C3 compounds

For C3 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 1-propanol					
Pathway 1: $CH_3CH_2CH_2(OH) + HO^\bullet \rightarrow C^\bullet H_2CH_2CH_2(OH) + H_2O$		$4.3\ 10^8$			BR: 15% - 1
$C^\bullet H_2CH_2CH_2(OH) + O_2 \rightarrow CH_2(OH)CH_2CH_2(OO^\bullet)$		$4.7{\cdot}10^9$		Adams and Willson, 1969	
Pathway 2: $CH_3CH_2CH_2(OH) + HO^\bullet \rightarrow CH_3C^\bullet HCH_2(OH) + H_2O$		$4.3\ 10^8$			BR: 15% - 1
$CH_3C^\bullet HCH_2(OH) + O_2 \rightarrow CH_3CH(OO^\bullet)CH_2(OH)$		$4.7{\cdot}10^9$		Adams and Willson, 1969	
Pathway 3: $CH_3CH_2CH_2(OH) + HO^\bullet \rightarrow CH_3CH_2C^\bullet H(OH) + H_2O$		$1.9\ 10^9$			BR: 70% - 1
$CH_3CH_2C^\bullet H(OH) + O_2 \rightarrow CH_3CH_2CH(OH)(OO^\bullet)$		$4.7{\cdot}10^9$		Adams and Willson, 1969	
$CH_3CH_2CH_2(OH) + HO^\bullet \rightarrow 0.15\ CH_2(OH)CH_2CH_2(OO^\bullet) + 0.15\ CH_3CH(OO^\bullet)CH_2(OH) + 0.70\ CH_3CH_2CH(OH)(OO^\bullet) + H_2O - O_2$	R(389)	$2.7{\cdot}10^9$	782	Monod et al., 2005	
Pathway 1: $CH_3CH_2CH_2(OH) + NO_3^\bullet \rightarrow C^\bullet H_2CH_2CH_2(OH) + NO_3^- + H^+$		$5.1\ 10^5$			BR: 15%
$C^\bullet H_2CH_2CH_2(OH) + O_2 \rightarrow CH_2(OH)CH_2CH_2(OO^\bullet)$		$4.7{\cdot}10^9$		Adams and Willson, 1969	
Pathway 2: $CH_3CH_2CH_2(OH) + NO_3^\bullet \rightarrow CH_3C^\bullet HCH_2(OH) + NO_3^- + H^+$		$5.1\ 10^5$			BR: 15%
$CH_3C^\bullet HCH_2(OH) + O_2 \rightarrow CH_3CH(OO^\bullet)CH_2(OH)$		$4.7{\cdot}10^9$		Adams and Willson, 1969	
Pathway 3: $CH_3CH_2CH_2(OH) + NO_3^\bullet \rightarrow CH_3CH_2C^\bullet H(OH) + NO_3^- + H^+$		$2.2\ 10^6$			BR: 70%
$CH_3CH_2C^\bullet H(OH) + O_2 \rightarrow CH_3CH_2CH(OH)(OO^\bullet)$		$4.7{\cdot}10^9$		Adams and Willson, 1969	
$CH_3CH_2CH_2(OH) + NO_3^\bullet \rightarrow 0.15\ CH_2(OH)CH_2CH_2(OO^\bullet) + 0.15\ CH_3CH(OO^\bullet)CH_2(OH) + 0.70\ CH_3CH_2CH(OH)(OO^\bullet) + NO_3^- + H^+ - O_2$	R(390)	$3.2{\cdot}10^6$		Herrmann et al., 1994	2
Pathway 1: $2\ CH_2(OH)CH_2CH_2(OO^\bullet) \rightarrow 2\ CH_2(OH)CH_2CHO + H_2O_2$		$3.0\ 10^7$			BR: 20% - 3
Pathway 2: $2\ CH_2(OH)CH_2CH_2(OO^\bullet) \rightarrow 2\ CH_2(OH)CH_2CH_2(O^\bullet) + O_2$		$1.3\ 10^8$			BR: 80% - 3
$CH_2(OH)CH_2CH_2(O^\bullet) \rightarrow CH_2(OH)CH_2C^\bullet H(OH)$					4
$CH_2(OH)CH_2C^\bullet H(OH) + O_2 \rightarrow CH_2(OH)CH_2CH(OH)(OO^\bullet)$		$2.0{\cdot}10^9$			5
$2\ CH_2(OH)CH_2CH_2(OO^\bullet) \rightarrow 0.40\ CH_2(OH)CH_2CHO + 1.60\ CH_2(OH)CH_2CH(OH)(OO^\bullet) + 0.20\ H_2O_2 - 0.80\ O_2$	R(391)	$1.6\ 10^8$	-1600		= k(2 $CH_3CH_2(OO^\bullet)$) - 8
Pathway 1: $2\ CH_3CH(OO^\bullet)CH_2(OH) \rightarrow 2\ CH_3COCH_2(OH) + H_2O_2$		$5.0\ 10^7$			BR: 50%
Pathway 2:$2\ CH_3CH(OO^\bullet)CH_2(OH) \rightarrow CH_3COCH_2(OH) + CH_3CH(OH)CH_2(OH) + O_2$		$3.3\ 10^7$			BR: 33%
Pathway 3:$2\ CH_3CH(OO^\bullet)CH_2(OH) \rightarrow 2\ CH_3CH(O^\bullet)CH_2(OH) + O_2$		$1.7\ 10^7$			BR:17%
$CH_3CH(O^\bullet)CH_2(OH) \rightarrow CH_3CHO + C^\bullet H_2(OH)$					6 - 7
$C^\bullet H_2(OH) + O_2 \rightarrow CH_2(OH)(OO^\bullet)$		$2.0{\cdot}10^9$			5
$2\ CH_3CH(OO^\bullet)CH_2(OH) \rightarrow 1.33\ CH_3COCH_2(OH) + 0.33\ CH_3CH(OH)CH_2(OH) + 0.34\ CH_2(OH)(OO^\bullet) + 0.34\ CH_3CHO + 0.50\ H_2O_2 + 0.16\ O_2$	R(392)	$1.0\ 10^8$			= k(2 $CH_2(OH)CH_2(OO^\bullet)$) - 8
$CH_3CH_2CH(OH)(OO^\bullet) + OH^- \rightarrow CH_3CH_2CH(O^-)(OO^\bullet) + H_2O$		$4.0\ 10^9$			
$CH_3CH_2CH(O^-)(OO^\bullet) \rightarrow CH_3CH_2CHO + O_2^{\bullet-}$					9
$CH_3CH_2CH(OH)(OO^\bullet) + OH^- \rightarrow CH_3CH_2CHO + O_2^{\bullet-} + H_2O$	R(393)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^\bullet)$ + OH^-)
$CH_3CH_2CH(OH)(OO^\bullet) \rightarrow CH_3CH_2CHO + HO_2^\bullet$	R(394)	52			10
$CH_2(OH)CH_2CH(OH)(OO^\bullet) + OH^- \rightarrow CH_2(OH)CH_2CH(O^-)(OO^\bullet) + H_2O$		$4.0\ 10^9$			
$CH_2(OH)CH_2CH(O^-)(OO^\bullet) \rightarrow CH_2(OH)CH_2CHO + O_2^{\bullet-}$					9
$CH_2(OH)CH_2CH(OH)(OO^\bullet) + OH^- \rightarrow CH_2(OH)CH_2CHO + O_2^{\bullet-} + H_2O$	R(395)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^\bullet)$ + OH^-)
$CH_2(OH)CH_2CH(OH)(OO^\bullet) \rightarrow CH_2(OH)CH_2CHO + HO_2^\bullet$	R(396)	52			10
Oxidation of 3-hydroxypropionaldehyde					11
Pathway 1: $CH_2(OH)CH_2CHO + HO^\bullet \rightarrow CH_2(OH)CH_2C^\bullet O + H_2O$		$2.6{\cdot}10^9$			BR: 62% - 12
$CH_2(OH)CH_2C^\bullet O + O_2 \rightarrow CH_2(OH)CH_2CO(OO^\bullet)$		$2.0{\cdot}10^9$			5
Pathway 2: $CH_2(OH)CH_2CHO + HO^\bullet \rightarrow C^\bullet H(OH)CH_2CHO + H_2O$		$1.5{\cdot}10^9$			BR: 38% - 12
$C^\bullet H(OH)CH_2CHO + O_2 \rightarrow CHOCH_2CH(OH)(OO^\bullet)$		$2.0{\cdot}10^9$			5

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CH_2(OH)CH_2CHO + HO^\bullet \rightarrow 0.62\ CH_2(OH)CH_2CO(OO^\bullet) + 0.38\ CHOCH_2CH(OH)(OO^\bullet) + H_2O - O_2$	R(397)	$4.1\ 10^9$			13
Pathway 1: $CH_2(OH)CH_2CHO + NO_3^\bullet \rightarrow CH_2(OH)CH_2C^\bullet O + NO_3^- + H^+$		$1.9{\cdot}10^6$			BR: 62%
$CH_2(OH)CH_2C^\bullet O + O_2 \rightarrow CH_2(OH)CH_2CO(OO^\bullet)$		$2.0{\cdot}10^9$			5
Pathway 2: $CH_2(OH)CH_2CHO + NO_3^\bullet \rightarrow C^\bullet H(OH)CH_2CHO + NO_3^- + H^+$		$1.2{\cdot}10^6$			BR: 38%
$C^\bullet H(OH)CH_2CHO + O_2 \rightarrow CHOCH_2CH(OH)(OO^\bullet)$		$2.0{\cdot}10^9$			5
$CH_2(OH)CH_2CHO + NO_3^\bullet \rightarrow 0.62\ CH_2(OH)CH_2CO(OO^\bullet) + 0.38\ CHOCH_2CH(OH)(OO^\bullet) + NO_3^- + H^+ - O_2$	R(398)	$3.1\ 10^6$			$= k(CH_2(OH)CHO + NO_3^\bullet) - 2$
Pathway 1: $CH_2(OH)CH_2CH(OH)(OH) + HO^\bullet \rightarrow CH_2(OH)CH_2C^\bullet(OH)(OH) + H_2O$		$1.1{\cdot}10^9$			BR: 33% - 14
$CH_2(OH)CH_2C^\bullet(OH)(OH) + O_2 \rightarrow CH_2(OH)CH_2C(OH)(OH)(OO^\bullet)$		$2.0{\cdot}10^9$			5
Pathway 2: $CH_2(OH)CH_2CH(OH)(OH) + HO^\bullet \rightarrow C^\bullet H(OH)CH_2CH(OH)(OH) + H_2O$		$2.1{\cdot}10^9$			BR: 67% - 14
$C^\bullet H(OH)CH_2CH(OH)(OH) + O_2 \rightarrow CH(OH)(OH)CH_2CH(OH)(OO^\bullet)$		$2.0{\cdot}10^9$			5
$CH_2(OH)CH_2CH(OH)(OH) + HO^\bullet \rightarrow 0.33\ CH_2(OH)CH_2C(OH)(OH)(OO^\bullet) + 0.67\ CH(OH)(OH)CH_2CH(OH)(OO^\bullet) + H_2O - O_2$	R(399)	$3.2\ 10^9$			13
Pathway 1: $CH_2(OH)CH_2CH(OH)(OH) + NO_3^\bullet \rightarrow CH_2(OH)CH_2C^\bullet(OH)(OH) + NO_3^- + H^+$		$3.6{\cdot}10^5$			BR: 33%
$CH_2(OH)CH_2C^\bullet(OH)(OH) + O_2 \rightarrow CH_2(OH)CH_2C(OH)(OH)(OO^\bullet)$		$2.0{\cdot}10^9$			5
Pathway 2: $CH_2(OH)CH_2CH(OH)(OH) + NO_3^\bullet \rightarrow C^\bullet H(OH)CH_2CH(OH)(OH) + NO_3^- + H^+$		$7.4{\cdot}10^5$			BR: 67%
$C^\bullet H(OH)CH_2CH(OH)(OH) + O_2 \rightarrow CH(OH)(OH)CH_2CH(OH)(OO^\bullet)$		$2.0{\cdot}10^9$			5
$CH_2(OH)CH_2CH(OH)(OH) + NO_3^\bullet \rightarrow 0.33\ CH_2(OH)CH_2C(OH)(OH)(OO^\bullet) + 0.67\ CH(OH)(OH)CH_2CH(OH)(OO^\bullet) + NO_3^- + H^+ - O_2$	R(400)	$1.1\ 10^6$			$= k(CH_2(OH)CH(OH)(OH) + NO_3^\bullet) - 2$
$2\ CH_2(OH)CH_2CO(OO^\bullet) \rightarrow 2\ CH_2(OH)CH_2CO(O^\bullet) + O_2$		$1.6{\cdot}10^8$			
$CH_2(OH)CH_2CO(O^\bullet) \rightarrow CH_2(OH)C^\bullet H_2 + CO_2$					6 - 7
$CH_2(OH)C^\bullet H_2 + O_2 \rightarrow CH_2(OH)CH_2(OO^\bullet)$		$2.0{\cdot}10^9$			5
$2\ CH_2(OH)CH_2CO(OO^\bullet) \rightarrow 2\ CH_2(OH)CH_2(OO^\bullet) + 2\ CO_2 - O_2$	R(401)	$1.6{\cdot}10^8$	-1600		$= k(2\ CH_3CH_2(OO^\bullet))$
$CHOCH_2CH(OH)(OO^\bullet) + OH^- \rightarrow CHOCH_2CH(O^-)(OO^\bullet) + H_2O$		$4.0\ 10^9$			
$CHOCH_2CH(O^-)(OO^\bullet) \rightarrow CHOCH_2CHO + O_2^{\bullet-}$					9
$CHOCH_2CH(OH)(OO^\bullet) + OH^- \rightarrow CHOCH_2CHO + O_2^{\bullet-} + H_2O$	R(402)	$4.0\ 10^9$			$= k(CH_3CH(OH)(OO^\bullet) + OH^-)$
$CHOCH_2CH(OH)(OO^\bullet) \rightarrow CHOCH_2CHO + HO_2^\bullet$	R(403)	52			10
$CH_2(OH)CH_2C(OH)(OH)(OO^\bullet) + OH^- \rightarrow CH_2(OH)CH_2C(OH)(O^-)(OO^\bullet) + H_2O$		$4.0\ 10^9$			
$CH_2(OH)CH_2C(OH)(O^-)(OO^\bullet) \rightarrow CH_2(OH)CH_2CO(OH) + O_2^{\bullet-}$					9
$CH_2(OH)CH_2C(OH)(OH)(OO^\bullet) + OH^- \rightarrow CH_2(OH)CH_2CO(OH) + O_2^{\bullet-} + H_2O$	R(404)	$4.0\ 10^9$			$= k(CH_3CH(OH)(OO^\bullet) + OH^-)$
$CH_2(OH)CH_2C(OH)(OH)(OO^\bullet) \rightarrow CH_2(OH)CH_2CO(OH) + HO_2^\bullet$	R(405)	$1.0\ 10^6$			15
$CH(OH)(OH)CH_2CH(OH)(OO^\bullet) + OH^- \rightarrow CH(OH)(OH)CH_2CH(O^-)(OO^\bullet) + H_2O$		$4.0\ 10^9$			
$CH(OH)(OH)CH_2CH(O^-)(OO^\bullet) \rightarrow CHOCH_2CH(OH)(OH) + O_2^{\bullet-}$					9
$CH(OH)(OH)CH_2CH(OH)(OO^\bullet) + OH^- \rightarrow CHOCH_2CH(OH)(OH) + O_2^{\bullet-} + H_2O$	R(406)	$4.0\ 10^9$			$= k(CH_3CH(OH)(OO^\bullet) + OH^-)$
$CH(OH)(OH)CH_2CH(OH)(OO^\bullet) \rightarrow CHOCH_2CH(OH)(OH) + HO_2^\bullet$	R(407)	52			10
Oxidation of propane-1,2-diol					
Pathway 1: $CH_3CH(OH)CH_2(OH) + HO^\bullet \rightarrow CH_3CH(OH)C^\bullet H(OH) + H_2O$		$1.0{\cdot}10^9$			BR: 60% - 16
$CH_3CH(OH)C^\bullet H(OH) + O_2 \rightarrow CH_3CH(OH)CH(OH)(OO^\bullet)$		$2.0{\cdot}10^9$			5
Pathway 2: $CH_3CH(OH)CH_2(OH) + HO^\bullet \rightarrow CH_3C^\bullet(OH)CH_2(OH) + H_2O$		$7.0{\cdot}10^8$			BR: 40% - 16
$CH_3C^\bullet(OH)CH_2(OH) + O_2 \rightarrow CH_3C(OH)(OO^\bullet)CH_2(OH)$		$2.0{\cdot}10^9$			5
$CH_3CH(OH)CH_2(OH) + HO^\bullet \rightarrow 0.60\ CH_3CH(OH)CH(OH)(OO^\bullet) + 0.40\ CH_3C(OH)(OO^\bullet)CH_2(OH) + H_2O - O_2$	R(408)	$1.7\ 10^9$		Hoffmann et al., 2009	
Pathway 1: $CH_3CH(OH)CH_2(OH) + NO_3^\bullet \rightarrow CH_3CH(OH)C^\bullet H(OH) + NO_3^- + H^+$		$5.9{\cdot}10^6$			BR: 60%
$CH_3CH(OH)C^\bullet H(OH) + O_2 \rightarrow CH_3CH(OH)CH(OH)(OO^\bullet)$		$2.0{\cdot}10^9$			5
Pathway 2: $CH_3CH(OH)CH_2(OH) + NO_3^\bullet \rightarrow CH_3C^\bullet(OH)CH_2(OH) + NO_3^- + H^+$		$4.0{\cdot}10^6$			BR: 40%
$CH_3C^\bullet(OH)CH_2(OH) + O_2 \rightarrow CH_3C(OH)(OO^\bullet)CH_2(OH)$		$2.0{\cdot}10^9$			5
$CH_3CH(OH)CH_2(OH) + NO_3^\bullet \rightarrow 0.60\ CH_3CH(OH)CH(OH)(OO^\bullet) + 0.40\ CH_3C(OH)(OO^\bullet)CH_2(OH) + NO_3^- + H^+ - O_2$	R(409)	$9.9\ 10^6$		Hoffmann et al., 2009	2
$CH_3CH(OH)CH(OH)(OO^\bullet) + OH^- \rightarrow CH_3CH(OH)CH(O^-)(OO^\bullet) + H_2O$		$4.0\ 10^9$			

