet)C(OH)(OH)COCO(O^-)$	T(348)	1.3			1 = $K_h(CH_3COCOCO(O^-)/CH_3C(OH)(OH)COCO(O^-))$
$CH_2(OO^\bullet)COCOCO(O^-) + H_2O \leftrightarrow CH_2(OO^\bullet)COC(OH)(OH)CO(O^-)$	T(349)	1.3			1 = $K_h(CH_3COCOCO(O^-)/CH_3COC(OH)(OH)CO(O^-))$
$CH_2(OO^\bullet)COCOCO(O^-) + 2\ H_2O \leftrightarrow CH_2(OO^\bullet)C(OH)(OH)C(OH)(OH)CO(O^-)$	T(350)	$3.9\ 10^{-1}$			1 = $K_h(CH_3COCOCO(O^-)/CH_3C(OH)(OH)C(OH)(OH)CO(O^-))$
2,3-dioxo-4-hydroxybutanal					
$CH_2(OH)COCOCHO + H_2O \leftrightarrow CH_2(OH)COCOCH(OH)(OH)$	T(351)	$8.0\ 10^{2}$		Estimated with GROMHE	
$CH_2(OH)COCOCHO + H_2O \leftrightarrow CH_2(OH)C(OH)(OH)COCHO$	T(352)	$4.5\ 10^{1}$		Estimated with GROMHE	
$CH_2(OH)COCOCHO + H_2O \leftrightarrow CH_2(OH)COC(OH)(OH)CHO$	T(353)	$4.1\ 10^{2}$		Estimated with GROMHE	
$CH_2(OH)COCOCHO + 2\ H_2O \leftrightarrow CH_2(OH)C(OH)(OH)COCH(OH)(OH)$	T(354)	$1.7\ 10^{4}$		Estimated with GROMHE	
$CH_2(OH)COCOCHO + 2\ H_2O \leftrightarrow CH_2(OH)COC(OH)(OH)CH(OH)(OH)$	T(355)	$5.5\ 10^{4}$		Estimated with GROMHE	
$CH_2(OH)COCOCHO + 2\ H_2O \leftrightarrow CH_2(OH)C(OH)(OH)C(OH)(OH)CHO$	T(356)	$4.7\ 10^{3}$		Estimated with GROMHE	
$CH_2(OH)COCOCHO + 3\ H_2O \leftrightarrow CH_2(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OH)$	T(357)	$3.0\ 10^{5}$		Estimated with GROMHE	
$CHOCOCOCH(OH)(OO^\bullet) + H_2O \leftrightarrow CH(OH)(OH)COCOCH(OH)(OO^\bullet)$	T(358)	$8.0\ 10^{2}$			1 = $K_h(CH_2(OH)COCOCHO/CH_2(OH)COCOCH(OH)(OH))$
$CHOCOCOCH(OH)(OO^\bullet) + H_2O \leftrightarrow CHOCOC(OH)(OH)CH(OH)(OO^\bullet)$	T(359)	$4.5\ 10^{1}$			1 = $K_h(CH_2(OH)COCOCHO/CH_2(OH)C(OH)(OH)COCHO)$
$CHOCOCOCH(OH)(OO^\bullet) + H_2O \leftrightarrow CHOC(OH)(OH)COCH(OH)(OO^\bullet)$	T(360)	$4.1\ 10^{2}$			1 = $K_h(CH_2(OH)COCOCHO/CH_2(OH)COC(OH)(OH)CHO)$
$CHOCOCOCH(OH)(OO^\bullet) + 2\ H_2O \leftrightarrow CH(OH)(OH)COC(OH)(OH)CH(OH)(OO^\bullet)$	T(361)	$1.7\ 10^{4}$			1 = $K_h(CH_2(OH)COCOCHO/CH_2(OH)C(OH)(OH)COCH(OH)(OH))$
$CHOCOCOCH(OH)(OO^\bullet) + 2\ H_2O \leftrightarrow CH(OH)(OH)C(OH)(OH)COCH(OH)(OO^\bullet)$	T(362)	$5.5\ 10^{4}$			1 = $K_h(CH_2(OH)COCOCHO/CH_2(OH)COC(OH)(OH)CH(OH)(OH))$
$CHOCOCOCH(OH)(OO^\bullet) + 2\ H_2O \leftrightarrow CHOC(OH)(OH)C(OH)(OH)CH(OH)(OO^\bullet)$	T(363)	$4.7\ 10^{3}$			1 = $K_h(CH_2(OH)COCOCHO/CH_2(OH)C(OH)(OH)C(OH)(OH)CHO)$
$CHOCOCOCH(OH)(OO^\bullet) + 3\ H_2O \leftrightarrow CH(OH)(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OO^\bullet)$	T(364)	$3.0\ 10^{5}$			1 = $K_h(CH_2(OH)COCOCHO/CH_2(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OH))$
$CH_2(OH)COCOCO(OO^\bullet) + H_2O \leftrightarrow CH_2(OH)COCOC(OH)(OH)(OO^\bullet)$	T(365)	$1.0\ 10^{-3}$			2
$CH_2(OH)COCOCO(OO^\bullet) + H_2O \leftrightarrow CH_2(OH)C(OH)(OH)COCO(OO^\bullet)$	T(366)	$4.5\ 10^{1}$			1 = $K_h(CH_2(OH)COCOCHO/CH_2(OH)C(OH)(OH)COCHO)$
$CH_2(OH)COCOCO(OO^\bullet) + H_2O \leftrightarrow CH_2(OH)COC(OH)(OH)CO(OO^\bullet)$	T(367)	$4.1\ 10^{2}$			1 = $K_h(CH_2(OH)COCOCHO/CH_2(OH)COC(OH)(OH)CHO)$
$CH_2(OH)COCOCO(OO^\bullet) + 2\ H_2O \leftrightarrow CH_2(OH)C(OH)(OH)COC(OH)(OH)(OO^\bullet)$	T(368)	$1.7\ 10^{4}$			1