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CH_3CH(OH)CH(O^-)(OO^\bullet) \rightarrow CH_3CH(OH)CHO + O_2^{\bullet-}$					9
$CH_3CH(OH)CH(OH)(OO^\bullet) + OH^- \rightarrow CH_3CH(OH)CHO + O_2^{\bullet-} + H_2O$	R(410)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^\bullet) + OH^-$)
$CH_3CH(OH)CH(OH)(OO^\bullet) \rightarrow CH_3CH(OH)CHO + HO_2^\bullet$	R(411)	$1.9\ 10^2$			10
$CH_3C(OH)(OO^\bullet)CH_2(OH) + OH^- \rightarrow CH_3C(O^-)(OO^\bullet)CH_2(OH) + H_2O$		$4.0\ 10^9$			
$CH_3C(O^-)(OO^\bullet)CH_2(OH) \rightarrow CH_3COCH_2(OH) + O_2^{\bullet-}$					9
$CH_3C(OH)(OO^\bullet)CH_2(OH) + OH^- \rightarrow CH_3COCH_2(OH) + O_2^{\bullet-} + H_2O$	R(412)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^\bullet) + OH^-$)
$CH_3C(OH)(OO^\bullet)CH_2(OH) \rightarrow CH_3COCH_2(OH) + HO_2^\bullet$	R(413)	$1.9\ 10^2$			10
Oxidation of 2-hydroxypropionaldehyde					17
Pathway 1: $CH_3CH(OH)CH(OH)(OH) + HO^\bullet \rightarrow CH_3CH(OH)CH(OH)(O^\bullet) + H_2O$		$4.8\ 10^8$			BR: 37% - 18
$CH_3CH(OH)CH(OH)(O^\bullet) \rightarrow CH_3C^\bullet H(OH) + CHO(OH)$					6 - 7
$CH_3C^\bullet H(OH) + O_2 \rightarrow CH_3CH(OH)(OO^\bullet)$		$2.0{\cdot}10^9$			5
Pathway 2: $CH_3CH(OH)CH(OH)(OH) + HO^\bullet \rightarrow CH_3CH(OH)C^\bullet(OH)(OH) + H_2O$		$4.6\ 10^8$			BR: 35% - 18
$CH_3CH(OH)C^\bullet(OH)(OH) + O_2 \rightarrow CH_3CH(OH)C(OH)(OH)(OO^\bullet)$		$2.0{\cdot}10^9$			5
Pathway 3: $CH_3CH(OH)CH(OH)(OH) + HO^\bullet \rightarrow CH_3C^\bullet(OH)CH(OH)(OH) + H_2O$		$3.6\ 10^8$			BR: 28% - 18
$CH_3C^\bullet(OH)CH(OH)(OH) + O_2 \rightarrow CH_3C(OH)(OO^\bullet)CH(OH)(OH)$		$2.0{\cdot}10^9$			5
$CH_3CH(OH)CH(OH)(OH) + HO^\bullet \rightarrow 0.37\ CH_3CH(OH)(OO^\bullet) + 0.37\ CHO(OH) + 0.35\ CH_3CH(OH)C(OH)(OH)(OO^\bullet) + 0.28\ CH_3C(OH)(OO^\bullet)CH(OH)(OH) + H_2O - O_2$	R(414)	$1.3\ 10^9$			13
Pathway 1: $CH_3CH(OH)CH(OH)(OH) + NO_3^\bullet \rightarrow CH_3CH(OH)C^\bullet(OH)(OH) + NO_3^- + H^+$		$6.2\ 10^5$			BR: 56%
$CH_3CH(OH)C^\bullet(OH)(OH) + O_2 \rightarrow CH_3CH(OH)C(OH)(OH)(OO^\bullet)$		$2.0{\cdot}10^9$			5
Pathway 2: $CH_3CH(OH)CH(OH)(OH) + NO_3^\bullet \rightarrow CH_3C^\bullet(OH)CH(OH)(OH) + NO_3^- + H^+$		$4.8\ 10^5$			BR: 44%
$CH_3C^\bullet(OH)CH(OH)(OH) + O_2 \rightarrow CH_3C(OH)(OO^\bullet)CH(OH)(OH)$		$2.0{\cdot}10^9$			5
$CH_3CH(OH)CH(OH)(OH) + NO_3^\bullet \rightarrow 0.56\ CH_3CH(OH)C(OH)(OH)(OO^\bullet) + 0.44\ CH_3C(OH)(OO^\bullet)CH(OH)(OH) + NO_3^- + H^+ - O_2$	R(415)	$1.1\ 10^6$			= k($CH_2(OH)CH(OH)(OH) + NO_3^\bullet$) - 2
$CH_3CH(OH)C(OH)(OH)(OO^\bullet) + OH^- \rightarrow CH_3CH(OH)C(OH)(O^-)(OO^\bullet) + H_2O$		$4.0\ 10^9$			
$CH_3CH(OH)C(OH)(O^-)(OO^\bullet) \rightarrow CH_3CH(OH)CO(OH) + O_2^{\bullet-}$					9
$CH_3CH(OH)C(OH)(OH)(OO^\bullet) + OH^- \rightarrow CH_3CH(OH)CO(OH) + O_2^{\bullet-} + H_2O$	R(416)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^\bullet) + OH^-$)
$CH_3CH(OH)C(OH)(OH)(OO^\bullet) \rightarrow CH_3CH(OH)CO(OH) + HO_2^\bullet$	R(417)	$1.0\ 10^6$			15
$CH_3C(OH)(OO^\bullet)CH(OH)(OH) + OH^- \rightarrow CH_3C(O^-)(OO^\bullet)CH(OH)(OH) + H_2O$		$4.0\ 10^9$			
$CH_3C(O^-)(OO^\bullet)CH(OH)(OH) \rightarrow CH_3COCH(OH)(OH) + O_2^{\bullet-}$					9
$CH_3C(OH)(OO^\bullet)CH(OH)(OH) + OH^- \rightarrow CH_3COCH(OH)(OH) + O_2^{\bullet-} + H_2O$	R(418)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^\bullet) + OH^-$)
$CH_3C(OH)(OO^\bullet)CH(OH)(OH) \rightarrow CH_3COCH(OH)(OH) + HO_2^\bullet$	R(419)	$1.9\ 10^2$			10
Oxidation of propanedial					19
Pathway 1: $CH(OH)(OH)CH_2CH(OH)(OH) + HO^\bullet \rightarrow CH(OH)(OH)CH_2C^\bullet(OH)(OH) + H_2O$		$1.7\ 10^9$			BR: 67% - 20
$CH(OH)(OH)CH_2C^\bullet(OH)(OH) + O_2 \rightarrow CH(OH)(OH)CH_2C(OH)(OH)(OO^\bullet)$		$2.0{\cdot}10^9$			5
Pathway 2: $CH(OH)(OH)CH_2CH(OH)(OH) + HO^\bullet \rightarrow CH(OH)(OH)CH_2CH(OH)(O^\bullet) + H_2O$		$8.0\ 10^8$			BR: 33% - 20
$CH(OH)(OH)CH_2CH(OH)(O^\bullet) \rightarrow CH(OH)(OH)CH_2C^\bullet(OH)(OH)$					4
$CH(OH)(OH)CH_2C^\bullet(OH)(OH) + O_2 \rightarrow CH(OH)(OH)CH_2C(OH)(OH)(OO^\bullet)$		$2.0{\cdot}10^9$			5
$CH(OH)(OH)CH_2CH(OH)(OH) + HO^\bullet \rightarrow CH(OH)(OH)CH_2C(OH)(OH)(OO^\bullet) + H_2O - O_2$	R(420)	$2.5\ 10^9$			13
$CH(OH)(OH)CH_2CH(OH)(OH) + NO_3^\bullet \rightarrow CH(OH)(OH)CH_2C^\bullet(OH)(OH) + NO_3^- + H^+$		$1.0\ 10^6$			BR: 100%
$CH(OH)(OH)CH_2C^\bullet(OH)(OH) + O_2 \rightarrow CH(OH)(OH)CH_2C(OH)(OH)(OO^\bullet)$		$2.0{\cdot}10^9$			5
$CH(OH)(OH)CH_2CH(OH)(OH) + NO_3^\bullet \rightarrow CH(OH)(OH)CH_2C(OH)(OH)(OO^\bullet) + NO_3^- + H^+$	R(421)	$1.0\ 10^6$			= k($CH(OH)(OH)CH(OH)(OH) + NO_3^\bullet$) - 2
$CH(OH)(OH)CH_2C(OH)(OH)(OO^\bullet) + OH^- \rightarrow CH(OH)(OH)CH_2C(OH)(O^-)(OO^\bullet) + H_2O$		$4.0\ 10^9$			
$CH(OH)(OH)CH_2C(OH)(O^-)(OO^\bullet) \rightarrow CO(OH)CH_2CH(OH)(OH) + O_2^{\bullet-}$					9
$CH(OH)(OH)CH_2C(OH)(OH)(OO^\bullet) + OH^- \rightarrow CO(OH)CH_2CH(OH)(OH) + O_2^{\bullet-} + H_2O$	R(422)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^\bullet) + OH^-$)

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CH(OH)(OH)CH_2C(OH)(OH)(OO^•) \rightarrow CO(OH)CH_2CH(OH)(OH) + HO_2^•$	R(423)	$1.0\ 10^6$			15
Oxidation of 3-hydroxypropionic acid					
Pathway 1: $CH_2(OH)CH_2CO(OH) + HO^• \rightarrow C^•H(OH)CH_2CO(OH) + H_2O$		$1.3\ 10^9$			BR: 100% - 21
$C^•H(OH)CH_2CO(OH) + O_2 \rightarrow CH(OH)(OO^•)CH_2CO(OH)$		$2.0 \cdot 10^9$			5
$CH_2(OH)CH_2CO(OH) + HO^• \rightarrow CH(OH)(OO^•)CH_2CO(OH) + H_2O - O_2$	R(424)	$1.3\ 10^9$			13
Pathway 1: $CH_2(OH)CH_2CO(OH) + NO_3^• \rightarrow C^•H(OH)CH_2CO(OH) + NO_3^- + H^+$		$2.1\ 10^6$			BR: 100%
$C^•H(OH)CH_2CO(OH) + O_2 \rightarrow CH(OH)(OO^•)CH_2CO(OH)$		$2.0 \cdot 10^9$			5
$CH_2(OH)CH_2CO(OH) + NO_3^• \rightarrow CH(OH)(OO^•)CH_2CO(OH) + NO_3^- + H^+ - O_2$	R(425)	$2.1 \cdot 10^6$	3248		= k($CH_3CH(OH)CO(OH)$ + $NO_3^•$) - 2
Pathway 1: $CH_2(OH)CH_2CO(O^-) + HO^• \rightarrow C^•H(OH)CH_2CO(O^-) + H_2O$		$2.5\ 10^9$			BR: 100% - 22
$C^•H(OH)CH_2CO(O^-) + O_2 \rightarrow CH(OH)(OO^•)CH_2CO(O^-)$		$2.0 \cdot 10^9$			5
$CH_2(OH)CH_2CO(O^-) + HO^• \rightarrow CH(OH)(OO^•)CH_2CO(O^-) + H_2O - O_2$	R(426)	$2.5\ 10^9$			13
Pathway 1: $CH_2(OH)CH_2CO(O^-) + NO_3^• \rightarrow C^•H(OH)CH_2CO(O^-) + NO_3^- + H^+$		$1.0\ 10^7$			BR: 100%
$C^•H(OH)CH_2CO(O^-) + O_2 \rightarrow CH(OH)(OO^•)CH_2CO(O^-)$		$2.0 \cdot 10^9$			5
$CH_2(OH)CH_2CO(O^-) + NO_3^• \rightarrow CH(OH)(OO^•)CH_2CO(O^-) + NO_3^- + H^+ - O_2$	R(427)	$1.0 \cdot 10^7$	2646		= k($CH_3CH(OH)CO(O^-) + NO_3^•$) - 2
$CH(OH)(OO^•)CH_2CO(OH) + OH^- \rightarrow CH(O^-)(OO^•)CH_2CO(OH) + H_2O$		$4.0\ 10^9$			
$CH(O^-)(OO^•)CH_2CO(OH) \rightarrow CO(OH)CH_2CHO + O_2^{•-}$					9
$CH(OH)(OO^•)CH_2CO(OH) + OH^- \rightarrow CO(OH)CH_2CHO + O_2^{•-} + H_2O$	R(428)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^•) + OH^-$)
$CH(OH)(OO^•)CH_2CO(OH) \rightarrow CO(OH)CH_2CHO + HO_2^•$	R(429)	52			10
$CH(OH)(OO^•)CH_2CO(O^-) + OH^- \rightarrow CH(O^-)(OO^•)CH_2CO(O^-) + H_2O$		$4.0\ 10^9$			
$CH(O^-)(OO^•)CH_2CO(O^-) \rightarrow CO(O^-)CH_2CHO + O_2^{•-}$					9
$CH(OH)(OO^•)CH_2CO(O^-) + OH^- \rightarrow CO(O^-)CH_2CHO + O_2^{•-} + H_2O$	R(430)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^•) + OH^-$)
$CH(OH)(OO^•)CH_2CO(O^-) \rightarrow CO(O^-)CH_2CHO + HO_2^•$	R(431)	52			10
Oxidation of 2-propanol					
Pathway 1: $CH_3CH(OH)CH_3 + HO^• \rightarrow CH_3CH(OH)C^•H_2 + H_2O$		$2.0\ 10^8$		Padmaja et al., 1993	BR: 13% - 23
$CH_3CH(OH)C^•H_2 + O_2 \rightarrow CH_3CH(OH)CH_2(OO^•)$		$4.2 \cdot 10^9$		Schaefer et al., 2014	
Pathway 2: $CH_3CH(OH)CH_3 + HO^• \rightarrow CH_3C^•(OH)CH_3 + H_2O$		$1.7\ 10^9$			BR: 87% - 23
$CH_3C^•(OH)CH_3 + O_2 \rightarrow CH_3C(OH)(OO^•)CH_3$		$4.2 \cdot 10^9$		Schaefer et al., 2014	
$CH_3CH(OH)CH_3 + HO^• \rightarrow 0.87\ CH_3C(OH)(OO^•)CH_3 + 0.13\ CH_3CH(OH)CH_2(OO^•) + H_2O - O_2$	R(432)	$1.9 \cdot 10^9$		Monod et al., 2005	
Pathway 1: $CH_3CH(OH)CH_3 + NO_3^• \rightarrow CH_3CH(OH)C^•H_2 + NO_3^- + H^+$		$5.0\ 10^5$			BR: 13%
$CH_3CH(OH)C^•H_2 + O_2 \rightarrow CH_3CH(OH)CH_2(OO^•)$		$4.2 \cdot 10^9$		Schaefer et al., 2014	
Pathway 2: $CH_3CH(OH)CH_3 + NO_3^• \rightarrow CH_3C^•(OH)CH_3 + NO_3^- + H^+$		$3.2\ 10^6$			BR: 87%
$CH_3C^•(OH)CH_3 + O_2 \rightarrow CH_3C(OH)(OO^•)CH_3$		$4.2 \cdot 10^9$		Schaefer et al., 2014	
$CH_3CH(OH)CH_3 + NO_3^• \rightarrow 0.87\ CH_3C(OH)(OO^•)CH_3 + 0.13\ CH_3CH(OH)CH_2(OO^•) + NO_3^- + H^+ - O_2$	R(433)	$3.7 \cdot 10^6$		Herrmann et al., 1994	2
$CH_3C(OH)(OO^•)CH_3 + OH^- \rightarrow CH_3C(O^-)(OO^•)CH_3 + H_2O$		$5.2\ 10^9$			
$CH_3C(O^-)(OO^•)CH_3 \rightarrow CH_3COCH_3 + O_2^{•-}$					9
$CH_3C(OH)(OO^•)CH_3 + OH^- \rightarrow CH_3COCH_3 + O_2^{•-} + H_2O$	R(434)	$5.2\ 10^9$		Ilan et al., 1976	
$CH_3C(OH)(OO^•)CH_3 \rightarrow CH_3COCH_3 + HO_2^•$	R(435)	$7.0\ 10^2$		Ilan et al., 1976	
Pathway 1: $2\ CH_3CH(OH)CH_2(OO^•) \rightarrow 2\ CH_3CH(OH)CHO + H_2O_2$		$5.0\ 10^7$			BR: 50%
Pathway 2: $2\ CH_3CH(OH)CH_2(OO^•) \rightarrow CH_3CH(OH)CH_2(OH) + CH_3CH(OH)CHO + O_2$		$3.3\ 10^7$			BR: 33%
Pathway 3: $2\ CH_3CH(OH)CH_2(OO^•) \rightarrow 2\ CH_3CH(OH)CH_2(O^•) + O_2$		$1.7\ 10^7$			BR: 17%
$CH_3CH(OH)CH_2(O^•) \rightarrow CH_2O + CH_3C^•H(OH)$					6 - 7
$CH_3C^•H(OH) + O_2 \rightarrow CH_3CH(OH)(OO^•)$		$2.0 \cdot 10^9$			5
$2\ CH_3CH(OH)CH_2(OO^•) \rightarrow 1.33\ CH_3CH(OH)CHO + 0.33\ CH_3CH(OH)CH_2(OH) + 0.34\ CH_3CH(OH)(OO^•) + 0.34\ CH_2O + 0.50\ H_2O_2 + 0.16\ O_2$	R(436)	$1.0\ 10^8$			= k($2\ CH_2(OH)CH_2(OO^•)$) - 8

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
Oxidation of propionaldehyde - ethylperoxide formation					24
Pathway 1: $CH_3CH_2CHO + HO^\bullet \rightarrow CH_3CH_2C^\bullet O + H_2O$		$2.6\ 10^9$			BR: 87% - 25
$CH_3CH_2C^\bullet O + O_2 \rightarrow CH_3CH_2CO(OO^\bullet)$		$2.0{\cdot}10^9$			5
Pathway 2: $CH_3CH_2CHO + HO^\bullet \rightarrow C^\bullet H_2CH_2CHO + H_2O$		$4.0\ 10^8$			BR: 13% - 25
$C^\bullet H_2CH_2CHO + O_2 \rightarrow CHOCH_2CH_2(OO^\bullet)$		$2.0{\cdot}10^9$			5
$CH_3CH_2CHO + HO^\bullet \rightarrow 0.87\ CH_3CH_2CO(OO^\bullet) + 0.13\ CHOCH_2CH_2(OO^\bullet) + H_2O - O_2$	R(437)	$3.2{\cdot}10^9$			13
Pathway 1: $CH_3CH_2CHO + NO_3^\bullet \rightarrow CH_3CH_2C^\bullet O + NO_3^- + H^+$		$5.0\ 10^7$			BR: 87%
$CH_3CH_2C^\bullet O + O_2 \rightarrow CH_3CH_2CO(OO^\bullet)$		$2.0{\cdot}10^9$			5
Pathway 2: $CH_3CH_2CHO + NO_3^\bullet \rightarrow C^\bullet H_2CH_2CHO + NO_3^- + H^+$		$8.0\ 10^6$			BR: 13%
$C^\bullet H_2CH_2CHO + O_2 \rightarrow CHOCH_2CH_2(OO^\bullet)$		$2.0{\cdot}10^9$			5
$CH_3CH_2CHO + NO_3^\bullet \rightarrow 0.87\ CH_3CH_2CO(OO^\bullet) + 0.13\ CHOCH_2CH_2(OO^\bullet) + NO_3^- + H^+ - O_2$	R(438)	$5.8{\cdot}10^7$	2646	De Semainville et al., 2007	2
Pathway 1: $CH_3CH_2CH(OH)(OH) + HO^\bullet \rightarrow CH_3CH_2C^\bullet(OH)(OH) + H_2O$		$9.9\ 10^8$			BR: 52% - 26
$CH_3CH_2C^\bullet(OH)(OH) + O_2 \rightarrow CH_3CH_2C(OH)(OH)(OO^\bullet)$		$2.0{\cdot}10^9$			5
Pathway 2: $CH_3CH_2CH(OH)(OH) + HO^\bullet \rightarrow C^\bullet H_2CH_2CH(OH)(OH) + H_2O$		$4.8\ 10^8$			BR: 25% - 26
$C^\bullet H_2CH_2CH(OH)(OH) + O_2 \rightarrow CH(OH)(OH)CH_2CH_2(OO^\bullet)$		$2.0{\cdot}10^9$			5
Pathway 3: $CH_3CH_2CH(OH)(OH) + HO^\bullet \rightarrow CH_3CH_2CH(OH)(O^\bullet) + H_2O$		$4.3\ 10^8$			BR: 23% - 26
$CH_3CH_2CH(OH)(O^\bullet) \rightarrow CH_3CH_2C^\bullet(OH)(OH)$					4
$CH_3CH_2C^\bullet(OH)(OH) + O_2 \rightarrow CH_3CH_2C(OH)(OH)(OO^\bullet)$		$2.0{\cdot}10^9$			5
$CH_3CH_2CH(OH)(OH) + HO^\bullet \rightarrow 0.75\ CH_3CH_2C(OH)(OH)(OO^\bullet) + 0.25\ CH(OH)(OH)CH_2CH_2(OO^\bullet) + H_2O - O_2$	R(439)	$1.9{\cdot}10^9$			13
Pathway 1: $CH_3CH_2CH(OH)(OH) + NO_3^\bullet \rightarrow CH_3CH_2C^\bullet(OH)(OH) + NO_3^- + H^+$		$3.9\ 10^7$			BR: 67%
$CH_3CH_2C^\bullet(OH)(OH) + O_2 \rightarrow CH_3CH_2C(OH)(OH)(OO^\bullet)$		$2.0{\cdot}10^9$			5
Pathway 2: $CH_3CH_2CH(OH)(OH) + NO_3^\bullet \rightarrow C^\bullet H_2CH_2CH(OH)(OH) + NO_3^- + H^+$		$1.9\ 10^7$			BR: 33%
$C^\bullet H_2CH_2CH(OH)(OH) + O_2 \rightarrow CH(OH)(OH)CH_2CH_2(OO^\bullet)$		$2.0{\cdot}10^9$			5
$CH_3CH_2CH(OH)(OH) + NO_3^\bullet \rightarrow 0.67\ CH_3CH_2C(OH)(OH)(OO^\bullet) + 0.33\ CH(OH)(OH)CH_2CH_2(OO^\bullet) + NO_3^- + H^+ - O_2$	R(440)	$5.8{\cdot}10^7$	2646	De Semainville et al., 2007	2
$2\ CH_3CH_2CO(OO^\bullet) \rightarrow 2\ CH_3CH_2CO(O^\bullet){\cdot} + O_2$		$1.6{\cdot}10^8$			
$CH_3CH_2CO(O^\bullet){\cdot} \rightarrow CH_3CH_2^\bullet{\cdot} + CO_2$					6 - 7
$CH_3CH_2^\bullet + O_2 \rightarrow CH_3CH_2(OO^\bullet)$		$2.0{\cdot}10^9$			5
$2\ CH_3CH_2CO(OO^\bullet) \rightarrow 2\ CH_3CH_2(OO^\bullet) + 2\ CO_2 - O_2$	R(441)	$1.6{\cdot}10^8$	-1600		= k(2 $CH_3CH_2(OO^\bullet)$) - 8
Pathway 1: $2\ CHOCH_2CH_2(OO^\bullet) \rightarrow 2\ CHOCH_2CHO + H_2O_2$		$3.0\ 10^7$			BR: 20% - 3
Pathway 2: $2\ CHOCH_2CH_2(OO^\bullet) \rightarrow 2\ CHOCH_2CH_2(O^\bullet) + O_2$		$1.3\ 10^8$			BR: 80% - 3
$CHOCH_2CH_2(O^\bullet) \rightarrow CHOCH_2C^\bullet H(OH)$					4
$CHOCH_2C^\bullet H(OH) + O_2 \rightarrow CHOCH_2CH(OH)(OO^\bullet)$		$2.0{\cdot}10^9$			5
$2\ CHOCH_2CH_2(OO^\bullet) \rightarrow 0.40\ CHOCH_2CHO + 1.60\ CHOCH_2CH(OH)(OO^\bullet) + 0.20\ H_2O_2 - 0.80\ O_2$	R(442)	$1.6\ 10^8$	-1600		= k(2 $CH_3CH_2(OO^\bullet)$) - 8
$CH_3CH_2C(OH)(OH)(OO^\bullet) + OH^- \rightarrow CH_3CH_2C(OH)(O^-)(OO^\bullet) + H_2O$		$4.0\ 10^9$			
$CH_3CH_2C(OH)(O^-)(OO^\bullet) \rightarrow CH_3CH_2CO(OH) + O_2^{\bullet-}$					9
$CH_3CH_2C(OH)(OH)(OO^\bullet) + OH^- \rightarrow CH_3CH_2CO(OH) + O_2^{\bullet-} + H_2O$	R(443)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^\bullet)$ + OH^-)
$CH_3CH_2C(OH)(OH)(OO^\bullet) \rightarrow CH_3CH_2CO(OH) + HO_2^\bullet$	R(444)	$1.0\ 10^6$			15
Pathway 1: $2\ CH(OH)(OH)CH_2CH_2(OO^\bullet) \rightarrow 2\ CHOCH_2CH(OH)(OH) + H_2O_2$		$3.0\ 10^7$			BR: 20% - 3
Pathway 2: $2\ CH(OH)(OH)CH_2CH_2(OO^\bullet) \rightarrow 2\ CH(OH)(OH)CH_2CH_2(O^\bullet) + O_2$		$1.3\ 10^8$			BR: 80% - 3
$CH(OH)(OH)CH_2CH_2(O^\bullet) \rightarrow CH(OH)(OH)CH_2C^\bullet H(OH)$					4
$CH(OH)(OH)CH_2C^\bullet H(OH) + O_2 \rightarrow CH(OH)(OH)CH_2CH(OH)(OO^\bullet)$		$2.0{\cdot}10^9$			5
$2\ CH(OH)(OH)CH_2CH_2(OO^\bullet) \rightarrow 0.40\ CHOCH_2CH(OH)(OH) + 1.60\ CH(OH)(OH)CH_2CH(OH)(OO^\bullet) + 0.20\ H_2O_2 - 0.80\ O_2$	R(445)	$1.6\ 10^8$	-1600		= k(2 $CH_3CH_2(OO^\bullet)$) - 8
Oxidation of methylglyoxal					27
Pathway 1: $CH_3COCH(OH)(OH) + HO^\bullet \rightarrow C^\bullet H_2COCH(OH)(OH) + H_2O$		$1.2\ 10^8$			BR: 14% - 28

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$C^{\bullet}H_2COCH(OH)(OH) + O_2 \rightarrow CH(OH)(OH)COCH_2(OO^{\bullet})$		$2.0\ 10^9$			5
Pathway 2: $CH_3COCH(OH)(OH) + HO^{\bullet} \rightarrow CH_3COC^{\bullet}(OH)(OH) + H_2O$		$2.7\ 10^8$			BR: 29% - 28
$CH_3COC^{\bullet}(OH)(OH) + O_2 \rightarrow CH_3COC(OH)(OH)(OO^{\bullet})$		$2.0\ 10^9$			5
Pathway 3: $CH_3COCH(OH)(OH) + HO^{\bullet} \rightarrow CH_3COCH(OH)(O^{\bullet}) + H_2O$		$5.3\ 10^8$			BR: 57% - 28
$CH_3COCH(OH)(O^{\bullet}) \rightarrow CH_3C^{\bullet}O + CHO(OH)$					6 - 7
$CH_3C^{\bullet}O + O_2 \rightarrow CH_3CO(OO^{\bullet})$		$2.0\ 10^9$			5
$CH_3COCH(OH)(OH) + HO^{\bullet} \rightarrow 0.14\ CH(OH)(OH)COCH_2(OO^{\bullet}) + 0.29\ CH_3COC(OH)(OH)(OO^{\bullet}) + 0.57\ CHO(OH) + 0.57\ CH_3CO(OO^{\bullet}) + H_2O - O_2$	R(446)	$9.2{\cdot}10^8$	1235	Schaefer et al., 2014	
Pathway 1: $CH_3COCH(OH)(OH) + NO_3^{\bullet} \rightarrow C^{\bullet}H_2COCH(OH)(OH) + NO_3^- + H^+$		$1.5\ 10^6$			BR: 33%
$C^{\bullet}H_2COCH(OH)(OH) + O_2 \rightarrow CH(OH)(OH)COCH_2(OO^{\bullet})$		$2.0\ 10^9$			5
Pathway 2: $CH_3COCH(OH)(OH) + NO_3^{\bullet} \rightarrow CH_3COC^{\bullet}(OH)(OH) + NO_3^- + H^+$		$3.0\ 10^6$			BR: 67%
$CH_3COC^{\bullet}(OH)(OH) + O_2 \rightarrow CH_3COC(OH)(OH)(OO^{\bullet})$		$2.0\ 10^9$			5
$CH_3COCH(OH)(OH) + NO_3^{\bullet} \rightarrow 0.33\ CH(OH)(OH)COCH_2(OO^{\bullet}) + 0.67\ CH_3COC(OH)(OH)(OO^{\bullet}) + NO_3^- + H^+ - O_2$	R(447)	$4.5{\cdot}10^6$	4213	Schaefer et al., 2014	2
Pathway 1: $CH_3C(OH)(OH)CH(OH)(OH) + HO^{\bullet} \rightarrow CH_3C(OH)(O^{\bullet})CH(OH)(OH) + H_2O$		$4.9\ 10^8$			BR: 53% - 29
$CH_3C(OH)(O^{\bullet})CH(OH)(OH) \rightarrow CH_3CO(OH) + C^{\bullet}H(OH)(OH)$					6 - 7
$C^{\bullet}H(OH)(OH) + O_2 \rightarrow CH(OH)(OH)(OO^{\bullet})$		$2.0\ 10^9$			5
Pathway 2: $CH_3C(OH)(OH)CH(OH)(OH) + HO^{\bullet} \rightarrow CH_3C(OH)(OH)CH(OH)(O^{\bullet}) + H_2O$		$4.3\ 10^8$			BR: 47% - 29
$CH_3C(OH)(OH)CH(OH)(O^{\bullet}) \rightarrow CH_3C^{\bullet}(OH)(OH) + CHO(OH)$					6- 7
$CH_3C^{\bullet}(OH)(OH) + O_2 \rightarrow CH_3C(OH)(OH)(OO^{\bullet})$		$2.0\ 10^9$			5
$CH_3C(OH)(OH)CH(OH)(OH) + HO^{\bullet} \rightarrow 0.53\ CH_3CO(OH) + 0.53\ CH(OH)(OH)(OO^{\bullet}) + 0.47\ CHO(OH) + 0.47\ CH_3C(OH)(OH)(OO^{\bullet}) + H_2O - O_2$	R(448)	$9.2{\cdot}10^8$	1235	Schaefer et al., 2014	
Pathway 1: $CH_3C(OH)(OH)CH(OH)(OH) + NO_3^{\bullet} \rightarrow CH_3C(OH)(OH)C^{\bullet}(OH)(OH) + NO_3^- + H^+$		$3.0\ 10^6$			BR: 67%
$CH_3C(OH)(OH)C^{\bullet}(OH)(OH) + O_2 \rightarrow CH_3C(OH)(OH)C(OH)(OH)(OO^{\bullet})$		$2.0\ 10^9$			5
Pathway 2: $CH_3C(OH)(OH)CH(OH)(OH) + NO_3^{\bullet} \rightarrow C^{\bullet}H_2C(OH)(OH)CH(OH)(OH) + NO_3^- + H^+$		$1.5\ 10^6$			BR: 33%
$C^{\bullet}H_2C(OH)(OH)CH(OH)(OH) + O_2 \rightarrow CH(OH)(OH)C(OH)(OH)CH_2(OO^{\bullet})$		$2.0\ 10^9$			5
$CH_3C(OH)(OH)CH(OH)(OH) + NO_3^{\bullet} \rightarrow 0.67\ CH_3C(OH)(OH)C(OH)(OH)(OO^{\bullet}) + 0.33\ CH(OH)(OH)C(OH)(OH)CH_2(OO^{\bullet}) + NO_3^- + H^+ - O_2$	R(449)	$4.5{\cdot}10^6$	4213	Schaefer et al., 2014	2
$CH_3COC(OH)(OH)(OO^{\bullet}) + OH^- \rightarrow CH_3COC(OH)(O^-)(OO^{\bullet}) + H_2O$		$4.0\ 10^9$			
$CH_3COC(OH)(O^-)(OO^{\bullet}) \rightarrow CH_3COCO(OH) + O_2^{\bullet-}$					9
$CH_3COC(OH)(OH)(OO^{\bullet}) + OH^- \rightarrow CH_3COCO(OH) + O_2^{\bullet-} + H_2O$	R(450)	$4.0\ 10^9$			$= k(CH_3CH(OH)(OO^{\bullet}) + OH^-)$
$CH_3COC(OH)(OH)(OO^{\bullet}) \rightarrow CH_3COCO(OH) + HO_2^{\bullet}$	R(451)	$1.0\ 10^6$			15
$CH_3C(OH)(OH)C(OH)(OH)(OO^{\bullet}) + OH^- \rightarrow CH_3C(OH)(OH)C(OH)(O^-)(OO^{\bullet}) + H_2O$		$4.0\ 10^9$			
$CH_3C(OH)(OH)C(OH)(O^-)(OO^{\bullet}) \rightarrow CH_3C(OH)(OH)CO(OH) + O_2^{\bullet-}$					9
$CH_3C(OH)(OH)C(OH)(OH)(OO^{\bullet}) + OH^- \rightarrow CH_3C(OH)(OH)CO(OH) + O_2^{\bullet-} + H_2O$	R(452)	$4.0\ 10^9$			
$CH_3C(OH)(OH)C(OH)(OH)(OO^{\bullet}) \rightarrow CH_3C(OH)(OH)CO(OH) + HO_2^{\bullet}$	R(453)	$1.0\ 10^6$			15
Pathway 1: $2\ CH(OH)(OH)COCH_2(OO^{\bullet}) \rightarrow 2\ CHOCOCH(OH)(OH) + H_2O_2$		$1.8\ 10^8$			BR: 45%
Pathway 2: $2\ CH(OH)(OH)COCH_2(OO^{\bullet}) \rightarrow CH_2(OH)COCH(OH)(OH) + CHOCOCH(OH)(OH) + O_2$		$8.0\ 10^7$			BR: 20%
Pathway 3: $2\ CH(OH)(OH)COCH_2(OO^{\bullet}) \rightarrow 2\ CH_2(O^{\bullet})COCH(OH)(OH) + O_2$		$1.4\ 10^8$			BR: 35%
$CH_2(O^{\bullet})COCH(OH)(OH) \rightarrow C^{\bullet}H(OH)COCH(OH)(OH)$					4
$C^{\bullet}H(OH)COCH(OH)(OH) + O_2 \rightarrow CH(OH)(OH)COCH(OH)(OO^{\bullet})$		$2.0{\cdot}10^9$			5
$2\ CH(OH)(OH)COCH_2(OO^{\bullet}) \rightarrow 1.10\ CHOCOCH(OH)(OH) + 0.20\ CH_2(OH)COCH(OH)(OH) + 0.70\ CH(OH)(OH)COCH(OH)(OO^{\bullet}) + 0.45\ H_2O_2 - 0.15\ O_2$	R(454)	$4.0\ 10^8$			$= k(2\ CH_3COCH_2(OO^{\bullet})) - 8$
Pathway 1: $2\ CH(OH)(OH)C(OH)(OH)CH_2(OO^{\bullet}) \rightarrow 2\ CHOC(OH)(OH)CH(OH)(OH) + H_2O_2$		$1.8\ 10^8$			BR: 45%
Pathway 2: $2\ CH(OH)(OH)C(OH)(OH)CH_2(OO^{\bullet}) \rightarrow CH_2(OH)C(OH)(OH)CH(OH)(OH) + CHOC(OH)(OH)CH(OH)(OH) + O_2$		$8.0\ 10^7$			BR: 20%
Pathway 3: $2\ CH(OH)(OH)C(OH)(OH)CH_2(OO^{\bullet}) \rightarrow 2\ CH_2(O^{\bullet})C(OH)(OH)CH(OH)(OH) + O_2$		$1.4\ 10^8$			BR: 35%
$CH_2(O^{\bullet})C(OH)(OH)CH(OH)(OH) \rightarrow C^{\bullet}H(OH)C(OH)(OH)CH(OH)(OH)$					4
$C^{\bullet}H(OH)C(OH)(OH)CH(OH)(OH) + O_2 \rightarrow CH(OH)(OH)C(OH)(OH)CH(OH)(OO^{\bullet})$		$2.0{\cdot}10^9$			5