Species		K_a or K_h	-ΔH/R (K)	References	Notes
					= K_h(CH_2(OH)COCOCHO/CH_2(OH)C(OH)(OH)COCH(OH)(OH))
CH_2(OH)COCOCO(OO•) + 2 H_2O ↔ CH_2(OH)COC(OH)(OH)C(OH)(OH)(OO•)	T(369)	5.5 10^4			1
					= K_h(CH_2(OH)COCOCHO/CH_2(OH)COC(OH)(OH)CH(OH)(OH))
CH_2(OH)COCOCO(OO•) + 2 H_2O ↔ CH_2(OH)C(OH)(OH)C(OH)(OH)CO(OO•)	T(370)	4.7 10^3			1
					= K_h(CH_2(OH)COCOCHO/CH_2(OH)C(OH)(OH)C(OH)(OH)CHO)
CH_2(OH)COCOCO(OO•) + 3 H_2O ↔ CH_2(OH)C(OH)(OH)C(OH)(OH)C(OH)(OH)(OO•)	T(371)	3.0 10^5			1
					= K_h(CH_2(OH)COCOCHO/CH_2(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OH))
2,3-dioxo-4-hydroxybutanoic acid					
CH_2(OH)COCOCO(OH) ↔ CH_2(OH)COCOCO(O^-) + H^+	T(372)	4.1 10^{-3}			= K_a(CH_3COCO(OH)/CH_3COCO(O^-))
CH_2(OH)COCOCO(OH) + H_2O ↔ CH_2(OH)C(OH)(OH)COCO(OH)	T(373)	4.2 10^1		Estimated with GROMHE	
CH_2(OH)COCOCO(OH) + H_2O ↔ CH_2(OH)COC(OH)(OH)CO(OH)	T(374)	3.5 10^2		Estimated with GROMHE	
CH_2(OH)COCOCO(OH) + 2 H_2O ↔ CH_2(OH)C(OH)(OH)C(OH)(OH)CO(OH)	T(375)	3.7 10^3		Estimated with GROMHE	
CH_2(OH)COCOCO(O^-) + H_2O ↔ CH_2(OH)C(OH)(OH)COCO(O^-)	T(376)	5.6		Estimated with GROMHE	
CH_2(OH)COCOCO(O^-) + H_2O ↔ CH_2(OH)COC(OH)(OH)CO(O^-)	T(377)	2.3		Estimated with GROMHE	
CH_2(OH)COCOCO(O^-) + 2 H_2O ↔ CH_2(OH)C(OH)(OH)C(OH)(OH)CO(O^-)	T(378)	3.2		Estimated with GROMHE	
CO(OH)COCOCH(OH)(OO•) ↔ CO(O^-)COCOCH(OH)(OO•) + H^+	T(379)	4.1 10^{-3}			= K_a(CH_2(OH)COCOCO(OH)/CH_2(OH)COCOCO(O^-))
CO(OH)COCOCH(OH)(OO•) + H_2O ↔ CO(OH)COC(OH)(OH)CH(OH)(OO•)	T(380)	4.2 10^1			1
					= K_h(CH_2(OH)COCOCO(OH)/CH_2(OH)C(OH)(OH)COCO(OH))
CO(OH)COCOCH(OH)(OO•) + H_2O ↔ CO(OH)C(OH)(OH)COCH(OH)(OO•)	T(381)	3.5 10^2			1
					= K_h(CH_2(OH)COCOCO(OH)/CH_2(OH)COC(OH)(OH)CO(OH))
CO(OH)COCOCH(OH)(OO•) + 2 H_2O ↔ CO(OH)C(OH)(OH)C(OH)(OH)CH(OH)(OO•)	T(382)	3.7 10^3			1
					= K_h(CH_2(OH)COCOCO(OH)/CH_2(OH)C(OH)(OH)C(OH)(OH)CO(OH))
CO(O^-)COCOCH(OH)(OO•) + H_2O ↔ CO(O^-)COC(OH)(OH)CH(OH)(OO•)	T(383)	5.6			1
					= K_h(CH_2(OH)COCOCO(O^-)/CH_2(OH)C(OH)(OH)COCO(O^-))
CO(O^-)COCOCH(OH)(OO•) + H_2O ↔ CO(O^-)C(OH)(OH)COCH(OH)(OO•)	T(384)	2.3			1
					= K_h(CH_2(OH)COCOCO(O^-)/CH_2(OH)COC(OH)(OH)CO(O^-))
CO(O^-)COCOCH(OH)(OO•) + 2 H_2O ↔ CO(O^-)C(OH)(OH)C(OH)(OH)CH(OH)(OO•)	T(385)	3.2			1
					= K_h(CH_2(OH)COCOCO(O^-)/CH_2(OH)C(OH)(OH)C(OH)(OH)CO(O^-))
2,3,4-trioxobutanoic acid					
CHOCOCOCO(OH) ↔ CHOCOCOCO(O^-) + H^+	T(386)	4.1 10^{-3}			= K_a(CH_3COCO(OH)/CH_3COCO(O^-))
CHOCOCOCO(OH) + H_2O ↔ CH(OH)(OH)COCOCO(OH)	T(387)	1.4 10^3		Estimated with GROMHE	
CHOCOCOCO(OH) + H_2O ↔ CHOCOC(OH)(OH)CO(OH)	T(388)	1.5 10^3		Estimated with GROMHE	
CHOCOCOCO(OH) + H_2O ↔ CHOC(OH)(OH)COCO(OH)	T(389)	1.7 10^3		Estimated with GROMHE	