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
2 $CH(OH)(OH)C(OH)(OH)CH_2(OO^•)$ → 1.10 $CHOC(OH)(OH)CH(OH)(OH)$ + 0.20 $CH_2(OH)C(OH)(OH)CH(OH)(OH)$ + 0.70 $CH(OH)(OH)C(OH)(OH)CH(OH)(OO^•)$ + 0.45 H_2O_2 - 0.15 O_2	R(455)	4.0 10^8			= k(2 $CH_3COCH_2(OO^•)$) - 8
Oxidation of 2-oxo, 3-hydroxypropanal					30
Pathway 1: $CH_2(OH)COCH(OH)(OH)$ + $HO^•$ → $CH_2(OH)COCH(OH)(O^•)$ + H_2O		3.6 10^8			BR: 41% - 31
$CH_2(OH)COCH(OH)(O^•)$ → $CH_2(OH)C^•O$ + CHO(OH)					6 - 7
$CH_2(OH)C^•O$ + O_2 → $CH_2(OH)CO(OO^•)$		$2.0 \cdot 10^9$			5
Pathway 2: $CH_2(OH)COCH(OH)(OH)$ + $HO^•$ → $C^•H(OH)COCH(OH)(OH)$ + H_2O		3.5 10^8			BR: 40% - 31
$C^•H(OH)COCH(OH)(OH)$ + O_2 → $CH(OH)(OH)COCH(OH)(OO^•)$		$2.0 \cdot 10^9$			5
Pathway 3: $CH_2(OH)COCH(OH)(OH)$ + $HO^•$ → $CH_2(OH)COC^•(OH)(OH)$ + H_2O		1.6 10^8			BR: 19% - 31
$CH_2(OH)COC^•(OH)(OH)$ + O_2 → $CH_2(OH)COC(OH)(OH)(OO^•)$		$2.0 \cdot 10^9$			5
$CH_2(OH)COCH(OH)(OH)$ + $HO^•$ → 0.41 CHO(OH) + 0.41 $CH_2(OH)CO(OO^•)$ + 0.40 $CH(OH)(OH)COCH(OH)(OO^•)$ + 0.19 $CH_2(OH)COC(OH)(OH)(OO^•)$ + H_2O - O_2	R(456)	8.7 10^8			13
Pathway 1: $CH_2(OH)COCH(OH)(OH)$ + $NO_3^•$ → $C^•H(OH)COCH(OH)(OH)$ + NO_3^- + H^+		7.4 10^5			BR: 67%
$C^•H(OH)COCH(OH)(OH)$ + O_2 → $CH(OH)(OH)COCH(OH)(OO^•)$		$2.0 \cdot 10^9$			5
Pathway 2: $CH_2(OH)COCH(OH)(OH)$ + $NO_3^•$ → $CH_2(OH)COC^•(OH)(OH)$ + NO_3^- + H^+		3.6 10^5			BR: 33%
$CH_2(OH)COC^•(OH)(OH)$ + O_2 → $CH_2(OH)COC(OH)(OH)(OO^•)$		$2.0 \cdot 10^9$			5
$CH_2(OH)COCH(OH)(OH)$ + $NO_3^•$ → 0.67 $CH(OH)(OH)COCH(OH)(OO^•)$ + 0.33 $CH_2(OH)COC(OH)(OH)(OO^•)$ + NO_3^- + H^+ - O_2	R(457)	1.1 10^6			= k($CH_2(OH)CH(OH)(OH)$ + $NO_3^•$) - 2
Pathway 1: $CH_2(OH)C(OH)(OH)CH(OH)(OH)$ + $HO^•$ → $CH_2(OH)C(OH)(O^•)CH(OH)(OH)$ + H_2O		4.6 10^8			BR: 38% - 32
$CH_2(OH)C(OH)(O^•)CH(OH)(OH)$ → $CH_2(OH)CO(OH)$ + $C^•H(OH)(OH)$					6 - 7
$C^•H(OH)(OH)$ + O_2 → $CH(OH)(OH)(OO^•)$		$2.0 \cdot 10^9$			5
Pathway 2: $CH_2(OH)C(OH)(OH)CH(OH)(OH)$ + $HO^•$ → $CH_2(OH)C(OH)(OH)CH(OH)(O^•)$ + H_2O		4.2 10^8			BR: 35% - 32
$CH_2(OH)C(OH)(OH)CH(OH)(O^•)$ → $CH_2(OH)C^•(OH)(OH)$ + CHO(OH)					6 - 7
$CH_2(OH)C^•(OH)(OH)$ + O_2 → $CH_2(OH)C(OH)(OH)(OO^•)$		$2.0 \cdot 10^9$			5
Pathway 3: $CH_2(OH)C(OH)(OH)CH(OH)(OH)$ + $HO^•$ → $C^•H(OH)C(OH)(OH)CH(OH)(OH)$ + H_2O		3.2 10^8			BR: 27% - 32
$C^•H(OH)C(OH)(OH)CH(OH)(OH)$ + O_2 → $CH(OH)(OH)C(OH)(OH)CH(OH)(OO^•)$		$2.0 \cdot 10^9$			5
$CH_2(OH)C(OH)(OH)CH(OH)(OH)$ + $HO^•$ → 0.38 $CH_2(OH)CO(OH)$ + 0.38 $CH(OH)(OH)(OO^•)$ + 0.35 CHO(OH) + 0.35 $CH_2(OH)C(OH)(OH)(OO^•)$ + 0.27 $CH(OH)(OH)C(OH)(OH)CH(OH)(OO^•)$ + H_2O - O_2	R(458)	1.2 10^9			13
Pathway 1: $CH_2(OH)C(OH)(OH)CH(OH)(OH)$ + $NO_3^•$ → $C^•H(OH)C(OH)(OH)CH(OH)(OH)$ + NO_3^- + H^+		1.0 10^6			BR: 100%
$C^•H(OH)C(OH)(OH)CH(OH)(OH)$ + O_2 → $CH(OH)(OH)C(OH)(OH)CH(OH)(OO^•)$		$2.0 \cdot 10^9$			5
$CH_2(OH)C(OH)(OH)CH(OH)(OH)$ + $NO_3^•$ → $CH(OH)(OH)C(OH)(OH)CH(OH)(OO^•)$ + NO_3^- + H^+ - O_2	R(459)	1.0 10^6			= k($CH(OH)(OH)CH(OH)(OH)$ + $NO_3^•$) - 2
$CH_2(OH)COC(OH)(OH)(OO^•)$ + OH^- → $CH_2(OH)COC(OH)(O^-)(OO^•)$ + H_2O		4.0 10^9			
$CH_2(OH)COC(OH)(O^-)(OO^•)$ → $CH_2(OH)COCO(OH)$ + $O_2^{•-}$					9
$CH_2(OH)COC(OH)(OH)(OO^•)$ + OH^- → $CH_2(OH)COCO(OH)$ + $O_2^{•-}$ + H_2O	R(460)	4.0 10^9			= k($CH_3CH(OH)(OO^•)$ + OH^-)
$CH_2(OH)COC(OH)(OH)(OO^•)$ → $CH_2(OH)COCO(OH)$ + $HO_2^•$	R(461)	1.0 10^6			15
$CH(OH)(OH)COCH(OH)(OO^•)$ + OH^- → $CH(OH)(OH)COCH(O^-)(OO^•)$ + H_2O		4.0 10^9			
$CH(OH)(OH)COCH(O^-)(OO^•)$ → $CHOCOCH(OH)(OH)$ + $O_2^{•-}$					9
$CH(OH)(OH)COCH(OH)(OO^•)$ + OH^- → $CHOCOCH(OH)(OH)$ + $O_2^{•-}$ + H_2O	R(462)	4.0 10^9			= k($CH_3CH(OH)(OO^•)$ + OH^-)
$CH(OH)(OH)COCH(OH)(OO^•)$ → $CHOCOCH(OH)(OH)$ + $HO_2^•$	R(463)	1.9 10^2			10
$CH(OH)(OH)C(OH)(OH)CH(OH)(OO^•)$ + OH^- → $CH(OH)(OH)C(OH)(OH)CH(O^-)(OO^•)$ + H_2O		4.0 10^9			
$CH(OH)(OH)C(OH)(OH)CH(O^-)(OO^•)$ → $CHOC(OH)(OH)CH(OH)(OH)$ + $O_2^{•-}$					9
$CH(OH)(OH)C(OH)(OH)CH(OH)(OO^•)$ + OH^- → $CHOC(OH)(OH)CH(OH)(OH)$ + $O_2^{•-}$ + H_2O	R(464)	4.0 10^9			
$CH(OH)(OH)C(OH)(OH)CH(OH)(OO^•)$ → $CHOC(OH)(OH)CH(OH)(OH)$ + $HO_2^•$	R(465)	1.0 10^6			15
$CH_2(OH)C(OH)(OH)C(OH)(OH)(OO^•)$ + OH^- → $CH_2(OH)C(OH)(OH)C(OH)(O^-)(OO^•)$ + H_2O		4.0 10^9			
$CH_2(OH)C(OH)(OH)C(OH)(O^-)(OO^•)$ → $CH_2(OH)C(OH)(OH)CO(OH)$ + $O_2^{•-}$					9

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CH_2(OH)C(OH)(OH)C(OH)(OH)(OO^•) + OH^- \rightarrow CH_2(OH)C(OH)(OH)CO(OH) + O_2^{•-} + H_2O$	R(466)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^•)$ + OH^-)
$CH_2(OH)C(OH)(OH)C(OH)(OH)(OO^•) \rightarrow CH_2(OH)C(OH)(OH)CO(OH) + HO_2^•$	R(467)	$1.0\ 10^6$			15
Oxidation of oxopropanedial					33
Pathway 1: $CH(OH)(OH)C(OH)(OH)CH(OH)(OH) + HO^• \rightarrow CH(OH)(OH)C(OH)(OH)CH(OH)(O^•) + H_2O$		$8.7\ 10^8$			BR: 67% - 34
$CH(OH)(OH)C(OH)(OH)CH(OH)(O^•) \rightarrow CH(OH)(OH)C^•(OH)(OH) + CHO(OH)$					6 - 7
$CH(OH)(OH)C^•(OH)(OH) + O_2 \rightarrow CH(OH)(OH)C(OH)(OH)(OO^•)$		$2.0{\cdot}10^9$			5
Pathway 2: $CH(OH)(OH)C(OH)(OH)CH(OH)(OH) + HO^• \rightarrow CH(OH)(OH)C(OH)(O^•)CH(OH)(OH) + H_2O$		$4.3\ 10^8$			BR: 33% - 34
$CH(OH)(OH)C(OH)(O^•)CH(OH)(OH) \rightarrow C^•H(OH)(OH) + CH(OH)(OH)CO(OH)$					6 - 7
$C^•H(OH)(OH) + O_2 \rightarrow CH(OH)(OH)(OO^•)$		$2.0{\cdot}10^9$			5
$CH(OH)(OH)C(OH)(OH)CH(OH)(OH) + HO^• \rightarrow 0.67\ CH(OH)(OH)C(OH)(OH)(OO^•) + 0.67\ CHO(OH) + 0.33\ CH(OH)(OH)CO(OH) + 0.33\ CH(OH)(OH)(OO^•) + H_2O - O_2$	R(468)	$1.3\ 10^9$			13
$CH(OH)(OH)C(OH)(OH)C(OH)(OH)(OO^•) + OH^- \rightarrow CH(OH)(OH)C(OH)(OH)C(OH)(O^-)(OO^•) + H_2O$		$4.0\ 10^9$			
$CH(OH)(OH)C(OH)(OH)C(OH)(O^-)(OO^•) \rightarrow CO(OH)C(OH)(OH)CH(OH)(OH) + O_2^{•-}$					9
$CH(OH)(OH)C(OH)(OH)C(OH)(OH)(OO^•) + OH^- \rightarrow CO(OH)C(OH)(OH)CH(OH)(OH) + O_2^{•-} + H_2O$	R(469)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^•)$ + OH^-)
$CH(OH)(OH)C(OH)(OH)C(OH)(OH)(OO^•) \rightarrow CO(OH)C(OH)(OH)CH(OH)(OH) + HO_2^•$	R(470)	$1.0\ 10^6$			15
Oxidation of acetone					35
$CH_3COCH_3 + HO^• \rightarrow CH_3COC^•H_2 + H_2O$		$1.8{\cdot}10^8$			
$CH_3COC^•H_2 + O_2 \rightarrow CH_3COCH_2(OO^•)$		$3.1\ 10^9$		Zegota et al., 1986a	
$CH_3COCH_3 + HO^• \rightarrow CH_3COCH_2(OO^•) + H_2O - O_2$	R(471)	$1.8{\cdot}10^8$		Gligorovski et al., 2009	
$CH_3COCH_3 + NO_3^• \rightarrow CH_3COC^•H_2 + NO_3^- + H^+$		$3.7\ 10^3$	4332		
$CH_3COC^•H_2 + O_2 \rightarrow CH_3COCH_2(OO^•)$		$3.1\ 10^9$		Zegota et al., 1986a	5
$CH_3COCH_3 + NO_3^• \rightarrow CH_3COCH_2(OO^•) + NO_3^- + H^+ - O_2$	R(472)	$3.7{\cdot}10^3$	4332	Herrmann and Zellner, 1998	
Pathway 1: $2\ CH_3COCH_2(OO^•) \rightarrow 2\ CH_3COCHO + H_2O_2$		$1.8\ 10^8$		Zegota et al., 1986a	BR: 45%
Pathway 2: $2\ CH_3COCH_2(OO^•) \rightarrow CH_3COCHO + CH_3COCH_2(OH) + O_2$		$8.0\ 10^7$		Zegota et al., 1986a	BR: 20%
Pathway 3: $2\ CH_3COCH_2(OO^•) \rightarrow 2\ CH_3COCH_2(O^•) + O_2$		$1.4\ 10^8$		Zegota et al., 1986a	BR: 35%
$CH_3COCH_2(O^•) \rightarrow CH_3COC^•H(OH)$					4
$CH_3COC^•H(OH) + O_2 \rightarrow CH_3COCH(OH)(OO^•)$		$2.0\ 10^9$			5
$2\ CH_3COCH_2(OO^•) \rightarrow 1.10\ CH_3COCHO + 0.20\ CH_3COCH_2(OH) + 0.70\ CH_3COCH(OH)(OO^•) + 0.45\ H_2O_2 - 0.15\ O_2$	R(473)	$4.0\ 10^8$		Zegota et al., 1986a	
Oxidation of hydroxyacetone					36
Pathway 1: $CH_3COCH_2(OH) + HO^• \rightarrow C^•H_2COCH_2(OH) + H_2O$		$8.5\ 10^7$			BR: 16% - 37
$C^•H_2COCH_2(OH) + O_2 \rightarrow CH_2(OH)COCH_2(OO^•)$		$2.0\ 10^9$			5
Pathway 2: $CH_3COCH_2(OH) + HO^• \rightarrow CH_3COC^•H(OH) + H_2O$		$3.5\ 10^8$			BR: 69% - 37
$CH_3COC^•H(OH) + O_2 \rightarrow CH_3COCH(OH)(OO^•)$		$2.0\ 10^9$			5
Pathway 3: $CH_3COCH_2(OH) + HO^• \rightarrow CH_3COCH_2(O^•) + H_2O$		$7.5\ 10^7$			BR: 15% - 37
$CH_3COCH_2(O^•) \rightarrow CH_3C^•O + CH_2O$					6 - 7
$CH_3C^•O + O_2 \rightarrow CH_3CO(OO^•)$		$2.0\ 10^9$			5
$CH_3COCH_2(OH) + HO^• \rightarrow 0.69\ CH_3COCH(OH)(OO^•) + 0.16\ CH_2(OH)COCH_2(OO^•) + 0.15\ CH_2O + 0.15\ CH_3CO(OO^•) + H_2O - O_2$	R(474)	$5.1\ 10^8$			13
$CH_3COCH_2(OH) + NO_3^• \rightarrow CH_3COC^•H(OH) + NO_3^- + H^+$		$1.8\ 10^7$			BR: 100%
$CH_3COC^•H(OH) + O_2 \rightarrow CH_3COCH(OH)(OO^•)$		$2.0\ 10^9$			5
$CH_3COCH_2(OH) + NO_3^• \rightarrow CH_3COCH(OH)(OO^•) + NO_3^- + H^+ - O_2$	R(475)	$1.8{\cdot}10^7$	1564	De Semainville et al., 2007	2
$CH_3COCH(OH)(OO^•) + OH^- \rightarrow CH_3COCH(O^-)(OO^•) + H_2O$		$4.0\ 10^9$			
$CH_3COCH(O^-)(OO^•) \rightarrow CH_3COCHO + O_2^{•-}$					9

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CH_3COCH(OH)(OO^\bullet) + OH^- \rightarrow CH_3COCHO + O_2^{\bullet-} + H_2O$	R(476)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^\bullet) + OH^-$)
$CH_3COCH(OH)(OO^\bullet) \rightarrow CH_3COCHO + HO_2^\bullet$	R(477)	$1.9\ 10^2$			10
Pathway 1: $2\ CH_2(OH)COCH_2(OO^\bullet) \rightarrow 2\ CH_2(OH)COCHO + H_2O_2$		$1.8\ 10^8$			BR: 45%
Pathway 2: $2\ CH_2(OH)COCH_2(OO^\bullet) \rightarrow CH_2(OH)COCH_2(OH) + CH_2(OH)COCHO + O_2$		$8.0\ 10^7$			BR: 20%
Pathway 3: $2\ CH_2(OH)COCH_2(OO^\bullet) \rightarrow 2\ CH_2(OH)COCH_2(O^\bullet) + O_2$		$1.4\ 10^8$			BR: 35%
$CH_2(OH)COCH_2(O^\bullet) \rightarrow CH_2(OH)COC^\bullet H(OH)$					4
$CH_2(OH)COC^\bullet H(OH) + O_2 \rightarrow CH_2(OH)COCH(OH)(OO^\bullet)$		$2.0\ 10^9$			5
$2\ CH_2(OH)COCH_2(OO^\bullet) \rightarrow 1.10\ CH_2(OH)COCHO + 0.20\ CH_2(OH)COCH_2(OH) + 0.70\ CH_2(OH)COCH(OH)(OO^\bullet) + 0.45\ H_2O_2 - 0.15\ O_2$	R(478)	$4.0\ 10^8$			= k($2\ CH_3COCH_2(OO^\bullet)$) - 8
Oxidation of dihydroxyacetone					38
$CH_2(OH)COCH_2(OH) + HO^\bullet \rightarrow CH_2(OH)COC^\bullet H(OH) + H_2O$		$8.1\ 10^8$			BR: 100% - 39
$CH_2(OH)COC^\bullet H(OH) + O_2 \rightarrow CH_2(OH)COCH(OH)(OO^\bullet)$		$2.0\ 10^9$			5
$CH_2(OH)COCH_2(OH) + HO^\bullet \rightarrow CH_2(OH)COCH(OH)(OO^\bullet) + H_2O - O_2$	R(479)	$8.1\ 10^8$			13
$CH_2(OH)COCH_2(OH) + NO_3^\bullet \rightarrow CH_2(OH)COC^\bullet H(OH) + NO_3^- + H^+$		$6.6{\cdot}10^6$			BR: 100%
$CH_2(OH)COC^\bullet H(OH) + O_2 \rightarrow CH_2(OH)COCH(OH)(OO^\bullet)$		$2.0\ 10^9$			5
$CH_2(OH)COCH_2(OH) + NO_3^\bullet \rightarrow CH_2(OH)COCH(OH)(OO^\bullet) + NO_3^- + H^+ - O_2$	R(480)	$6.6{\cdot}10^6$	2117		= k($CH_2(OH)CH_2(OH) + NO_3^\bullet$) - 2
$CH_2(OH)COCH(OH)(OO^\bullet) + OH^- \rightarrow CH_2(OH)COCH(O^-)(OO^\bullet) + H_2O$		$4.0\ 10^9$			
$CH_2(OH)COCH(O^-)(OO^\bullet) \rightarrow CH_2(OH)COCHO + O_2^{\bullet-}$					9
$CH_2(OH)COCH(OH)(OO^\bullet) + OH^- \rightarrow CH_2(OH)COCHO + O_2^{\bullet-} + H_2O$	R(481)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^\bullet) + OH^-$)
$CH_2(OH)COCH(OH)(OO^\bullet) \rightarrow CH_2(OH)COCHO + HO_2^\bullet$	R(482)	$1.9\ 10^2$			10
Oxidation of propionic acid					
Pathway 1: $CH_3CH_2CO(OH) + HO^\bullet \rightarrow CH_3C^\bullet HCO(OH) + H_2O$		$5.0\ 10^7$			BR: 17% - 40
$CH_3C^\bullet HCO(OH) + O_2 \rightarrow CH_3CH(OO^\bullet)CO(OH)$		$2.0\ 10^9$			5
Pathway 2: $CH_3CH_2CO(OH) + HO^\bullet \rightarrow C^\bullet H_2CH_2CO(OH) + H_2O$		$2.7\ 10^8$			BR: 83% - 40
$C^\bullet H_2CH_2CO(OH) + O_2 \rightarrow CH_2(OO^\bullet)CH_2CO(OH)$		$2.0\ 10^9$			5
$CH_3CH_2CO(OH) + HO^\bullet \rightarrow 0.17\ CH_3CH(OO^\bullet)CO(OH) + 0.83\ CH_2(OO^\bullet)CH_2CO(OH) + H_2O - O_2$	R(483)	$3.2{\cdot}10^8$	2300	Ervens et al., 2003	
Pathway 1: $CH_3CH_2CO(OH) + NO_3^\bullet \rightarrow CH_3C^\bullet HCO(OH) + NO_3^- + H^+$		$1.3\ 10^4$			BR: 17%
$CH_3C^\bullet HCO(OH) + O_2 \rightarrow CH_3CH(OO^\bullet)CO(OH)$		$2.0\ 10^9$			5
Pathway 2: $CH_3CH_2CO(OH) + NO_3^\bullet \rightarrow C^\bullet H_2CH_2CO(OH) + NO_3^- + H^+$		$6.1\ 10^4$			BR: 83%
$C^\bullet H_2CH_2CO(OH) + O_2 \rightarrow CH_2(OO^\bullet)CH_2CO(OH)$		$2.0\ 10^9$			5
$CH_3CH_2CO(OH) + NO_3^\bullet \rightarrow 0.17\ CH_3CH(OO^\bullet)CO(OH) + 0.83\ CH_2(OO^\bullet)CH_2CO(OH) + NO_3^- + H^+ - O_2$	R(484)	$7.4{\cdot}10^4$		Rousse and George, 2004	2
Pathway 1: $CH_3CH_2CO(O^-) + HO^\bullet \rightarrow CH_3C^\bullet HCO(O^-) + H_2O$		$2.0\ 10^8$			BR: 28% - 41
$CH_3C^\bullet HCO(O^-) + O_2 \rightarrow CH_3CH(OO^\bullet)CO(O^-)$		$2.0\ 10^9$			5
Pathway 2: $CH_3CH_2CO(O^-) + HO^\bullet \rightarrow C^\bullet H_2CH_2CO(O^-) + H_2O$		$5.3\ 10^8$			BR: 72% - 41
$C^\bullet H_2CH_2CO(O^-) + O_2 \rightarrow CH_2(OO^\bullet)CH_2CO(O^-)$		$2.0\ 10^9$			5
$CH_3CH_2CO(O^-) + HO^\bullet \rightarrow 0.28\ CH_3CH(OO^\bullet)CO(O^-) + 0.72\ CH_2(OO^\bullet)CH_2CO(O^-) + H_2O - O_2$	R(485)	$7.3{\cdot}10^8$	1800	Ervens et al., 2003	
Pathway 1: $CH_3CH_2CO(O^-) + NO_3^\bullet \rightarrow CH_3C^\bullet HCO(O^-) + NO_3^- + H^+$		$2.1\ 10^4$			BR: 28%
$CH_3C^\bullet HCO(O^-) + O_2 \rightarrow CH_3CH(OO^\bullet)CO(O^-)$		$2.0\ 10^9$			5
Pathway 2: $CH_3CH_2CO(O^-) + NO_3^\bullet \rightarrow C^\bullet H_2CH_2CO(O^-) + NO_3^- + H^+$		$5.3\ 10^4$			BR: 72%
$C^\bullet H_2CH_2CO(O^-) + O_2 \rightarrow CH_2(OO^\bullet)CH_2CO(O^-)$		$2.0\ 10^9$			5
$CH_3CH_2CO(O^-) + NO_3^\bullet \rightarrow 0.28\ CH_3CH(OO^\bullet)CO(O^-) + 0.72\ CH_2(OO^\bullet)CH_2CO(O^-) + NO_3^- + H^+ - O_2$	R(486)	$7.4{\cdot}10^4$			= k($CH_3CH_2CO(OH) + NO_3^\bullet$) - 2
Pathway 1: $2\ CH_3CH(OO^\bullet)CO(OH) \rightarrow 2\ CH_3COCO(OH) + H_2O_2$		$2.2\ 10^7$			BR: 30%
Pathway 2: $2\ CH_3CH(OO^\bullet)CO(OH)$ *(+ 2 H_2O)* $\rightarrow 2\ CH_3CHO + 2\ CO_2 + H_2O_2 + 2\ H_2O$		$2.2\ 10^7$			BR: 30%
Pathway 3: $2\ CH_3CH(OO^\bullet)CO(OH) \rightarrow CH_3COCO(OH) + CH_3CH(OH)CO(OH) + O_2$		$2.2\ 10^7$			BR: 30%
Pathway 4: $2\ CH_3CH(OO^\bullet)CO(OH) \rightarrow 2\ CH_3CH(O^\bullet)CO(OH) + O_2$		$9.0\ 10^6$			BR: 10%