Species		K_a or K_h	-ΔH/R (K)	References	Notes
CHOCOCOCO(OH) +2 H_2O ↔ CH(OH)(OH)C(OH)(OH)COCO(OH)	T(390)	$4.0\ 10^{5}$		Estimated with GROMHE	
CHOCOCOCO(OH) +2 H_2O ↔ CH(OH)(OH)COC(OH)(OH)CO(OH)	T(391)	$1.0\ 10^{6}$		Estimated with GROMHE	
CHOCOCOCO(OH) +2 H_2O ↔ CHOC(OH)(OH)C(OH)(OH)CO(OH)	T(392)	$6.5\ 10^{5}$		Estimated with GROMHE	
CHOCOCOCO(OH) +3 H_2O ↔ CH(OH)(OH)C(OH)(OH)C(OH)(OH)CO(OH)	T(393)	$7.5\ 10^{7}$		Estimated with GROMHE	
CHOCOCOCO(O^-) + H_2O ↔ CH(OH)(OH)COCOCO(O^-)	T(157)	$6.3\ 10^{2}$		Estimated with GROMHE	
CHOCOCOCO(O^-) + H_2O ↔ CHOCOC(OH)(OH)CO(O^-)	T(158)	$1.0\ 10^{1}$		Estimated with GROMHE	
CHOCOCOCO(O^-) + H_2O ↔ CHOC(OH)(OH)COCO(O^-)	T(159)	$2.3\ 10^{2}$		Estimated with GROMHE	
CHOCOCOCO(O^-) +2 H_2O ↔ CH(OH)(OH)C(OH)(OH)COCO(O^-)	T(160)	$2.4\ 10^{4}$		Estimated with GROMHE	
CHOCOCOCO(O^-) +2 H_2O ↔ CH(OH)(OH)COC(OH)(OH)CO(O^-)	T(161)	$3.0\ 10^{3}$		Estimated with GROMHE	
CHOCOCOCO(O^-) +2 H_2O ↔ CHOC(OH)(OH)C(OH)(OH)CO(O^-)	T(162)	$5.7\ 10^{2}$		Estimated with GROMHE	
CHOCOCOCO(O^-) +3 H_2O ↔ CH(OH)(OH)C(OH)(OH)C(OH)(OH)CO(O^-)	T(163)	$2.9\ 10^{4}$		Estimated with GROMHE	
CO(OH)COCOCO($OO^\bullet$) ↔ CO(O^-)COCOCO($OO^\bullet$) + H^+	T(394)	$4.1\ 10^{-3}$			= K_a(CHOCOCOCO(OH)/CHOCOCOCO(O^-))
CO(OH)COCOCO($OO^\bullet$) + H_2O ↔ CO(OH)COCOC(OH)(OH)($OO^\bullet$)	T(395)	$1.0\ 10^{-3}$			2
CO(OH)COCOCO($OO^\bullet$) + H_2O ↔ CO(OH)C(OH)(OH)COCO($OO^\bullet$)	T(396)	$1.5\ 10^{3}$			1 = K_h(CHOCOCOCO(OH)/CHOCOC(OH)(OH)CO(OH))
CO(OH)COCOCO($OO^\bullet$) + H_2O ↔ CO(OH)COC(OH)(OH)CO($OO^\bullet$)	T(397)	$1.7\ 10^{3}$			1 = K_h(CHOCOCOCO(OH)/CHOC(OH)(OH)COCO(OH))
CO(OH)COCOCO($OO^\bullet$) +2 H_2O ↔ CO(OH)COC(OH)(OH)C(OH)(OH)($OO^\bullet$)	T(398)	$4.0\ 10^{5}$			1 = K_h(CHOCOCOCO(OH)/CH(OH)(OH)C(OH)(OH)COCO(OH))
CO(OH)COCOCO($OO^\bullet$) +2 H_2O ↔ CO(OH)C(OH)(OH)COC(OH)(OH)($OO^\bullet$)	T(399)	$1.0\ 10^{6}$			1 = K_h(CHOCOCOCO(OH)/CH(OH)(OH)COC(OH)(OH)CO(OH))
CO(OH)COCOCO($OO^\bullet$) +2 H_2O ↔ CO(OH)C(OH)(OH)C(OH)(OH)CO($OO^\bullet$)	T(400)	$6.5\ 10^{5}$			1 = K_h(CHOCOCOCO(OH)/CHOC(OH)(OH)C(OH)(OH)CO(OH))
CO(OH)COCOCO($OO^\bullet$) +3 H_2O ↔ CO(OH)C(OH)(OH)C(OH)(OH)C(OH)(OH)($OO^\bullet$)	T(401)	$7.5\ 10^{7}$			1 = K_h(CHOCOCOCO(OH)/CH(OH)(OH)C(OH)(OH)C(OH)(OH)CO(OH))
CO(O^-)COCOCO($OO^\bullet$) + H_2O ↔ CO(O^-)COCOC(OH)(OH)($OO^\bullet$)	T(402)	$1.0\ 10^{-3}$			2
CO(O^-)COCOCO($OO^\bullet$) + H_2O ↔ CO(O^-)C(OH)(OH)COCO($OO^\bullet$)	T(403)	$1.0\ 10^{1}$			1 = K_h(CHOCOCOCO(O^-)/CHOCOC(OH)(OH)CO(O^-))
CO(O^-)COCOCO($OO^\bullet$) + H_2O ↔ CO(O^-)COC(OH)(OH)CO($OO^\bullet$)	T(404)	$2.3\ 10^{2}$			1 = K_h(CHOCOCOCO(O^-)/CHOC(OH)(OH)COCO(O^-))
CO(O^-)COCOCO($OO^\bullet$) +2 H_2O ↔ CO(O^-)COC(OH)(OH)C(OH)(OH)($OO^\bullet$)	T(405)	$2.4\ 10^{4}$			1