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CH_3CH(O^•)CO(OH) \rightarrow CH_3C^•(OH)CO(OH)$					4
$CH_3C^•(OH)CO(OH) + O_2 \rightarrow CH_3C(OH)(OO^•)CO(OH)$		$2.0 \cdot 10^9$			5
$2\ CH_3CH(OO^•)CO(OH) \rightarrow 0.90\ CH_3COCO(OH) + 0.30\ CH_3CH(OH)CO(OH) + 0.20\ CH_3C(OH)(OO^•)CO(OH) + 0.60\ CH_3CHO + 0.60\ CO_2 + 0.60\ H_2O_2 + 0.20\ O_2$	R(487)	$7.5 \cdot 10^7$			= k(2 $CH_2(OO^•)CO(O^-)$) - 8
Pathway 1: $2\ CH_3CH(OO^•)CO(O^-) \rightarrow 2\ CH_3COCO(O^-) + H_2O_2$		$2.2\ 10^7$			BR: 30%
Pathway 2: $2\ CH_3CH(OO^•)CO(O^-)$ *(+ 2 H_2O)* $\rightarrow 2\ CH_3CHO + 2\ CO_2 + H_2O_2 + 2\ OH^-$		$2.2\ 10^7$			BR: 30%
Pathway 3: $2\ CH_3CH(OO^•)CO(O^-) \rightarrow CH_3COCO(O^-) + CH_3CH(OH)CO(O^-) + O_2$		$2.2\ 10^7$			BR: 30%
Pathway 4: $2\ CH_3CH(OO^•)CO(O^-) \rightarrow 2\ CH_3CH(O^•)CO(O^-) + O_2$		$9.0\ 10^6$			BR: 10%
$CH_3CH(O^•)CO(O^-) \rightarrow CH_3C^•(OH)CO(O^-)$					4
$CH_3C^•(OH)CO(O^-) + O_2 \rightarrow CH_3C(OH)(OO^•)CO(O^-)$		$2.0 \cdot 10^9$			5
$2\ CH_3CH(OO^•)CO(O^-) \rightarrow 0.90\ CH_3COCO(O^-) + 0.30\ CH_3CH(OH)CO(O^-) + 0.20\ CH_3C(OH)(OO^•)CO(O^-) + 0.60\ CH_3CHO + 0.60\ CO_2 + 0.60\ H_2O_2 + 0.20\ O_2 - 0.60\ H_2O + 0.60\ OH^-$	R(488)	$7.5 \cdot 10^7$			= k(2 $CH_2(OO^•)CO(O^-)$) - 8
Pathway 1: $2\ CH_2(OO^•)CH_2CO(OH) \rightarrow 2\ CO(OH)CH_2CHO + H_2O_2$		$3.0\ 10^7$			BR: 20%
Pathway 2: $2\ CH_2(OO^•)CH_2CO(OH) \rightarrow 2\ CH_2(O^•)CH_2CO(OH) + O_2$		$1.3\ 10^8$			BR: 80%
$CH_2(O^•)CH_2CO(OH) \rightarrow C^•H(OH)CH_2CO(OH)$					4
$C^•H(OH)CH_2CO(OH) + O_2 \rightarrow CH(OH)(OO^•)CH_2CO(OH)$		$2.0 \cdot 10^9$			5
$2\ CH_2(OO^•)CH_2CO(OH) \rightarrow 0.40\ CO(OH)CH_2CHO + 1.60\ CH(OH)(OO^•)CH_2CO(OH) + 0.20\ H_2O_2 - 0.80\ O_2$	R(489)	$1.6\ 10^8$	-1600		= k(2 $CH_3CH_2(OO^•)$) - 8
Pathway 1: $2\ CH_2(OO^•)CH_2CO(O^-) \rightarrow 2\ CO(O^-)CH_2CHO + H_2O_2$		$3.0\ 10^7$			BR: 20%
Pathway 2: $2\ CH_2(OO^•)CH_2CO(O^-) \rightarrow 2\ CH_2(O^•)CH_2CO(O^-) + O_2$		$1.3\ 10^8$			BR: 80%
$CH_2(O^•)CH_2CO(O^-) \rightarrow C^•H(OH)CH_2CO(O^-)$					4
$C^•H(OH)CH_2CO(O^-) + O_2 \rightarrow CH(OH)(OO^•)CH_2CO(O^-)$		$2.0 \cdot 10^9$			5
$2\ CH_2(OO^•)CH_2CO(O^-) \rightarrow 0.40\ CO(O^-)CH_2CHO + 1.60\ CH(OH)(OO^•)CH_2CO(O^-) + 0.20\ H_2O_2 - 0.80\ O_2$	R(490)	$1.6\ 10^8$	-1600		= k(2 $CH_3CH_2(OO^•)$) - 8
Oxidation of 3-oxopropionic acid					42
Pathway 1: $CO(OH)CH_2CH(OH)(OH) + HO^• \rightarrow CO(OH)CH_2C^•(OH)(OH) + H_2O$		$5.5\ 10^8$			BR: 58% - 43
$CO(OH)CH_2C^•(OH)(OH) + O_2 \rightarrow CO(OH)CH_2C(OH)(OH)(OO^•)$		$2.0 \cdot 10^9$			5
Pathway 2: $CO(OH)CH_2CH(OH)(OH) + HO^• \rightarrow CO(OH)CH_2CH(OH)(O^•) + H_2O$		$4.0\ 10^8$			BR: 42% - 43
$CO(OH)CH_2CH(OH)(O^•) \rightarrow CO(OH)CH_2C^•(OH)(OH)$					4
$CO(OH)CH_2C^•(OH)(OH) + O_2 \rightarrow CO(OH)CH_2C(OH)(OH)(OO^•)$		$2.0 \cdot 10^9$			5
$CO(OH)CH_2CH(OH)(OH) + HO^• \rightarrow CO(OH)CH_2C(OH)(OH)(OO^•) + H_2O - O_2$	R(491)	$9.5\ 10^8$			13
$CO(OH)CH_2CH(OH)(OH) + NO_3^• \rightarrow CO(OH)CH_2C^•(OH)(OH) + NO_3^- + H^+$		$9.1\ 10^5$			BR: 100%
$CO(OH)CH_2C^•(OH)(OH) + O_2 \rightarrow CO(OH)CH_2C(OH)(OH)(OO^•)$		$2.0 \cdot 10^9$			5
$CO(OH)CH_2CH(OH)(OH) + NO_3^• \rightarrow CO(OH)CH_2C(OH)(OH)(OO^•) + NO_3^- + H^+ - O_2$	R(492)	$9.1\ 10^5$	3971		= k($CH_2(OH)CO(OH) + NO_3^•$) - 2
Pathway 1: $CO(O^-)CH_2CH(OH)(OH) + HO^• \rightarrow CO(O^-)CH_2C^•(OH)(OH) + H_2O$		$1.0\ 10^9$			BR: 59% - 44
$CO(O^-)CH_2C^•(OH)(OH) + O_2 \rightarrow CO(O^-)CH_2C(OH)(OH)(OO^•)$		$2.0 \cdot 10^9$			5
Pathway 2: $CO(O^-)CH_2CH(OH)(OH) + HO^• \rightarrow CO(O^-)CH_2CH(OH)(O^•) + H_2O$		$4.3\ 10^8$			BR: 25% - 44
$CO(O^-)CH_2CH(OH)(O^•) \rightarrow CO(O^-)CH_2C^•(OH)(OH)$					4
$CO(O^-)CH_2C^•(OH)(OH) + O_2 \rightarrow CO(O^-)CH_2C(OH)(OH)(OO^•)$		$2.0 \cdot 10^9$			5
Pathway 3: $CO(O^-)CH_2CH(OH)(OH) + HO^• \rightarrow CO(O^•)CH_2CH(OH)(OH) + OH^-$		$2.7\ 10^8$			BR: 16% - 44
$CO(O^•)CH_2CH(OH)(OH) \rightarrow C^•H_2CH(OH)(OH) + CO_2$					6 - 7
$C^•H_2CH(OH)(OH) + O_2 \rightarrow CH(OH)(OH)CH_2(OO^•)$		$2.0 \cdot 10^9$			5
$CO(O^-)CH_2CH(OH)(OH) + HO^• \rightarrow 0.84\ CO(O^-)CH_2C(OH)(OH)(OO^•) + 0.16\ CH(OH)(OH)CH_2(OO^•) + 0.16\ CO_2 + 0.84\ H_2O + 0.16\ OH^- - O_2$	R(493)	$1.7\ 10^9$			13
Pathway 1: $CO(O^-)CH_2CH(OH)(OH) + NO_3^• \rightarrow CO(O^-)CH_2C^•(OH)(OH) + NO_3^- + H^+$		$1.0 \cdot 10^7$			BR: 100%
$CO(O^-)CH_2C^•(OH)(OH) + O_2 \rightarrow CO(O^-)CH_2C(OH)(OH)(OO^•)$		$2.0 \cdot 10^9$			5
$CO(O^-)CH_2CH(OH)(OH) + NO_3^• \rightarrow CO(O^-)CH_2C(OH)(OH)(OO^•) + NO_3^- + H^+ - O_2$	R(494)	$1.0 \cdot 10^7$	3008		= k($CH_2(OH)CO(O^-) + NO_3^•$) - 2
$CO(O^-)CH_2CHO + HO^• \rightarrow CO(O^-)CH_2C^•O + H_2O$		$3.0\ 10^9$			BR: 100% - 45

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CO(O^-)CH_2C^\bullet O + O_2 \rightarrow CO(O^-)CH_2CO(OO^\bullet)$		$2.0 \cdot 10^9$			5
$CO(O^-)CH_2CHO + HO^\bullet \rightarrow CO(O^-)CH_2CO(OO^\bullet) + H_2O - O_2$	R(495)	$3.0\ 10^9$			13
$CO(O^-)CH_2CHO + NO_3^\bullet \rightarrow CO(O^-)CH_2C^\bullet O + NO_3^- + H^+$		$1.0 \cdot 10^7$			BR: 100%
$CO(O^-)CH_2C^\bullet O + O_2 \rightarrow CO(O^-)CH_2CO(OO^\bullet)$		$2.0 \cdot 10^9$			5
$CO(O^-)CH_2CHO + NO_3^\bullet \rightarrow CO(O^-)CH_2CO(OO^\bullet) + NO_3^- + H^+ - O_2$	R(496)	$1.0 \cdot 10^7$	3008		= k($CH_2(OH)CO(O^-) + NO_3^\bullet$) - 2
$CO(OH)CH_2C(OH)(OH)(OO^\bullet) + OH^- \rightarrow CO(OH)CH_2C(OH)(O\text{-})(OO^\bullet) + H_2O$		$4.0\ 10^9$			
$CO(OH)CH_2C(OH)(O\text{-})(OO^\bullet) \rightarrow CO(OH)CH_2CO(OH) + O_2^{\bullet-}$					9
$CO(OH)CH_2C(OH)(OH)(OO^\bullet) + OH^- \rightarrow CO(OH)CH_2CO(OH) + O_2^{\bullet-} + H_2O$	R(497)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^\bullet) + OH^-$)
$CO(OH)CH_2C(OH)(OH)(OO^\bullet) \rightarrow CO(OH)CH_2CO(OH) + HO_2^\bullet$	R(498)	$1.0\ 10^6$			15
$CO(O^-)CH_2C(OH)(OH)(OO^\bullet) + OH^- \rightarrow CO(O^-)CH_2C(OH)(O^-)(OO^\bullet) + H_2O$		$4.0\ 10^9$			
$CO(O^-)CH_2C(OH)(O^-)(OO^\bullet) \rightarrow CO(OH)CH_2CO(O^-) + O_2^{\bullet-}$					9
$CO(O^-)CH_2C(OH)(OH)(OO^\bullet) + OH^- \rightarrow CO(OH)CH_2CO(O^-) + O_2^{\bullet-} + H_2O$	R(499)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^\bullet) + OH^-$)
$CO(O^-)CH_2C(OH)(OH)(OO^\bullet) \rightarrow CO(OH)CH_2CO(O^-) + HO_2^\bullet$	R(500)	$1.0\ 10^6$			15
$2\ CO(O^-)CH_2CO(OO^\bullet) \rightarrow 2\ CO(O^-)CH_2CO(O^\bullet) + O_2$		$1.6 \cdot 10^8$			
$CO(O^-)CH_2CO(O^\bullet) \rightarrow CO(O^-)C^\bullet H_2 + CO_2$					6 - 7
$CO(O^-)C^\bullet H_2 + O_2 \rightarrow CH_2(OO^\bullet)CO(O^-)$		$2.0 \cdot 10^9$			5
$2\ CO(O^-)CH_2CO(OO^\bullet) \rightarrow 2\ CH_2(OO^\bullet)CO(O^-) + 2\ CO_2 - O_2$	R(501)	$1.6 \cdot 10^8$	-1600		= k($2\ CH_3CH_2(OO^\bullet)$) - 8
Oxidation of malonic acid					
$CO(OH)CH_2CO(OH) + HO^\bullet \rightarrow CO(OH)C^\bullet HCO(OH) + H_2O$		$1.9 \cdot 10^7$			BR: 100%
$CO(OH)C^\bullet HCO(OH) + O_2 \rightarrow CO(OH)CH(OO^\bullet)CO(OH)$		$2.0 \cdot 10^9$			5
$CO(OH)CH_2CO(OH) + HO^\bullet \rightarrow CO(OH)CH(OO^\bullet)CO(OH) + H_2O - O_2$	R(502)	$1.9 \cdot 10^7$		Wang et al., 2001	
$CO(OH)CH_2CO(OH) + NO_3^\bullet \rightarrow CO(OH)C^\bullet HCO(OH) + NO_3^- + H^+$		$5.1 \cdot 10^4$			BR: 100%
$CO(OH)C^\bullet HCO(OH) + O_2 \rightarrow CO(OH)CH(OO^\bullet)CO(OH)$		$2.0 \cdot 10^9$			5
$CO(OH)CH_2CO(OH) + NO_3^\bullet \rightarrow CO(OH)CH(OO^\bullet)CO(OH) + NO_3^- + H^+ - O_2$	R(503)	$5.1 \cdot 10^4$		De Semainville et al., 2010	2
Pathway 1: $CO(OH)CH_2CO(O^-) + HO^\bullet \rightarrow CO(OH)C^\bullet HCO(O^-) + H_2O$		$4.0 \cdot 10^6$			BR: 6% - 46
$CO(OH)C^\bullet HCO(O^-) + O_2 \rightarrow CO(OH)CH(OO^\bullet)CO(O^-)$		$2.0 \cdot 10^9$			5
Pathway 2: $CO(OH)CH_2CO(O^-) + HO^\bullet \rightarrow CO(O^\bullet)CH_2CO(OH) + OH^-$		$5.6\ 10^7$			BR: 94% - 46
$CO(O^\bullet)CH_2CO(OH) \rightarrow C^\bullet H_2CO(OH) + CO_2$					6 - 7
$C^\bullet H_2CO(OH) + O_2 \rightarrow CH_2(OO^\bullet)CO(OH)$		$2.0 \cdot 10^9$			5
$CO(OH)CH_2CO(O^-) + HO^\bullet \rightarrow 0.06\ CO(OH)CH(OO^\bullet)CO(O^-) + 0.94\ CH_2(OO^\bullet)CO(OH) + 0.94\ CO_2 + 0.06\ H_2O + 0.94\ OH^- - O_2$	R(504)	$6.0 \cdot 10^7$	1300	Ervens et al., 2003	
Pathway 1: $CO(OH)CH_2CO(O^-) + NO_3^\bullet \rightarrow CO(OH)C^\bullet HCO(O^-) + NO_3^- + H^+$		$5.6\ 10^6$	3369		
$CO(OH)C^\bullet HCO(O^-) + O_2 \rightarrow CO(OH)CH(OO^\bullet)CO(O^-)$		$2.0 \cdot 10^9$			5
$CO(OH)CH_2CO(O^-) + NO_3^\bullet \rightarrow CO(OH)CH(OO^\bullet)CO(O^-) + NO_3^- + H^+ - O_2$	R(505)	$5.6 \cdot 10^6$	3369	De Semainville et al., 2010	2
Pathway 1: $CO(O^-)CH_2CO(O^-) + HO^\bullet \rightarrow CO(O^-)C^\bullet HCO(O^-) + H_2O$		$1.0 \cdot 10^7$			BR: 6% - 47
$CO(O^-)C^\bullet HCO(O^-) + O_2 \rightarrow CO(O^-)CH(OO^\bullet)CO(O^-)$		$2.0 \cdot 10^9$			5
Pathway 2: $CO(O^-)CH_2CO(O^-) + HO^\bullet \rightarrow CO(O^\bullet)CH_2CO(O^-) + OH^-$		$1.0\ 10^8$			BR: 94% - 47
$CO(O^\bullet)CH_2CO(O^-) \rightarrow C^\bullet H_2CO(O^-) + CO_2$					6 - 7
$C^\bullet H_2CO(O^-) + O_2 \rightarrow CH_2(OO^\bullet)CO(O^-)$		$2.0 \cdot 10^9$			5
$CO(O^-)CH_2CO(O^-) + HO^\bullet \rightarrow 0.06\ CO(O^-)CH(OO^\bullet)CO(O^-) + 0.94\ CH_2(OO^\bullet)CO(O^-) + 0.94\ CO_2 + 0.06\ H_2O + 0.94\ OH^- - O_2$	R(506)	$1.1 \cdot 10^8$		Wang et al., 2001	
Pathway 1: $CO(O^-)CH_2CO(O^-) + NO_3^\bullet \rightarrow CO(O^-)C^\bullet HCO(O^-) + NO_3^- + H^+$		$2.3\ 10^7$	3008		
$CO(O^-)C^\bullet HCO(O^-) + O_2 \rightarrow CO(O^-)CH(OO^\bullet)CO(O^-)$		$2.0 \cdot 10^9$			5