Species		K_a or K_h	-ΔH/R (K)	References	Notes
					= K_h(CHOCOCOCO(O^-)/CH(OH)(OH)C(OH)(OH)COCO(O^-))
CO(O^-)COCOCO($OO^\bullet$) +2 H_2O ↔ CO(O^-)C(OH)(OH)COC(OH)(OH)($OO^\bullet$)	T(406)	$3.0\ 10^3$			1
					= K_h(CHOCOCOCO(O^-)/CH(OH)(OH)COC(OH)(OH)CO(O^-))
CO(O^-)COCOCO($OO^\bullet$) +2 H_2O ↔ CO(O^-)C(OH)(OH)C(OH)(OH)CO($OO^\bullet$)	T(407)	$5.7\ 10^2$			1
					= K_h(CHOCOCOCO(O^-)/CHOC(OH)(OH)C(OH)(OH)CO(O^-))
CO(O^-)COCOCO($OO^\bullet$) +3 H_2O ↔ CO(O^-)C(OH)(OH)C(OH)(OH)C(OH)(OH)($OO^\bullet$)	T(408)	$2.9\ 10^4$			1
					= K_h(CHOCOCOCO(O^-)/CH(OH)(OH)C(OH)(OH)C(OH)(OH)CO(O^-))
2- Methylglyceric Acid (2-MG)					
CH_2(OH)C(OH)(CH_3)CO(OH) ↔ CH_2(OH)C(OH)(CH_3)CO(O^-) + H^+	T(409)	$3.0\ 10^{-4}$			= K_a(CH_2(OH)CH(OH)CO(OH)/CH_2(OH)CH(OH)CO(O^-))
CH(OH)($OO^\bullet$)C(OH)(CH_3)CO(OH) ↔ CH(OH)($OO^\bullet$)C(OH)(CH_3)CO(O^-) + H^+	T(410)	$3.0\ 10^{-4}$			3
					= K_a(CH_2(OH)C(OH)(CH_3)CO(OH)/CH_2(OH)C(OH)(CH_3)CO(O^-)
CH_2(OH)C(OH)(CH_2($OO^\bullet$))CO(OH) ↔ CH_2(OH)C(OH)(CH_2($OO^\bullet$))CO(O^-) + H^+	T(411)	$3.0\ 10^{-4}$			3
					= K_a(CH_2(OH)C(OH)(CH_3)CO(OH)/CH_2(OH)C(OH)(CH_3)CO(O^-)
2-hydroxy,3-oxomethylpropanoic acid					
CHOC(OH)(CH_3)CO(OH) ↔ CHOC(OH)(CH_3)CO(O^-) + H^+	T(412)	$3.0\ 10^{-4}$			= K_a(CH_2(OH)CH(OH)CO(OH)/CH_2(OH)CH(OH)CO(O^-))
CHOC(OH)(CH_3)CO(OH) + H_2O ↔ CH(OH)(OH)C(OH)(CH_3)CO(OH)	T(413)	$4.6\ 10^1$		Estimated with GROMHE	
CHOC(OH)(CH_3)CO(O^-) + H_2O ↔ CH(OH)(OH)C(OH)(CH_3)CO(O^-)	T(414)	6.1		Estimated with GROMHE	
CO($OO^\bullet$)C(OH)(CH_3)CO(OH) ↔ CO($OO^\bullet$)C(OH)(CH_3)CO(O^-) + H^+	T(415)	$3.0\ 10^{-4}$			3
					= K_a(CHOC(OH)(CH_3)CO(OH)/CHOC(OH)(CH_3)CO(O^-))
CO($OO^\bullet$)C(OH)(CH_3)CO(OH) + H_2O ↔ C(OH)(OH)($OO^\bullet$)C(OH)(CH_3)CO(OH)	T(416)	$1.0\ 10^{-3}$			2
CO($OO^\bullet$)C(OH)(CH_3)CO(O^-) + H_2O ↔ C(OH)(OH)($OO^\bullet$)C(OH)(CH_3)CO(O^-)	T(417)	$1.0\ 10^{-3}$			2
CHOC(OH)(CH_2($OO^\bullet$))CO(OH) ↔ CHOC(OH)(CH_2($OO^\bullet$))CO(O^-) + H^+	T(418)	$3.0\ 10^{-4}$			3
					= K_a(CHOC(OH)(CH_3)CO(OH)/CHOC(OH)(CH_3)CO(O^-))
CHOC(OH)(CH_2($OO^\bullet$))CO(OH) + H_2O ↔ CH(OH)(OH)C(OH)(CH_2($OO^\bullet$))CO(OH)	T(419)	$4.6\ 10^1$			1
					= K_h(CHOC(OH)(CH_3)CO(OH)/CH(OH)(OH)C(OH)(CH_3)CO(OH))
CHOC(OH)(CH_2($OO^\bullet$))CO(O^-) + H_2O ↔ CH(OH)(OH)C(OH)(CH_2($OO^\bullet$))CO(O^-)	T(420)	6.1			1
					= K_h(CHOC(OH)(CH_3)CO(O^-)/CH(OH)(OH)C(OH)(CH_3)CO(O^-))
2-hydroxy-2-(hydroxymethyl)-3-oxopropanoic acid					
CHOC(OH)(CH_2(OH))CO(OH) ↔ CHOC(OH)(CH_2(OH))CO(O^-) + H^+	T(421)	$3.0\ 10^{-4}$			= K_a(CH_2(OH)CH(OH)CO(OH)/CH_2(OH)CH(OH)CO(O^-))
CHOC(OH)(CH_2(OH))CO(OH) + H_2O ↔ CH(OH)(OH)C(OH)(CH_2(OH))CO(OH)	T(422)	$8.4\ 10^1$		Estimated with GROMHE	
CHOC(OH)(CH_2(OH))CO(O^-) + H_2O ↔ CH(OH)(OH)C(OH)(CH_2(OH))CO(O^-)	T(423)	$1.1\ 10^1$		Estimated with GROMHE	
CHOC(OH)(CH(OH)($OO^\bullet$))CO(OH) ↔ CHOC(OH)(CH(OH)($OO^\bullet$))CO(O^-) + H^+	T(424)	$3.0\ 10^{-4}$			3
					= K_a(CHOC(OH)(CH_2(OH))CO(OH)/CHOC(OH)(CH_2(OH))CO(O^-))
CHOC(OH)(CH(OH)($OO^\bullet$))CO(OH) + H_2O ↔ CH(OH)(OH)C(OH)(CH(OH)($OO^\bullet$))CO(OH)	T(425)	$8.4\ 10^1$			1 = K_h(CHOC(OH)(CH_2(OH))CO(OH)/CH(OH)(OH)C(OH)(CH_2(OH))CO(OH))
CHOC(OH)(CH(OH)($OO^\bullet$))CO(O^-) + H_2O ↔ CH(OH)(OH)C(OH)(CH(OH)($OO^\bullet$))CO(O^-)	T(426)	$1.1\ 10^1$			1