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CO(O^-)CH_2CO(O^-) + NO_3^\bullet \rightarrow CO(O^-)CH(OO^\bullet)CO(O^-) + NO_3^- + H^+ - O_2$	R(507)	$2.3 \cdot 10^7$	3008	De Semainville et al., 2010	2
Pathway 1: $2\ CO(OH)CH(OO^\bullet)CO(OH) \rightarrow 2\ CO(OH)COCO(OH) + H_2O_2$		$2.2\ 10^7$			BR: 30%
Pathway 2: $2\ CO(OH)CH(OO^\bullet)CO(OH)$ *(+ 2 H_2O)* $\rightarrow 2\ CHOCO(OH) + 2\ CO_2 + H_2O_2 + 2\ H_2O$		$2.2\ 10^7$			BR: 30%
Pathway 3: $2\ CO(OH)CH(OO^\bullet)CO(OH) \rightarrow CO(OH)COCO(OH) + CO(OH)CH(OH)CO(OH) + O_2$		$2.2\ 10^7$			BR: 30%
Pathway 4: $2\ CO(OH)CH(OO^\bullet)CO(OH) \rightarrow 2\ CO(OH)CH(O^\bullet)CO(OH) + O_2$		$9.0\ 10^6$			BR: 10%
$CO(OH)CH(O^\bullet)CO(OH) \rightarrow CO(OH)C^\bullet(OH)CO(OH)$					4
$CO(OH)C^\bullet(OH)CO(OH) + O_2 \rightarrow CO(OH)C(OH)(OO^\bullet)CO(OH)$		$2.0 \cdot 10^9$			5
$2\ CO(OH)CH(OO^\bullet)CO(OH) \rightarrow 0.90\ CO(OH)COCO(OH) + 0.30\ CO(OH)CH(OH)CO(OH) + 0.20\ CO(OH)C(OH)(OO^\bullet)CO(OH) + 0.60\ CHOCO(OH) + 0.60\ CO_2 + 0.60\ H_2O_2 + 0.20\ O_2$	R(508)	$7.5 \cdot 10^7$			= k(2 $CH_2(OO^\bullet)CO(O^-)$) - 8
Pathway 1: $2\ CO(OH)CH(OO^\bullet)CO(O^-) \rightarrow 2\ CO(OH)COCO(O^-) + H_2O_2$		$2.2\ 10^7$			BR: 30%
Pathway 2: $2\ CO(OH)CH(OO^\bullet)CO(O^-)$ *(+ 2 H_2O)* $\rightarrow 2\ CHOCO(OH) + 2\ CO_2 + H_2O_2 + 2\ OH^-$		$2.2\ 10^7$			BR: 30%
Pathway 3: $2\ CO(OH)CH(OO^\bullet)CO(O^-) \rightarrow CO(OH)COCO(O^-) + CO(OH)CH(OH)CO(O^-) + O_2$		$2.2\ 10^7$			BR: 30%
Pathway 4: $2\ CO(OH)CH(OO^\bullet)CO(O^-) \rightarrow 2\ CO(OH)CH(O^\bullet)CO(O^-) + O_2$		$9.0\ 10^6$			BR: 10%
$CO(OH)CH(O^\bullet)CO(O^-) \rightarrow CO(OH)C^\bullet(OH)CO(O^-)$					4
$CO(OH)C^\bullet(OH)CO(O^-) + O_2 \rightarrow CO(OH)C(OH)(OO^\bullet)CO(O^-)$		$2.0 \cdot 10^9$			5
$2\ CO(OH)CH(OO^\bullet)CO(O^-) \rightarrow 0.90\ CO(OH)COCO(O^-) + 0.30\ CO(OH)CH(OH)CO(O^-) + 0.20\ CO(OH)C(OH)(OO^\bullet)CO(O^-) + 0.60\ CHOCO(OH) + 0.60\ CO_2 + 0.60\ H_2O_2 + 0.60\ OH^- + 0.20\ O_2 - 0.60\ H_2O$	R(509)	$7.5 \cdot 10^7$			= k(2 $CH_2(OO^\bullet)CO(O^-)$) - 8
Pathway 1: $2\ CO(O^-)CH(OO^\bullet)CO(O^-) \rightarrow 2\ CO(O^-)COCO(O^-) + H_2O_2$		$2.2\ 10^7$			BR: 30%
Pathway 2: $2\ CO(O^-)CH(OO^\bullet)CO(O^-)$ *(+ 2 H_2O)* $\rightarrow 2\ CHOCO(O^-) + 2\ CO_2 + H_2O_2 + 2\ OH^-$		$2.2\ 10^7$			BR: 30%
Pathway 3: $2\ CO(O^-)CH(OO^\bullet)CO(O^-) \rightarrow CO(O^-)COCO(O^-) + CO(O^-)CH(OH)CO(O^-) + O_2$		$2.2\ 10^7$			BR: 30%
Pathway 4: $2\ CO(O^-)CH(OO^\bullet)CO(O^-) \rightarrow 2\ CO(O^-)CH(O^\bullet)CO(O^-) + O_2$		$9.0\ 10^6$			BR: 10%
$CO(O^-)CH(O^\bullet)CO(O^-) \rightarrow CO(O^-)C^\bullet(OH)CO(O^-)$					4
$CO(O^-)C^\bullet(OH)CO(O^-) + O_2 \rightarrow CO(O^-)C(OH)(OO^\bullet)CO(O^-)$		$2.0 \cdot 10^9$			5
$2\ CO(O^-)CH(OO^\bullet)CO(O^-) \rightarrow 0.90\ CO(O^-)COCO(O^-) + 0.30\ CO(O^-)CH(OH)CO(O^-) + 0.20\ CO(O^-)C(OH)(OO^\bullet)CO(O^-) + 0.60\ CHOCO(O^-) + 0.60\ CO_2 + 0.60\ H_2O_2 + 0.60\ OH^- + 0.20\ O_2 - 0.60\ H_2O$	R(510)	$7.5 \cdot 10^7$			= k(2 $CH_2(OO^\bullet)CO(O^-)$) - 8
Oxidation of tartronic acid					
Pathway 1: $CO(OH)CH(OH)CO(OH) + HO^\bullet \rightarrow CO(OH)C^\bullet(OH)CO(OH) + H_2O$		$2.0 \cdot 10^7$			BR: 11% - 48
$CO(OH)C^\bullet(OH)CO(OH) + O_2 \rightarrow CO(OH)C(OH)(OO^\bullet)CO(OH)$		$2.0 \cdot 10^9$			5
Pathway 2: $CO(OH)CH(OH)CO(OH) + HO^\bullet \rightarrow CO(OH)CH(O^\bullet)CO(OH) + H_2O$		$1.5\ 10^8$			BR: 89% - 48
$CO(OH)CH(O^\bullet)CO(OH) \rightarrow C^\bullet O(OH) + CHOCO(OH)$					6 - 7
$C^\bullet O(OH) + O_2 \rightarrow CO(OH)(OO^\bullet)$		$2.0 \cdot 10^9$			5
$CO(OH)CH(OH)CO(OH) + HO^\bullet \rightarrow 0.11\ CO(OH)C(OH)(OO^\bullet)CO(OH) + 0.89\ CHOCO(OH) + 0.89\ CO(OH)(OO^\bullet) + H_2O - O_2$	R(511)	$1.7 \cdot 10^8$		Schuchmann et al., 1995	
$CO(OH)CH(OH)CO(OH) + NO_3^\bullet \rightarrow CO(OH)C^\bullet(OH)CO(OH) + NO_3^- + H^+$		$5.1 \cdot 10^4$			BR: 100%
$CO(OH)C^\bullet(OH)CO(OH) + O_2 \rightarrow CO(OH)C(OH)(OO^\bullet)CO(OH)$		$2.0 \cdot 10^9$			5
$CO(OH)CH(OH)CO(OH) + NO_3^\bullet \rightarrow CO(OH)C(OH)(OO^\bullet)CO(OH) + NO_3^- + H^+ - O_2$	R(512)	$5.1 \cdot 10^4$			= k($CO(OH)CH_2CO(OH)$ + $NO_3^\bullet$) - 2
Pathway 1: $CO(OH)CH(OH)CO(O^-) + HO^\bullet \rightarrow CO(OH)C^\bullet(OH)CO(O^-) + H_2O$		$4.0 \cdot 10^7$			BR: 11% - 49
$CO(OH)C^\bullet(OH)CO(O^-) + O_2 \rightarrow CO(OH)C(OH)(OO^\bullet)CO(O^-)$		$2.0 \cdot 10^9$			5
Pathway 2: $CO(OH)CH(OH)CO(O^-) + HO^\bullet \rightarrow CO(OH)CH(O^\bullet)CO(O^-) + H_2O$		$1.5\ 10^8$			BR: 43% - 49
$CO(OH)CH(O^\bullet)CO(O^-) \rightarrow C^\bullet O(OH) + CHOCO(O^-)$					6 - 7
$C^\bullet O(OH) + O_2 \rightarrow CO(OH)(OO^\bullet)$		$2.0 \cdot 10^9$			5
Pathway 3: $CO(OH)CH(OH)CO(O^-) + HO^\bullet \rightarrow CO(OH)CH(OH)CO(O^\bullet) + OH^-$		$1.7\ 10^8$			BR: 46% - 49
$CO(OH)CH(OH)CO(O^\bullet) \rightarrow CO(OH)C^\bullet H(OH) + CO_2$					6 - 7
$CO(OH)C^\bullet H(OH) + O_2 \rightarrow CH(OH)(OO^\bullet)CO(OH)$		$2.0 \cdot 10^9$			5

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CO(OH)CH(OH)CO(O^-) + HO^\bullet \rightarrow 0.11\ CO(OH)C(OH)(OO^\bullet)CO(O^-) + 0.46\ CH(OH)(OO^\bullet)CO(OH) + 0.43\ CO(OH)(OO^\bullet) + 0.46\ CO_2 + 0.43\ CHOCO(O^-) + 0.46\ OH^- + 0.54\ H_2O - O_2$	R(513)	$3.6 \cdot 10^8$		Schuchmann et al., 1995	
Pathway 1: $CO(OH)CH(OH)CO(O^-) + NO_3^\bullet \rightarrow CO(OH)C^\bullet(OH)CO(O^-) + NO_3^- + H^+$		$5.6 \cdot 10^6$	3369		BR: 100%
$CO(OH)C^\bullet(OH)CO(O^-) + O_2 \rightarrow CO(OH)C(OH)(OO^\bullet)CO(O^-)$		$2.0 \cdot 10^9$			5
$CO(OH)CH(OH)CO(O^-) + NO_3^\bullet \rightarrow CO(OH)C(OH)(OO^\bullet)CO(O^-) + NO_3^- + H^+ - O_2$	R(514)	$5.6 \cdot 10^6$	3369		= k($CO(OH)CH_2CO(O^-) + NO_3^\bullet$) - 2
Pathway 1: $CO(O^-)CH(OH)CO(O^-) + HO^\bullet \rightarrow CO(O^-)C^\bullet(OH)CO(O^-) + H_2O$		$6.0 \cdot 10^7$			BR: 13% - 50
$CO(O^-)C^\bullet(OH)CO(O^-) + O_2 \rightarrow CO(O^-)C(OH)(OO^\bullet)CO(O^-)$		$2.0 \cdot 10^9$			5
Pathway 2: $CO(O^-)CH(OH)CO(O^-) + HO^\bullet \rightarrow CO(O^-)CH(O^\bullet)CO(O^-) + H_2O$		$1.2\ 10^8$			BR: 27% - 50
$CO(O^-)CH(O^\bullet)CO(O^-) \rightarrow C^\bullet O(O^-) + CHOCO(O^-)$					6 - 7
$C^\bullet O(O^-) + O_2 \rightarrow CO(O^-)(OO^\bullet)$		$2.0 \cdot 10^9$			5
$CO(O^-)(OO^\bullet) \rightarrow CO_2 + O_2^{\bullet-}$					9
Pathway 3: $CO(O^-)CH(OH)CO(O^-) + HO^\bullet \rightarrow CO(O^-)CH(OH)CO(O^\bullet) + OH^-$		$2.6\ 10^8$			BR: 60% - 50
$CO(O^-)CH(OH)CO(O^\bullet) \rightarrow CO(O^-)C^\bullet H(OH) + CO_2$					6 - 7
$CO(O^-)C^\bullet H(OH) + O_2 \rightarrow CH(OH)(OO^\bullet)CO(O^-)$		$2.0 \cdot 10^9$			5
$CO(O^-)CH(OH)CO(O^-) + HO^\bullet \rightarrow 0.13\ CO(O^-)C(OH)(OO^\bullet)CO(O^-) + 0.27\ CHOCO(O^-) + 0.60\ CH(OH)(OO^\bullet)CO(O^-) + 0.87\ CO_2 + 0.27\ O_2^{\bullet-} + 0.60\ OH^- + 0.40\ H_2O - O_2$	R(515)	$4.4 \cdot 10^8$		Schuchmann et al., 1995	
$CO(O^-)CH(OH)CO(O^-) + NO_3^\bullet \rightarrow CO(O^-)C^\bullet(OH)CO(O^-) + NO_3^- + H^+$		$2.3 \cdot 10^7$	3008		BR: 100%
$CO(O^-)C^\bullet(OH)CO(O^-) + O_2 \rightarrow CO(O^-)C(OH)(OO^\bullet)CO(O^-)$		$2.0 \cdot 10^9$			5
$CO(O^-)CH(OH)CO(O^-) + NO_3^\bullet \rightarrow CO(O^-)C(OH)(OO^\bullet)CO(O^-) + NO_3^- + H^+ - O_2$	R(516)	$2.3 \cdot 10^7$	3008		= k($CO(O^-)CH_2CO(O^-) + NO_3^\bullet$) - 2
$CO(OH)C(OH)(OO^\bullet)CO(OH) + OH^- \rightarrow CO(OH)C(O^-)(OO^\bullet)CO(OH) + H_2O$		$4.0\ 10^9$			
$CO(OH)C(O^-)(OO^\bullet)CO(OH) \rightarrow CO(OH)COCO(OH) + O_2^{\bullet-}$					9
$CO(OH)C(OH)(OO^\bullet)CO(OH) + OH^- \rightarrow CO(OH)COCO(OH) + O_2^{\bullet-} + H_2O$	R(517)	$4.0 \cdot 10^9$			= k($CH_3CH(OH)(OO^\bullet) + OH^-$)
$CO(OH)C(OH)(OO^\bullet)CO(OH) \rightarrow CO(OH)COCO(OH) + HO_2^\bullet$	R(518)	$1.1 \cdot 10^4$			= k($CO(O^-)C(OH)(OO^\bullet)CO(O^-)$)
$CO(OH)C(OH)(OO^\bullet)CO(O^-) + OH^- \rightarrow CO(OH)C(O^-)(OO^\bullet)CO(O^-) + H_2O$		$4.0\ 10^9$			
$CO(OH)C(O^-)(OO^\bullet)CO(O^-) \rightarrow CO(OH)COCO(O^-) + O_2^{\bullet-}$					9
$CO(OH)C(OH)(OO^\bullet)CO(O^-) + OH^- \rightarrow CO(OH)COCO(O^-) + O_2^{\bullet-} + H_2O$	R(519)	$4.0 \cdot 10^9$			= k($CH_3CH(OH)(OO^\bullet) + OH^-$)
$CO(OH)C(OH)(OO^\bullet)CO(O^-) \rightarrow CO(OH)COCO(O^-) + HO_2^\bullet$	R(520)	$1.1 \cdot 10^4$			= k($CO(O^-)C(OH)(OO^\bullet)CO(O^-)$)
$CO(O^-)C(OH)(OO^\bullet)CO(O^-) + OH^- \rightarrow CO(O^-)C(O^-)(OO^\bullet)CO(O^-) + H_2O$		$4.0\ 10^9$			
$CO(O^-)C(O^-)(OO^\bullet)CO(O^-) \rightarrow CO(O^-)COCO(O^-) + O_2^{\bullet-}$					9
$CO(O^-)C(OH)(OO^\bullet)CO(O^-) + OH^- \rightarrow CO(O^-)COCO(O^-) + O_2^{\bullet-} + H_2O$	R(521)	$4.0 \cdot 10^9$			= k($CH_3CH(OH)(OO^\bullet) + OH^-$)
$CO(O^-)C(OH)(OO^\bullet)CO(O^-) \rightarrow CO(O^-)COCO(O^-) + HO_2^\bullet$	R(522)	$1.1 \cdot 10^4$		Schuchmann et al., 1995	
Oxidation of mesoxalic acid (or ketomalonic acid)					51
$CO(OH)C(OH)(OH)CO(OH) + HO^\bullet \rightarrow CO(OH)C(O^\bullet)(OH)CO(OH) + H_2O$		$1.4\ 10^8$			BR: 100%
$CO(OH)C(O^\bullet)(OH)CO(OH) \rightarrow CO(OH)CO(OH) + C^\bullet O(OH)$					6 - 7
$C^\bullet O(OH) + O_2 \rightarrow CO(OH)(OO^\bullet)$		$2.0 \cdot 10^9$			5
$CO(OH)C(OH)(OH)CO(OH) + HO^\bullet \rightarrow CO(OH)CO(OH) + CO(OH)(OO^\bullet) + H_2O - O_2$	R(523)	$1.4\ 10^8$		Schaefer, 2012	
$CO(OH)COCO(O^-) + HO^\bullet \rightarrow CO(OH)COCO(O^\bullet) + OH^-$		$3.2\ 10^8$			BR: 100%
$CO(OH)COCO(O^\bullet) \rightarrow CO(OH)C^\bullet O + CO_2$					6 - 7
$CO(OH)C^\bullet O + O_2 \rightarrow CO(OH)CO(OO^\bullet)$		$2.0 \cdot 10^9$			5
$CO(OH)COCO(O^-) + HO^\bullet \rightarrow CO(OH)CO(OO^\bullet) + CO_2 + OH^- - O_2$	R(524)	$3.2\ 10^8$			13
$CO(OH)C(OH)(OH)CO(O^-) + HO^\bullet \rightarrow CO(OH)C(O^\bullet)(OH)CO(O^-) + H_2O$		$1.4\ 10^8$			BR: 100%
$CO(OH)C(O^\bullet)(OH)CO(O^-) \rightarrow CO(OH)CO(O^-) + C^\bullet O(OH)$					6 - 7
$C^\bullet O(OH) + O_2 \rightarrow CO(OH)(OO^\bullet)$		$2.0 \cdot 10^9$			5