Species		K_a or K_h	-ΔH/R (K)	References	Notes
					= K_h(CHOC(OH)(CH_2(OH))CO(O^-)/CH(OH)(OH)C(OH)(CH_2(OH))CO(O^-))
CO(OO•)C(OH)(CH_2(OH))CO(OH) ↔ CO(OO•)C(OH)(CH_2(OH))CO(O^-) + H^+	T(427)	3.0 10^{-4}			3 = K_a(CHOC(OH)(CH_2(OH))CO(OH)/CHOC(OH)(CH_2(OH))CO(O^-))
CO(OO•)C(OH)(CH_2(OH))CO(OH) + H_2O ↔ C(OH)(OH)(OO•)C(OH)(CH_2(OH))CO(OH)	T(428)	1.0 10^{-3}			2
CO(OO•)C(OH)(CH_2(OH))CO(O^-) + H_2O ↔ C(OH)(OH)(OO•)C(OH)(CH_2(OH))CO(O^-)	T(429)	1.0 10^{-3}			2
2,3-hydroxy-2-(hydroxymethyl)propanoic acid					
CH_2(OH)C(OH)(CH_2(OH))CO(OH) ↔ CH_2(OH)C(OH)(CH_2(OH))CO(O^-) + H^+	T(430)	3.0 10^{-4}			= K_a(CH_2(OH)CH(OH)CO(OH)/CH_2(OH)CH(OH)CO(O^-))
CH(OH)(OO•)C(OH)(CH_2(OH))CO(OH) ↔ CH(OH)(OO•)C(OH)(CH_2(OH))CO(O^-) + H^+	T(431)	3.0 10^{-4}			3 = K_a(CH_2(OH)C(OH)(CH_2(OH))CO(OH)/CH_2(OH)C(OH)(CH_2(OH))CO(O^-))
Methyltartronic acid					
CO(OH)C(OH)(CH_3)CO(OH) ↔ CO(OH)C(OH)(CH_3)CO(O^-) + H^+	T(432)	3.8 10^{-3}			= K_a(CO(OH)CH(OH)CO(OH)/CO(OH)CH(OH)CO(O^-))
CO(OH)C(OH)(CH_3)CO(O^-) ↔ CO(O^-)C(OH)(CH_3)CO(O^-) + H^+	T(433)	2.9 10^{-5}			= K_a(CO(OH)CH(OH)CO(O^-)/CO(O^-)CH(OH)CO(O^-))
CO(OH)C(OH)(CH_2(OO•))CO(OH) ↔ CO(OH)C(OH)(CH_2(OO•))CO(O^-) + H^+	T(434)	3.8 10^{-3}			3 = K_a(CO(OH)C(OH)(CH_3)CO(OH)/CO(OH)C(OH)(CH_3)CO(O^-))
CO(OH)C(OH)(CH_2(OO•))CO(O^-) ↔ CO(O^-)C(OH)(CH_2(OO•))CO(O^-) + H^+	T(435)	2.9 10^{-5}			3 = K_a(CO(OH)C(OH)(CH_3)CO(O^-)/CO(O^-)C(OH)(CH_3)CO(O^-))
2- hydroxyl-2-(oxomethyl)-3-oxopropanoic acid					
CHOC(OH)(CHO)CO(OH) ↔ CHOC(OH)(CHO)CO(O^-) + H^+	T(436)	3.0 10^{-4}			= K_a(CH_2(OH)CH(OH)CO(OH)/CH_2(OH)CH(OH)CO(O^-))
CHOC(OH)(CHO)CO(OH) + H_2O ↔ CH(OH)(OH)C(OH)(CHO)CO(OH)	T(437)	7.3 10^{2}		Estimated with GROMHE	
CHOC(OH)(CHO)CO(OH) + 2 H_2O ↔ CH(OH)(OH)C(OH)(CH(OH)(OH))CO(OH)	T(438)	1.1 10^{5}		Estimated with GROMHE	
CHOC(OH)(CHO)CO(O^-) + H_2O ↔ CH(OH)(OH)C(OH)(CHO)CO(O^-)	T(439)	9.8 10^{1}		Estimated with GROMHE	
CHOC(OH)(CHO)CO(O^-) + 2 H_2O ↔ CH(OH)(OH)C(OH)(CH(OH)(OH))CO(O^-)	T(440)	2.0 10^{3}		Estimated with GROMHE	
CO(OO•)C(OH)(CHO)CO(OH) ↔ CO(OO•)C(OH)(CHO)CO(O^-) + H^+	T(441)	3.0 10^{-4}			3 = K_a(CHOC(OH)(CHO)CO(OH)/CHOC(OH)(CHO)CO(O^-))
CO(OO•)C(OH)(CHO)CO(OH) + H_2O ↔ C(OH)(OH)(OO•)C(OH)(CHO)CO(OH)	T(442)	1.0 10^{-3}			2
CO(OO•)C(OH)(CHO)CO(OH) + H_2O ↔ CO(OO•)C(OH)(CH(OH)(OH))CO(OH)	T(443)	7.3 10^{2}			1 = K_h(CHOC(OH)(CHO)CO(OH)/CH(OH)(OH)C(OH)(CHO)CO(OH))
CO(OO•)C(OH)(CHO)CO(OH) + 2 H_2O ↔ C(OH)(OH)(OO•)C(OH)(CH(OH)(OH))CO(OH)	T(444)	1.1 10^{5}			1 = K_h(CHOC(OH)(CHO)CO(OH)/CH(OH)(OH)C(OH)(CH(OH)(OH))CO(OH))
CO(OO•)C(OH)(CHO)CO(O^-) + H_2O ↔ C(OH)(OH)(OO•)C(OH)(CHO)CO(O^-)	T(445)	1.0 10^{-3}			2
CO(OO•)C(OH)(CHO)CO(O^-) + H_2O ↔ CO(OO•)C(OH)(CH(OH)(OH))CO(O^-)	T(446)	9.8 10^{1}			1 = K_h(CHOC(OH)(CHO)CO(O^-)/CH(OH)(OH)C(OH)(CHO)CO(O^-))