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CO(OH)C(OH)(OH)CO(O^-) + HO^\bullet \rightarrow CO(OH)CO(O^-) + CO(OH)(OO^\bullet) + H_2O - O_2$	R(525)	$1.4\ 10^8$		Schaefer, 2012	
$CO(O^-)COCO(O^-) + HO^\bullet \rightarrow CO(O^-)COCO(O^\bullet) + OH^-$		$1.6\ 10^8$			BR: 100%
$CO(O^-)COCO(O^\bullet) \rightarrow CO(O^-)C^\bullet O + CO_2$					6 - 7
$CO(O^-)C^\bullet O + O_2 \rightarrow CO(O^-)CO(OO^\bullet)$		$2.0{\cdot}10^9$			5
$CO(O^-)COCO(O^-) + HO^\bullet \rightarrow CO(O^-)CO(OO^\bullet) + CO_2 + OH^- - O_2$	R(526)	$1.6\ 10^8$		Schaefer, 2012	
Oxidation of lactic acid					
Pathway 1: $CH_3CH(OH)CO(OH) + HO^\bullet \rightarrow CH_3C^\bullet(OH)CO(OH) + H_2O$		$1.8\ 10^8$			BR: 34% - 52
$CH_3C^\bullet(OH)CO(OH) + O_2 \rightarrow CH_3C(OH)(OO^\bullet)CO(OH)$		$2.0\ 10^9$			5
Pathway 2: $CH_3CH(OH)CO(OH) + HO^\bullet \rightarrow C^\bullet H_2CH(OH)CO(OH) + H_2O$		$2.3\ 10^8$			BR: 44% - 52
$C^\bullet H_2CH(OH)CO(OH) + O_2 \rightarrow CH_2(OO^\bullet)CH(OH)CO(OH)$		$2.0\ 10^9$			5
Pathway 3: $CH_3CH(OH)CO(OH) + HO^\bullet \rightarrow CH_3CH(O^\bullet)CO(OH) + H_2O$		$1.1\ 10^8$			BR: 22% - 52
$CH_3CH(O^\bullet)CO(OH) \rightarrow CH_3CHO + C^\bullet O(OH)$					6 - 7
$C^\bullet O(OH) + O_2 \rightarrow CO(OH)(OO^\bullet)$		$2.0\ 10^9$			5
$CH_3CH(OH)CO(OH) + HO^\bullet \rightarrow 0.34\ CH_3C(OH)(OO^\bullet)CO(OH) + 0.44\ CH_2(OO^\bullet)CH(OH)CO(OH) + 0.22\ CH_3CHO + 0.22\ CO(OH)(OO^\bullet) + H_2O - O_2$	R(527)	$5.3{\cdot}10^8$	1120	Martin et al., 2008	
Pathway 1: $CH_3CH(OH)CO(OH) + NO_3^\bullet \rightarrow CH_3C^\bullet(OH)CO(OH) + NO_3^- + H^+$		$9.0\ 10^5$			BR: 43%
$CH_3C^\bullet(OH)CO(OH) + O_2 \rightarrow CH_3C(OH)(OO^\bullet)CO(OH)$		$2.0\ 10^9$			5
Pathway 2: $CH_3CH(OH)CO(OH) + NO_3^\bullet \rightarrow C^\bullet H_2CH(OH)CO(OH) + NO_3^- + H^+$		$1.2\ 10^6$			BR: 57%
$C^\bullet H_2CH(OH)CO(OH) + O_2 \rightarrow CH_2(OO^\bullet)CH(OH)CO(OH)$		$2.0\ 10^9$			5
$CH_3CH(OH)CO(OH) + NO_3^\bullet \rightarrow 0.43\ CH_3C(OH)(OO^\bullet)CO(OH) + 0.57\ CH_2(OO^\bullet)CH(OH)CO(OH) + NO_3^- + H^+ - O_2$	R(528)	$2.1{\cdot}10^6$	3248	De Semainville et al., 2007	2
Pathway 1: $CH_3CH(OH)CO(O^-) + HO^\bullet \rightarrow CH_3C^\bullet(OH)CO(O^-) + H_2O$		$3.3\ 10^8$			BR: 42% - 53
$CH_3C^\bullet(OH)CO(O^-) + O_2 \rightarrow CH_3C(OH)(OO^\bullet)CO(O^-)$		$2.0\ 10^9$			5
Pathway 2: $CH_3CH(OH)CO(O^-) + HO^\bullet \rightarrow C^\bullet H_2CH(OH)CO(O^-) + H_2O$		$2.2\ 10^8$			BR: 28% - 53
$C^\bullet H_2CH(OH)CO(O^-) + O_2 \rightarrow CH_2(OO^\bullet)CH(OH)CO(O^-)$		$2.0\ 10^9$			5
Pathway 3: $CH_3CH(OH)CO(O^-) + HO^\bullet \rightarrow CH_3CH(O^\bullet)CO(O^-) + H_2O$		$1.1\ 10^8$			BR: 14% - 53
$CH_3CH(O^\bullet)CO(O^-) \rightarrow CH_3CHO + C^\bullet O(O^-)$					6 - 7
$C^\bullet O(O^-) + O_2 \rightarrow CO(O^-)(OO^\bullet)$		$2.0\ 10^9$			5
$CO(O^-)(OO^\bullet) \rightarrow CO_2 + O_2^{\bullet-}$					9
Pathway 4: $CH_3CH(OH)CO(O^-) + HO^\bullet \rightarrow CH_3CH(OH)CO(O^\bullet) + OH^-$		$1.2\ 10^8$			BR: 16% - 53
$CH_3CH(OH)CO(O^\bullet) \rightarrow CH_3C^\bullet H(OH) + CO_2$					6 - 7
$CH_3C^\bullet H(OH) + O_2 \rightarrow CH_3CH(OH)(OO^\bullet)$		$2.0{\cdot}10^9$			5
$CH_3CH(OH)CO(O^-) + HO^\bullet \rightarrow 0.42\ CH_3C(OH)(OO^\bullet)CO(O^-) + 0.28\ CH_2(OO^\bullet)CH(OH)CO(O^-) + 0.14\ CH_3CHO + 0.16\ CH_3CH(OH)(OO^\bullet) + 0.30\ CO_2 + 0.14\ O_2^{\bullet-} + 0.16\ OH^- + 0.84\ H_2O - O_2$	R(529)	$7.9{\cdot}10^8$	1294	Martin et al., 2008	
Pathway 1: $CH_3CH(OH)CO(O^-) + NO_3^\bullet \rightarrow CH_3C^\bullet(OH)CO(O^-) + NO_3^- + H^+$		$6.0\ 10^6$			BR: 60%
$CH_3C^\bullet(OH)CO(O^-) + O_2 \rightarrow CH_3C(OH)(OO^\bullet)CO(O^-)$		$2.0\ 10^9$			5
Pathway 2: $CH_3CH(OH)CO(O^-) + NO_3^\bullet \rightarrow C^\bullet H_2CH(OH)CO(O^-) + NO_3^- + H^+$		$4.0\ 10^6$			BR: 40%
$C^\bullet H_2CH(OH)CO(O^-) + O_2 \rightarrow CH_2(OO^\bullet)CH(OH)CO(O^-)$		$2.0\ 10^9$			5
$CH_3CH(OH)CO(O^-) + NO_3^\bullet \rightarrow 0.60\ CH_3C(OH)(OO^\bullet)CO(O^-) + 0.40\ CH_2(OO^\bullet)CH(OH)CO(O^-) + NO_3^- + H^+ - O_2$	R(530)	$1.0{\cdot}10^7$	2646	De Semainville et al., 2007	2
$CH_3C(OH)(OO^\bullet)CO(OH) + OH^- \rightarrow CH_3C(O^-)(OO^\bullet)CO(OH) + H_2O$		$4.0\ 10^9$			
$CH_3C(O^-)(OO^\bullet)CO(OH) \rightarrow CH_3COCO(OH) + O_2^{\bullet-}$					9
$CH_3C(OH)(OO^\bullet)CO(OH) + OH^- \rightarrow CH_3COCO(OH) + O_2^{\bullet-} + H_2O$	R(531)	$4.0\ 10^9$			= $k(CH_3CH(OH)(OO^\bullet) + OH^-)$
$CH_3C(OH)(OO^\bullet)CO(OH) \rightarrow CH_3COCO(OH) + HO_2^\bullet$	R(532)	665			10
$CH_3C(OH)(OO^\bullet)CO(O^-) + OH^- \rightarrow CH_3C(O^-)(OO^\bullet)CO(O^-) + H_2O$		$4.0\ 10^9$			
$CH_3C(O^-)(OO^\bullet)CO(O^-) \rightarrow CH_3COCO(O^-) + O_2^{\bullet-}$					9
$CH_3C(OH)(OO^\bullet)CO(O^-) + OH^- \rightarrow CH_3COCO(O^-) + O_2^{\bullet-} + H_2O$	R(533)	$4.0\ 10^9$			= $k(CH_3CH(OH)(OO^\bullet) + OH^-)$

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CH_3C(OH)(OO^•)CO(O^-) \rightarrow CH_3COCO(O^-) + HO_2^•$	R(534)	665			10
Pathway 1: 2 $CH_2(OO^•)CH(OH)CO(OH) \rightarrow$ 2 $CHOCH(OH)CO(OH) + H_2O_2$		$5.0\ 10^7$			BR: 50%
Pathway 2: 2 $CH_2(OO^•)CH(OH)CO(OH) \rightarrow CHOCH(OH)CO(OH) + CH_2(OH)CH(OH)CO(OH) + O_2$		$3.3\ 10^7$			BR: 33%
Pathway 3: 2 $CH_2(OO^•)CH(OH)CO(OH) \rightarrow$ 2 $CH_2(O^•)CH(OH)CO(OH) + O_2$		$1.7\ 10^7$			BR: 17%
$CH_2(O^•)CH(OH)CO(OH) \rightarrow CH_2O + C^•H(OH)CO(OH)$					6 - 7
$C^•H(OH)CO(OH) + O_2 \rightarrow CH(OH)(OO^•)CO(OH)$		$2.0{\cdot}10^9$			5
2 $CH_2(OO^•)CH(OH)CO(OH) \rightarrow 1.33\ CHOCH(OH)CO(OH) + 0.33\ CH_2(OH)CH(OH)CO(OH) + 0.34\ CH(OH)(OO^•)CO(OH) + 0.34\ CH_2O + 0.50\ H_2O_2 + 0.16\ O_2$	R(535)	$1.0\ 10^8$			= k(2 $CH_2(OH)CH_2(OO^•)$) - 8
Pathway 1: 2 $CH_2(OO^•)CH(OH)CO(O^-) \rightarrow$ 2 $CHOCH(OH)CO(O^-) + H_2O_2$		$5.0\ 10^7$			BR: 50%
Pathway 2: 2 $CH_2(OO^•)CH(OH)CO(O^-) \rightarrow CHOCH(OH)CO(O^-) + CH_2(OH)CH(OH)CO(O^-) + O_2$		$3.3\ 10^7$			BR: 33%
Pathway 3: 2 $CH_2(OO^•)CH(OH)CO(O^-) \rightarrow$ 2 $CH_2(O^•)CH(OH)CO(O^-) + O_2$		$1.7\ 10^7$			BR: 17%
$CH_2(O^•)CH(OH)CO(O^-) \rightarrow CH_2O + C^•H(OH)CO(O^-)$					6 - 7
$C^•H(OH)CO(O^-) + O_2 \rightarrow CH(OH)(OO^•)CO(O^-)$		$2.0{\cdot}10^9$			5
2 $CH_2(OO^•)CH(OH)CO(O^-) \rightarrow 1.33\ CHOCH(OH)CO(O^-) + 0.33\ CH_2(OH)CH(OH)CO(O^-) + 0.34\ CH(OH)(OO^•)CO(O^-) + 0.34\ CH_2O + 0.50\ H_2O_2 + 0.16\ O_2$	R(536)	$1.0\ 10^8$			= k(2 $CH_2(OH)CH_2(OO^•)$) - 8
Oxidation of 2,3-dihydroxypropanoic acid					
Pathway 1: $CH_2(OH)CH(OH)CO(OH) + HO^• \rightarrow C^•H(OH)CH(OH)CO(OH) + H_2O$		$5.5{\cdot}10^8$			BR: 85% - 54
$C^•H(OH)CH(OH)CO(OH) + O_2 \rightarrow CH(OH)(OO^•)CH(OH)CO(OH)$		$2.0{\cdot}10^9$			5
Pathway 2: $CH_2(OH)CH(OH)CO(OH) + HO^• \rightarrow CH_2(O^•)CH(OH)CO(OH) + H_2O$		$1.0{\cdot}10^8$			BR: 15% - 54
$CH_2(O^•)CH(OH)CO(OH) \rightarrow CH_2O + C^•H(OH)CO(OH)$					6 - 7
$C^•H(OH)CO(OH) + O_2 \rightarrow CH(OH)(OO^•)CO(OH)$		$2.0{\cdot}10^9$			5
$CH_2(OH)CH(OH)CO(OH) + HO^• \rightarrow 0.85\ CH(OH)(OO^•)CH(OH)CO(OH) + 0.15\ CH_2O + 0.15\ CH(OH)(OO^•)CO(OH) + H_2O - O_2$	R(537)	$6.5\ 10^8$			13
$CH_2(OH)CH(OH)CO(OH) + NO_3^• \rightarrow C^•H(OH)CH(OH)CO(OH) + NO_3^- + H^+$		$9.1\ 10^5$			BR: 100%
$C^•H(OH)CH(OH)CO(OH) + O_2 \rightarrow CH(OH)(OO^•)CH(OH)CO(OH)$		$2.0{\cdot}10^9$			5
$CH_2(OH)CH(OH)CO(OH) + NO_3^• \rightarrow CH(OH)(OO^•)CH(OH)CO(OH) + NO_3^- + H^+ - O_2$	R(538)	$9.1\ 10^5$	3971		= k($CH_2(OH)CO(OH) + NO_3^•$) - 2
Pathway 1: $CH_2(OH)CH(OH)CO(O^-) + HO^• \rightarrow C^•H(OH)CH(OH)CO(O^-) + H_2O$		$1.1{\cdot}10^9$			BR: 87% - 55
$C^•H(OH)CH(OH)CO(O^-) + O_2 \rightarrow CH(OH)(OO^•)CH(OH)CO(O^-)$		$2.0{\cdot}10^9$			5
Pathway 2: $CH_2(OH)CH(OH)CO(O^-) + HO^• \rightarrow CH_2(OH)C^•(OH)CO(O^-) + H_2O$		$2.0{\cdot}10^8$			BR: 13% - 55
$CH_2(OH)C^•(OH)CO(O^-) + O_2 \rightarrow CH_2(OH)C(OH)(OO^•)CO(O^-)$		$2.0{\cdot}10^9$			5
$CH_2(OH)CH(OH)CO(O^-) + HO^• \rightarrow 0.87\ CH(OH)(OO^•)CH(OH)CO(O^-) + 0.13\ CH_2(OH)C(OH)(OO^•)CO(O^-) + H_2O - O_2$	R(539)	$1.3\ 10^9$			13
Pathway 1: $CH_2(OH)CH(OH)CO(O^-) + NO_3^• \rightarrow C^•H(OH)CH(OH)CO(O^-) + NO_3^- + H^+$		$8.7{\cdot}10^6$			BR: 87%
$C^•H(OH)CH(OH)CO(O^-) + O_2 \rightarrow CH(OH)(OO^•)CH(OH)CO(O^-)$		$2.0{\cdot}10^9$			5
Pathway 2: $CH_2(OH)CH(OH)CO(O^-) + NO_3^• \rightarrow CH_2(OH)C^•(OH)CO(O^-) + NO_3^- + H^+$		$1.3{\cdot}10^6$			BR: 13%
$CH_2(OH)C^•(OH)CO(O^-) + O_2 \rightarrow CH_2(OH)C(OH)(OO^•)CO(O^-)$		$2.0{\cdot}10^9$			5
$CH_2(OH)CH(OH)CO(O^-) + NO_3^• \rightarrow 0.87\ CH(OH)(OO^•)CH(OH)CO(O^-) + 0.13\ CH_2(OH)C(OH)(OO^•)CO(O^-) + NO_3^- + H^+ - O_2$	R(540)	$1.0\ 10^7$	3008		= k($CH_2(OH)CO(O^-) + NO_3^•$) - 2
$CH(OH)(OO^•)CH(OH)CO(OH) + OH^- \rightarrow CH(O^-)(OO^•)CH(OH)CO(OH) + H_2O$		$4.0\ 10^9$			
$CH(O^-)(OO^•)CH(OH)CO(OH) \rightarrow CHOCH(OH)CO(OH) + O_2^{•-}$					9
$CH(OH)(OO^•)CH(OH)CO(OH) + OH^- \rightarrow CHOCH(OH)CO(OH) + O_2^{•-} + H_2O$	R(541)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^•) + OH^-$)
$CH(OH)(OO^•)CH(OH)CO(OH) \rightarrow CHOCH(OH)CO(OH) + HO_2^•$	R(542)	$1.9\ 10^2$			10
$CH(OH)(OO^•)CH(OH)CO(O^-) + OH^- \rightarrow CH(O^-)(OO^•)CH(OH)CO(O^-) + H_2O$		$4.0\ 10^9$			
$CH(O^-)(OO^•)CH(OH)CO(O^-) \rightarrow CHOCH(OH)CO(O^-) + O_2^{•-}$					9
$CH(OH)(OO^•)CH(OH)CO(O^-) + OH^- \rightarrow CHOCH(OH)CO(O^-) + O_2^{•-} + H_2O$	R(543)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^•) + OH^-$)
$CH(OH)(OO^•)CH(OH)CO(O^-) \rightarrow CHOCH(OH)CO(O^-) + HO_2^•$	R(544)	$1.9\ 10^2$			10