Species		K_a or K_h	-ΔH/R (K)	References	Notes
$CO(OO^•)C(OH)(CHO)CO(O^-)$ + 2 H_2O ↔ $C(OH)(OH)(OO^•)C(OH)(CH(OH)(OH))CO(O^-)$	T(447)	2.0 10^3			1 = K_h(CHOC(OH)(CHO)CO(O^-)/CH(OH)(OH)C(OH)(CH(OH)(OH))CO(O^-))
2-(hydroxymethyl)-tartronic acid					
$CO(OH)C(OH)(CH_2(OH))CO(OH)$ ↔ $CO(OH)C(OH)(CH_2(OH))CO(O^-)$ + H^+	T(448)	3.8 10^{-3}			= K_a(CO(OH)CH(OH)CO(OH)/CO(OH)CH(OH)CO(O^-))
$CO(OH)C(OH)(CH_2(OH))CO(O^-)$ ↔ $CO(O^-)C(OH)(CH_2(OH))CO(O^-)$ + H^+	T(449)	2.9 10^{-5}			= K_a(CO(OH)CH(OH)CO(O^-)/CO(O^-)CH(OH)CO(O^-))
$CO(OH)C(OH)(CH(OH)(OO^•))CO(OH)$ ↔ $CO(OH)C(OH)(CH(OH)(OO^•))CO(O^-)$ + H^+	T(450)	3.8 10^{-3}			3 = K_a(CO(OH)C(OH)(CH_2(OH))CO(OH)/CO(OH)C(OH)(CH_2(OH))CO(O^-))
$CO(OH)C(OH)(CH(OH)(OO^•))CO(O^-)$ ↔ $CO(O^-)C(OH)(CH(OH)(OO^•))CO(O^-)$ + H^+	T(451)	2.9 10^{-5}			3 = K_a(CO(OH)C(OH)(CH_2(OH))CO(O^-)/CO(O^-)C(OH)(CH_2(OH))CO(O^-))
2-(oxomethyl)-tartronic acid					
$CO(OH)C(OH)(CHO)CO(OH)$ ↔ $CO(OH)C(OH)(CHO)CO(O^-)$ + H^+	T(452)	3.8 10^{-3}			= K_a(CO(OH)CH(OH)CO(OH)/CO(OH)CH(OH)CO(O^-))
$CO(OH)C(OH)(CHO)CO(O^-)$ ↔ $CO(O^-)C(OH)(CHO)CO(O^-)$ + H^+	T(453)	2.9 10^{-5}			
$CO(OH)C(OH)(CHO)CO(OH)$ + H_2O ↔ $CO(OH)C(OH)(CH(OH)(OH))CO(OH)$	T(454)	3.4 10^2		Estimated with GROMHE	
$CO(OH)C(OH)(CHO)CO(O^-)$ + H_2O ↔ $CO(OH)C(OH)(CH(OH)(OH))CO(O^-)$	T(455)	4.6 10^1		Estimated with GROMHE	
$CO(O^-)C(OH)(CHO)CO(O^-)$ + H_2O ↔ $CO(O^-)C(OH)(CH(OH)(OH))CO(O^-)$	T(456)	6.1		Estimated with GROMHE	
$CO(OH)C(OH)(CO(OO^•))CO(OH)$ ↔ $CO(OH)C(OH)(CO(OO^•))CO(O^-)$ + H^+	T(457)	3.8 10^{-3}			3 = K_a(CO(OH)C(OH)(CHO)CO(OH)/CO(OH)C(OH)(CHO)CO(O^-))
$CO(OH)C(OH)(CO(OO^•))CO(O^-)$ ↔ $CO(O^-)C(OH)(CO(OO^•))CO(O^-)$ + H^+	T(458)	2.9 10^{-5}			3 = K_a(CO(OH)C(OH)(CHO)CO(O^-)/CO(O^-)C(OH)(CHO)CO(O^-))
$CO(OH)C(OH)(CO(OO^•))CO(OH)$ + H_2O ↔ $CO(OH)C(OH)(C(OH)(OH)(OO^•))CO(OH)$	T(459)	1.0 10^{-3}			2
$CO(OH)C(OH)(CO(OO^•))CO(O^-)$ + H_2O ↔ $CO(OH)C(OH)(C(OH)(OH)(OO^•))CO(O^-)$	T(460)	1.0 10^{-3}			2
$CO(O^-)C(OH)(CO(OO^•))CO(O^-)$ + H_2O ↔ $CO(O^-)C(OH)(C(OH)(OH)(OO^•))CO(O^-)$	T(461)	1.0 10^{-3}			2
Hydroxymethanetricarboxylic acid					
$CO(OH)C(OH)(CO(OH))CO(OH)$ ↔ $CO(OH)C(OH)(CO(OH))CO(O^-)$ + H^+	T(462)	7.2 10^{-4}			= K_{a1}(citric acid)
$CO(OH)C(OH)(CO(OH))CO(O^-)$ ↔ $CO(OH)C(OH)(CO(O^-))CO(O^-)$ + H^+	T(463)	1.7 10^{-5}			= K_{a2}(citric acid)
$CO(OH)C(OH)(CO(O^-))CO(O^-)$ ↔ $CO(O^-)C(OH)(CO(O^-))CO(O^-)$ + H^+	T(464)	4.0 10^{-7}			= K_{a3}(citric acid)
Methacrylic acid					
CH_2=C(CH_3)CO(OH) ↔ CH_2=C(CH_3)CO(O^-) + H^+	T(465)	1.3 10^{-5}			= K_a($CH_3CH_2CO(OH)$/$CH_3CH_2CO(O^-)$)

1 - For peroxy radicals, we assumed that the hydration constant is similar to the parent species.

2 - For acyl peroxylradicals, we assumed that hydration is not favored on the -CO($OO^•$) moiety. This is based on the similarity between the CO moiety in this function and the CO moiety in carboxylic (-CO(OH)) or percarboxylic acid (-CO(OOH)) organic functions which is not readily hydrated. Therefore we apply an arbitrarily low value (K_h = 1.0 10^{-3}) to the hydration constant of these species.

3 - For peroxy radicals, we assumed that the acidity constant is similar to the parent species.

Species		H (298K) ($M\ atm^{-1}$)	-ΔH/R (K)	References	Notes
C4 compounds					
Methacrolein					
$CH_2=C(CH_3)CHO$	T(70)	$4.8\ 10^{-2}$	4300	Ji and Evans, 2007	
Hydroxymethacrolein					
$CH_2=C(CH_2(OH))CHO$	T(71)	$6.9\ 10^{4}$	6014	Estimated	1 - 2 - 3
Methylvinylketone					
$CH_2=CHCOCH_3$	T(72)	$2.6\ 10^{-1}$	4800	Ji and Evans, 2007	
Hydroxymethylvinylketone					
$CH_2=CHCOCH_2(OH)$	T(73)	$1.3\ 10^{3}$	6014	Estimated	1 - 2 - 3
Hydroxybutandione					
$CH_3COCOCH_2(OH)$	T(74)	$5.4\ 10^{5}$	6014	Estimated	1 - 3
3,4-dihydroxybutan-2-one					
$CH_2(OH)CH(OH)COCH_3$	T(75)	$1.1\ 10^{5}$	6014	Estimated	1 - 2 - 3
1,4-dihydroxybutanedione					
$CH_2(OH)COCOCH_2(OH)$	T(76)	$1.9\ 10^{8}$	6014	Estimated	1 - 2 - 3
1,3,4-trihydroxybutanone					
$CH_2(OH)COCH(OH)CH_2(OH)$	T(77)	$9.1\ 10^{8}$	6014	Estimated	1 - 2 - 3
2,4-dihidroxy-3-oxobutanal					
$CH_2(OH)COCH(OH)CHO$	T(78)	$3.5\ 10^{8}$	6014	Estimated	1 - 2 - 3
2-oxo-3,4-dihidroxybutanal					
$CH_2(OH)CH(OH)COCHO$	T(79)	$1.5\ 10^{9}$	6014	Estimated	1 - 2 - 3
2-oxo-3-hydroxybutanedial					
$CHOCH(OH)COCHO$	T(80)	$3.6\ 10^{9}$	6014	Estimated	1 - 2 - 3
2,4-dioxo-3-hydroxybutanoic acid					
$CHOCH(OH)COCO(OH)$	T(81)	$5.2\ 10^{9}$	6014	Estimated	1 - 2 - 3
2,3-dioxobutanal					
$CH_3COCOCHO$	T(82)	$6.3\ 10^{8}$	6014	Estimated	1 - 2 - 3
2-hydroxy, 3-oxobutanal					
$CH_3COCH(OH)CHO$	T(83)	$2.0\ 10^{4}$	6014	Estimated	1 - 2 - 3
2-hydroxy,3-oxobutanoïc acid					
$CH_3COCH(OH)CO(OH)$	T(84)	$2.0\ 10^{5}$	6014	Estimated	1 - 2 - 3
2,4-dihydroxy, 3-oxobutanoic acid					
$CO(OH)CH(OH)COCH_2(OH)$	T(85)	$2.3\ 10^{9}$	6014	Estimated	1 - 2 - 3
2-hydroxy, 3,4-dioxobutanoic acid					
$CO(OH)CH(OH)COCHO$	T(86)	$5.8\ 10^{9}$	6014	Estimated	1 - 2 - 3

Species		H (298K) ($M\ atm^{-1}$)	-ΔH/R (K)	References	Notes
2-oxomalic acid					
$CO(OH)CH(OH)COCO(OH)$	T(87)	$2.0\ 10^{10}$	6014	Estimated	1 - 2 - 3
Dioxosuccinic acid					
$CO(OH)COCOCO(OH)$	T(88)	$1.3\ 10^{16}$	6014	Estimated	1 - 2 - 3
2,4-dioxobutanedial					
$CHOCOCOCHO$	T(89)	$3.5\ 10^{6}$	6014	Estimated	1 - 2 - 3
2,3-dioxobutanoic acid					
$CH_3COCOCO(OH)$	T(90)	$3.9\ 10^{9}$	6014	Estimated	1 - 2 - 3
2,3-dioxo-4-hydroxybutanal					
$CH_2(OH)COCOCHO$	T(91)	$1.3\ 10^{12}$	6014	Estimated	1 - 2 - 3
2,3-dioxo-4-hydroxybutanoic acid					
$CH_2(OH)COCOCO(OH)$	T(92)	$1.4\ 10^{12}$	6014	Estimated	1 - 2 - 3
2,3,4-trioxobutanoic acid					
$CHOCOCOCO(OH)$	T(93)	$2.1\ 10^{17}$	6014	Estimated	1 - 2 - 3
Methacrylic Acid Epoxide					
$CH_3C1(CO(OH))\text{-}O\text{-}C1H_2$	T(94)	$3.4\ 10^{2}$	6014	Estimated	1 - 3
Hydroxymethyl-methyl-α-lactone					
$CH_3C1(CH_2(OH))\text{-}O\text{-}C1O$	T(95)	6.5	6014	Estimated	1 - 3
2- Methylglyceric Acid					
$CH_2(OH)C(OH)(CH_3)CO(OH)$	T(96)	$6.0\ 10^{6}$	6014	Estimated	1 - 3
2-hydroxy-3-oxomethylpropanoic acid					
$CHOC(OH)(CH_3)CO(OH)$	T(97)	$1.1\ 10^{6}$	6014	Estimated	1 - 2 - 3
2-hydroxy-2-(hydroxymethyl)-3-oxopropanoic acid					
$CHOC(OH)(CH_2(OH))CO(OH)$	T(98)	$2.4\ 10^{10}$	6014	Estimated	1 - 2 - 3
2,3-hydroxy-2-(hydroxymethyl)-propanoic acid					
$CH_2(OH)C(OH)(CH_2(OH))CO(OH)$	T(99)	$8.8\ 10^{9}$	6014	Estimated	1 - 3
Methyltartronic acid					
$CO(OH)C(OH)(CH_3)CO(OH)$	T(100)	$7.6\ 10^{6}$	6014	Estimated	1 - 3
2- hydroxy-2-(oxomethyl)-3-oxopropanoic acid					
$CHOC(OH)(CHO)CO(OH)$	T(101)	$2.2\ 10^{11}$	6014	Estimated	1 - 2 - 3
2-(hydroxymethyl)-tartronic acid					
$CO(OH)C(OH)(CH_2(OH))CO(OH)$	T(102)	$9.2\ 10^{9}$	6014	Estimated	1 - 3
2-(oxomethyl)-tartronic acid					
$CO(OH)C(OH)(CHO)CO(OH)$	T(103)	$2.2\ 10^{11}$	6014	Estimated	1 - 2 - 3
Hydroxymethanetricarboxylic acid					
$CO(OH)C(OH)(CO(OH))CO(OH)$	T(104)	$2.0\ 10^{11}$	6014	Estimated	1 - 3
Methacrylic Acid					
$CH_2{=}C(CH_3)CO(OH)$	T(105)	$1.3\ 10^{3}$	6014	Estimated	1 - 3

1 - Estimated by the SAR GROMHE (Raventos-Duran et al., 2010).
2 - Effective Henry's law constant.
3 - When unavailable, the temperature dependence (enthalpy of dissolution) is set at 50 kJ mol^{-1}; -ΔH/R = 6014 K.

References:

Ji, C., Evans, E. M.: Using an internal standard method to determine Henry's law constants, Environmental Toxicology and Chemistry, 26-2, 231-236, 2007.

Accommodation coefficients

Species		α (298K)	-ΔH (J/mol)	-ΔS (J/mol/K)	References	Notes
C4 compounds		1				
Methacrolein						
$CH_2=C(CH_3)CHO$	T(70)	$5.0\ 10^{-2}$			Estimated	2
Hydroxymethacrolein						
$CH_2=C(CH_2(OH))CHO$	T(71)	$5.0\ 10^{-2}$			Estimated	2
Methylvinylketone						
$CH_2=CHCOCH_3$	T(72)	$5.0\ 10^{-2}$			Estimated	2
Hydroxymethylvinylketone						
$CH_2=CHCOCH_2(OH)$	T(73)	$5.0\ 10^{-2}$			Estimated	2
Hydroxybutandione						
$CH_3COCOCH_2(OH)$	T(74)	$5.0\ 10^{-2}$			Estimated	2
3,4-dihydroxybutan-2-one						
$CH_2(OH)CH(OH)COCH_3$	T(75)	$5.0\ 10^{-2}$			Estimated	2
1,4-dihydroxybutanedione						
$CH_2(OH)COCOCH_2(OH)$	T(76)	$5.0\ 10^{-2}$			Estimated	2
1,3,4-trihydroxybutanone						
$CH_2(OH)COCH(OH)CH_2(OH)$	T(77)	$5.0\ 10^{-2}$			Estimated	2
2,4-dihidroxy-3-oxobutanal						
$CH_2(OH)COCH(OH)CHO$	T(78)	$5.0\ 10^{-2}$			Estimated	2
2-oxo-3,4-dihidroxybutanal						
$CH_2(OH)CH(OH)COCHO$	T(79)	$5.0\ 10^{-2}$			Estimated	2
2-oxo-3-hydroxybutanedial						
$CHOCH(OH)COCHO$	T(80)	$5.0\ 10^{-2}$			Estimated	2
2,4-dioxo-3-hydroxybutanoic acid						
$CHOCH(OH)COCO(OH)$	T(81)	$5.0\ 10^{-2}$			Estimated	2
2,3-dioxobutanal						
$CH_3COCOCHO$	T(82)	$5.0\ 10^{-2}$			Estimated	2
2-hydroxy, 3-oxobutanal						
$CH_3COCH(OH)CHO$	T(83)	$5.0\ 10^{-2}$			Estimated	2
2-hydroxy,3-oxobutanoïc acid						
$CH_3COCH(OH)CO(OH)$	T(84)	$5.0\ 10^{-2}$			Estimated	2
2,4-dihydroxy, 3-oxobutanoic acid						
$CO(OH)CH(OH)COCH_2(OH)$	T(85)	$5.0\ 10^{-2}$			Estimated	2
2-hydroxy, 3,4-dioxobutanoic acid						
$CO(OH)CH(OH)COCHO$	T(86)	$5.0\ 10^{-2}$			Estimated	2

Species		α (298K)	-ΔH (J/mol)	-ΔS (J/mol/K)	References	Notes
2-oxomalic acid						
$CO(OH)CH(OH)COCO(OH)$	T(87)	$5.0\ 10^{-2}$			Estimated	2
Dioxosuccinic acid						
$CO(OH)COCOCO(OH)$	T(88)	$5.0\ 10^{-2}$			Estimated	2
2,4-dioxobutanedial						
$CHOCOCOCHO$	T(89)	$5.0\ 10^{-2}$			Estimated	2
2,3-dioxobutanoic acid						
$CH_3COCOCO(OH)$	T(90)	$5.0\ 10^{-2}$			Estimated	2
2,3-dioxo-4-hydroxybutanal						
$CH_2(OH)COCOCHO$	T(91)	$5.0\ 10^{-2}$			Estimated	2
2,3-dioxo-4-hydroxybutanoic acid						
$CH_2(OH)COCOCO(OH)$	T(92)	$5.0\ 10^{-2}$			Estimated	2
2,3,4-trioxobutanoic acid						
$CHOCOCOCO(OH)$	T(93)	$5.0\ 10^{-2}$			Estimated	2
Methacrylic Acid Epoxide						
$CH_3C1(CO(OH))\text{-}O\text{-}C1H_2$	T(94)	$5.0\ 10^{-2}$			Estimated	2
Hydroxymethyl-methyl-α-lactone						
$CH_3C1(CH_2(OH))\text{-}O\text{-}C1O$	T(95)	$5.0\ 10^{-2}$			Estimated	2
2- Methylglyceric Acid						
$CH_2(OH)C(OH)(CH_3)CO(OH)$	T(96)	$5.0\ 10^{-2}$			Estimated	2
2-hydroxy-3-oxomethylpropanoic acid						
$CHOC(OH)(CH_3)CO(OH)$	T(97)	$5.0\ 10^{-2}$			Estimated	2
2-hydroxy-2-(hydroxymethyl)-3-oxopropanoic acid						
$CHOC(OH)(CH_2(OH))CO(OH)$	T(98)	$5.0\ 10^{-2}$			Estimated	2
2,3-hydroxy-2-(hydroxymethyl)-propanoic acid						
$CH_2(OH)C(OH)(CH_2(OH))CO(OH)$	T(99)	$5.0\ 10^{-2}$			Estimated	2
Methyltartronic acid						
$CO(OH)C(OH)(CH_3)CO(OH)$	T(100)	$5.0\ 10^{-2}$			Estimated	2
2- hydroxy-2-(oxomethyl)-3-oxopropanoic acid						
$CHOC(OH)(CHO)CO(OH)$	T(101)	$5.0\ 10^{-2}$			Estimated	2
2-(hydroxymethyl)-tartronic acid						
$CO(OH)C(OH)(CH_2(OH))CO(OH)$	T(102)	$5.0\ 10^{-2}$			Estimated	2
2-(oxomethyl)-tartronic acid						
$CO(OH)C(OH)(CHO)CO(OH)$	T(103)	$5.0\ 10^{-2}$			Estimated	2
Hydroxymethanetricarboxylic acid						
$CO(OH)C(OH)(CO(OH))CO(OH)$	T(104)	$5.0\ 10^{-2}$			Estimated	2
Methacrylic Acid						
$CH_2{=}C(CH_3)CO(OH)$	T(105)	$5.0\ 10^{-2}$			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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