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CH_2(OH)C(OH)(OO^•)CO(OH) + OH^- \rightarrow CH_2(OH)C(O^-)(OO^•)CO(OH) + H_2O$		$4.0\ 10^9$			
$CH_2(OH)C(O^-)(OO^•)CO(OH) \rightarrow CH_2(OH)COCO(OH) + O_2^{•-}$					9
$CH_2(OH)C(OH)(OO^•)CO(OH) + OH^- \rightarrow CH_2(OH)COCO(OH) + O_2^{•-} + H_2O$	R(545)	$4.0\ 10^9$			= $k(CH_3CH(OH)(OO^•) + OH^-)$
$CH_2(OH)C(OH)(OO^•)CO(OH) \rightarrow CH_2(OH)COCO(OH) + HO_2^•$	R(546)	665			10
$CH_2(OH)C(OH)(OO^•)CO(O^-) + OH^- \rightarrow CH_2(OH)C(O^-)(OO^•)CO(O^-) + H_2O$		$4.0\ 10^9$			
$CH_2(OH)C(O^-)(OO^•)CO(O^-) \rightarrow CH_2(OH)COCO(O^-) + O_2^{•-}$					9
$CH_2(OH)C(OH)(OO^•)CO(O^-) + OH^- \rightarrow CH_2(OH)COCO(O^-) + O_2^{•-} + H_2O$	R(547)	$4.0\ 10^9$			= $k(CH_3CH(OH)(OO^•) + OH^-)$
$CH_2(OH)C(OH)(OO^•)CO(O^-) \rightarrow CH_2(OH)COCO(O^-) + HO_2^•$	R(548)	665			10
Oxidation of 2-hydroxy, 3-oxopropanoïc acid					56
Pathway 1: $CH(OH)(OH)CH(OH)CO(OH) + HO^• \rightarrow CH(OH)(O^•)CH(OH)CO(OH) + H_2O$		$4.2{\cdot}10^8$			BR: 63% - 57
$CH(OH)(O^•)CH(OH)CO(OH) \rightarrow CHO(OH) + C^•H(OH)CO(OH)$					6 - 7
$C^•H(OH)CO(OH) + O_2 \rightarrow CH(OH)(OO^•)CO(OH)$		$2.0{\cdot}10^9$			5
Pathway 2: $CH(OH)(OH)CH(OH)CO(OH) + HO^• \rightarrow C^•(OH)(OH)CH(OH)CO(OH) + H_2O$		$2.5{\cdot}10^8$			BR: 37% - 57
$C^•(OH)(OH)CH(OH)CO(OH) + O_2 \rightarrow CO(OH)CH(OH)C(OH)(OH)(OO^•)$		$2.0{\cdot}10^9$			5
$CH(OH)(OH)CH(OH)CO(OH) + HO^• \rightarrow 0.37\ CO(OH)CH(OH)C(OH)(OH)(OO^•) + 0.63\ CHO(OH) + 0.63\ CH(OH)(OO^•)CO(OH) + H_2O - O_2$	R(549)	$6.7\ 10^8$			13
$CH(OH)(OH)CH(OH)CO(OH) + NO_3^• \rightarrow C^•(OH)(OH)CH(OH)CO(OH) + NO_3^- + H^+$		$1.1\ 10^6$			BR: 100%
$C^•(OH)(OH)CH(OH)CO(OH) + O_2 \rightarrow CO(OH)CH(OH)C(OH)(OH)(OO^•)$		$2.0{\cdot}10^9$			5
$CH(OH)(OH)CH(OH)CO(OH) + NO_3^• \rightarrow CO(OH)CH(OH)C(OH)(OH)(OO^•) + NO_3^- + H^+ - O_2$	R(550)	$1.1\ 10^6$			= $k(CH_2(OH)CH(OH)(OH) + NO_3^•)$ - 2
Pathway 1: $CH(OH)(OH)CH(OH)CO(O^-) + HO^• \rightarrow CH(OH)(O^•)CH(OH)CO(O^-) + H_2O$		$4.9{\cdot}10^8$			BR: 49% - 58
$CH(OH)(O^•)CH(OH)CO(O^-) \rightarrow CHO(OH) + C^•H(OH)CO(O^-)$					6 - 7
$C^•H(OH)CO(O^-) + O_2 \rightarrow CH(OH)(OO^•)CO(O^-)$		$2.0{\cdot}10^9$			5
Pathway 2: $CH(OH)(OH)CH(OH)CO(O^-) + HO^• \rightarrow C^•(OH)(OH)CH(OH)CO(O^-) + H_2O$		$5.1{\cdot}10^8$			BR: 51% - 58
$C^•(OH)(OH)CH(OH)CO(O^-) + O_2 \rightarrow CO(O^-)CH(OH)C(OH)(OH)(OO^•)$		$2.0{\cdot}10^9$			5
$CH(OH)(OH)CH(OH)CO(O^-) + HO^• \rightarrow 0.51\ CO(O^-)CH(OH)C(OH)(OH)(OO^•) + 0.49\ CH(OH)(OO^•)CO(O^-) + 0.49\ CHO(OH) + H_2O - O_2$	R(551)	$1.0\ 10^9$			13
$CH(OH)(OH)CH(OH)CO(O^-) + NO_3^• \rightarrow C^•(OH)(OH)CH(OH)CO(O^-) + NO_3^- + H^+$		$1.1\ 10^6$			BR: 100%
$C^•(OH)(OH)CH(OH)CO(O^-) + O_2 \rightarrow CO(O^-)CH(OH)C(OH)(OH)(OO^•)$		$2.0{\cdot}10^9$			5
$CH(OH)(OH)CH(OH)CO(O^-) + NO_3^• \rightarrow CO(O^-)CH(OH)C(OH)(OH)(OO^•) + NO_3^- + H^+ - O_2$	R(552)	$1.1\ 10^6$			= $k(CH_2(OH)CH(OH)(OH) + NO_3^•)$ - 2
$CO(OH)CH(OH)C(OH)(OH)(OO^•) + OH^- \rightarrow CO(OH)CH(OH)C(OH)(O^-)(OO^•) + H_2O$		$4.0\ 10^9$			
$CO(OH)CH(OH)C(OH)(O^-)(OO^•) \rightarrow CO(OH)CH(OH)CO(OH) + O_2^{•-}$					9
$CO(OH)CH(OH)C(OH)(OH)(OO^•) + OH^- \rightarrow CO(OH)CH(OH)CO(OH) + O_2^{•-} + H_2O$	R(553)	$4.0\ 10^9$			= $k(CH_3CH(OH)(OO^•) + OH^-)$
$CO(OH)CH(OH)C(OH)(OH)(OO^•) \rightarrow CO(OH)CH(OH)CO(OH) + HO_2^•$	R(554)	$1.0\ 10^6$			15
$CO(O^-)CH(OH)C(OH)(OH)(OO^•) + OH^- \rightarrow CO(O^-)CH(OH)C(OH)(O^-)(OO^•) + H_2O$		$4.0\ 10^9$			
$CO(O^-)CH(OH)C(OH)(O^-)(OO^•) \rightarrow CO(OH)CH(OH)CO(O^-) + O_2^{•-}$					9
$CO(O^-)CH(OH)C(OH)(OH)(OO^•) + OH^- \rightarrow CO(OH)CH(OH)CO(O^-) + O_2^{•-} + H_2O$	R(555)	$4.0\ 10^9$			= $k(CH_3CH(OH)(OO^•) + OH^-)$
$CO(O^-)CH(OH)C(OH)(OH)(OO^•) \rightarrow CO(OH)CH(OH)CO(O^-) + HO_2^•$	R(556)	$1.0\ 10^6$			15
$CH(OH)(OH)C(OH)(OO^•)CO(OH) + OH^- \rightarrow CH(OH)(OH)C(O^-)(OO^•)CO(OH) + H_2O$		$4.0\ 10^9$			
$CH(OH)(OH)C(O^-)(OO^•)CO(OH) \rightarrow CH(OH)(OH)COCO(OH) + O_2^{•-}$					9
$CH(OH)(OH)C(OH)(OO^•)CO(OH) + OH^- \rightarrow CH(OH)(OH)COCO(OH) + O_2^{•-} + H_2O$	R(557)	$4.0\ 10^9$			= $k(CH_3CH(OH)(OO^•) + OH^-)$
$CH(OH)(OH)C(OH)(OO^•)CO(OH) \rightarrow CH(OH)(OH)COCO(OH) + HO_2^•$	R(558)	$1.9\ 10^2$			15
$CH(OH)(OH)C(OH)(OO^•)CO(O^-) + OH^- \rightarrow CH(OH)(OH)C(O^-)(OO^•)CO(O^-) + H_2O$		$4.0\ 10^9$			
$CH(OH)(OH)C(O^-)(OO^•)CO(O^-) \rightarrow CH(OH)(OH)COCO(O^-) + O_2^{•-}$					9
$CH(OH)(OH)C(OH)(OO^•)CO(O^-) + OH^- \rightarrow CH(OH)(OH)COCO(O^-) + O_2^{•-} + H_2O$	R(559)	$4.0\ 10^9$			= $k(CH_3CH(OH)(OO^•) + OH^-)$

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CH(OH)(OH)C(OH)(OO^{\bullet})CO(O^{-}) \rightarrow CH(OH)(OH)COCO(O^{-}) + HO_2^{\bullet}$	R(560)	$1.9\ 10^{2}$			15
Oxidation of 3-oxopyruvic acid					59
Pathway 1: $CO(OH)C(OH)(OH)CH(OH)(OH) + HO^{\bullet} \rightarrow CO(OH)C(OH)(OH)CH(OH)(O^{\bullet}) + H_2O$		$3.6\ 10^{8}$			BR: 52% - 60
$CO(OH)C(OH)(OH)CH(OH)(O^{\bullet}) \rightarrow CO(OH)C^{\bullet}(OH)(OH) + CHO(OH)$					6 - 7
$CO(OH)C^{\bullet}(OH)(OH) + O_2 \rightarrow CO(OH)C(OH)(OH)(OO^{\bullet})$		$2.0\ 10^{9}$			5
Pathway 2: $CO(OH)C(OH)(OH)CH(OH)(OH) + HO^{\bullet} \rightarrow CO(OH)C(OH)(O^{\bullet})CH(OH)(OH) + H_2O$		$2.4\ 10^{8}$			BR: 35% - 60
$CO(OH)C(OH)(O^{\bullet})CH(OH)(OH) \rightarrow CH(OH)(OH)CO(OH) + C^{\bullet}O(OH)$					6 - 7
$C^{\bullet}O(OH) + O_2 \rightarrow CO(OH)(OO^{\bullet})$		$2.0\ 10^{9}$			5
Pathway 3: $CO(OH)C(OH)(OH)CH(OH)(OH) + HO^{\bullet} \rightarrow CO(OH)C(OH)(OH)C^{\bullet}(OH)(OH) + H_2O$		$9.0\ 10^{7}$			BR: 13% - 60
$CO(OH)C(OH)(OH)C^{\bullet}(OH)(OH) + O_2 \rightarrow CO(OH)C(OH)(OH)C(OH)(OH)(OO^{\bullet})$		$2.0\ 10^{9}$			5
$CO(OH)C(OH)(OH)CH(OH)(OH) + HO^{\bullet} \rightarrow 0.52\ CHO(OH) + 0.52\ CO(OH)C(OH)(OH)(OO^{\bullet}) + 0.13\ CO(OH)C(OH)(OH)C(OH)(OH)(OO^{\bullet}) + 0.35\ CH(OH)(OH)CO(OH) + 0.35\ CO(OH)(OO^{\bullet}) + H_2O - O_2$	R(561)	$6.9\ 10^{8}$			13
$CO(OH)C(OH)(OH)CH(OH)(OH) + NO_3^{\bullet} \rightarrow CO(OH)C(OH)(OH)C^{\bullet}(OH)(OH) + NO_3^{-} + H^{+}$		$1.1\ 10^{6}$			BR:100%
$CO(OH)C(OH)(OH)C^{\bullet}(OH)(OH) + O_2 \rightarrow CO(OH)C(OH)(OH)C(OH)(OH)(OO^{\bullet})$		$2.0\ 10^{9}$			5
$CO(OH)C(OH)(OH)CH(OH)(OH) + NO_3^{\bullet} \rightarrow CO(OH)C(OH)(OH)C(OH)(OH)(OO^{\bullet}) + NO_3^{-} + H^{+} - O_2$	R(562)	$1.0{\cdot}10^{6}$			= k(CH(OH)(OH)CO(OH) + $NO_3^{\bullet}$) - 2
Pathway 1: $CO(O^{-})COCH(OH)(OH) + HO^{\bullet} \rightarrow CO(O^{-})COCH(OH)(O^{\bullet}) + H_2O$		$3.6\ 10^{8}$			BR: 65% - 61
$CO(O^{-})COCH(OH)(O^{\bullet}) \rightarrow CO(O^{-})C^{\bullet}O + CHO(OH)$					6 - 7
$CO(O^{-})C^{\bullet}O + O_2 \rightarrow CO(O^{-})CO(OO^{\bullet})$		$2.0\ 10^{9}$			5
Pathway 2: $CO(O^{-})COCH(OH)(OH) + HO^{\bullet} \rightarrow CO(O^{-})COC^{\bullet}(OH)(OH) + H_2O$		$1.9\ 10^{8}$			BR: 35% - 61
$CO(O^{-})COC^{\bullet}(OH)(OH) + O_2 \rightarrow CO(O^{-})COC(OH)(OH)(OO^{\bullet})$		$2.0\ 10^{9}$			5
$CO(O^{-})COCH(OH)(OH) + HO^{\bullet} \rightarrow 0.65\ CHO(OH) + 0.65\ CO(O^{-})CO(OO^{\bullet}) + 0.35\ CO(O^{-})COC(OH)(OH)(OO^{\bullet}) + H_2O - O_2$	R(563)	$5.5\ 10^{8}$			13
Pathway 1: $CO(O^{-})COCH(OH)(OH) + NO_3^{\bullet} \rightarrow CO(O^{-})COC^{\bullet}(OH)(OH) + NO_3^{-} + H^{+}$		$1.8\ 10^{5}$			BR: 100%
$CO(O^{-})COC^{\bullet}(OH)(OH) + O_2 \rightarrow CO(O^{-})COC(OH)(OH)(OO^{\bullet})$		$2.0\ 10^{9}$			5
$CO(O^{-})COCH(OH)(OH) + NO_3^{\bullet} \rightarrow CO(O^{-})COC(OH)(OH)(OO^{\bullet}) + NO_3^{-} + H^{+} - O_2$	R(564)	$1.8{\cdot}10^{5}$			= k(CH(OH)(OH)CO(O^{-}) + $NO_3^{\bullet}$) - 2
Pathway 1: $CO(O^{-})C(OH)(OH)CH(OH)(OH) + HO^{\bullet} \rightarrow CO(O^{-})C(OH)(OH)CH(OH)(O^{\bullet}) + H_2O$		$3.8\ 10^{8}$			BR: 39% - 62
$CO(O^{-})C(OH)(OH)CH(OH)(O^{\bullet}) \rightarrow CO(O^{-})C^{\bullet}(OH)(OH) + CHO(OH)$					6 - 7
$CO(O^{-})C^{\bullet}(OH)(OH) + O_2 \rightarrow CO(O^{-})C(OH)(OH)(OO^{\bullet})$		$2.0\ 10^{9}$			5
Pathway 2: $CO(O^{-})C(OH)(OH)CH(OH)(OH) + HO^{\bullet} \rightarrow CO(O^{-})C(OH)(O^{\bullet})CH(OH)(OH) + H_2O$		$4.4\ 10^{8}$			BR: 45% - 62
$CO(O^{-})C(OH)(O^{\bullet})CH(OH)(OH) \rightarrow CH(OH)(OH)CO(OH) + CO_2^{\bullet-}$					6 - 7
$CO_2^{\bullet-} + O_2 \rightarrow CO_2 + O_2^{\bullet-}$		$2.4\ 10^{9}$		Hislop and Bolton, 1999	
Pathway 3: $CO(O^{-})C(OH)(OH)CH(OH)(OH) + HO^{\bullet} \rightarrow CO(O^{-})C(OH)(OH)C^{\bullet}(OH)(OH) + H_2O$		$1.6\ 10^{8}$			BR: 16% - 62
$CO(O^{-})C(OH)(OH)C^{\bullet}(OH)(OH) + O_2 \rightarrow CO(O^{-})C(OH)(OH)C(OH)(OH)(OO^{\bullet})$		$2.0\ 10^{9}$			5
$CO(O^{-})C(OH)(OH)CH(OH)(OH) + HO^{\bullet} \rightarrow 0.39\ CHO(OH) + 0.39\ CO(O^{-})C(OH)(OH)(OO^{\bullet}) + 0.16\ CO(O^{-})C(OH)(OH)C(OH)(OH)(OO^{\bullet}) + 0.45\ CH(OH)(OH)CO(OH) + 0.45\ CO_2 + 0.45\ O_2^{\bullet-} + H_2O - O_2$	R(565)	$9.8{\cdot}10^{8}$			13
$CO(OH)C(OH)(OH)CH(OH)(OH) + NO_3^{\bullet} \rightarrow CO(OH)C(OH)(OH)C^{\bullet}(OH)(OH) + NO_3^{-} + H^{+}$		$1.8{\cdot}10^{5}$			BR: 100%
$CO(OH)C(OH)(OH)C^{\bullet}(OH)(OH) + O_2 \rightarrow CO(OH)C(OH)(OH)C(OH)(OH)(OO^{\bullet})$		$2.0\ 10^{9}$			5
$CO(O^{-})C(OH)(OH)CH(OH)(OH) + NO_3^{\bullet} \rightarrow CO(O^{-})C(OH)(OH)C(OH)(OH)(OO^{\bullet}) + NO_3^{-} + H^{+} - O_2$	R(566)	$1.8{\cdot}10^{5}$			= k(CH(OH)(OH)CO(O^{-}) + $NO_3^{\bullet}$) - 2
$CO(OH)C(OH)(OH)C(OH)(OH)(OO^{\bullet}) + OH^{-} \rightarrow CO(OH)C(OH)(OH)C(OH)(O^{-})(OO^{\bullet}) + H_2O$		$4.0\ 10^{9}$			9
$CO(OH)C(OH)(OH)C(OH)(O^{-})(OO^{\bullet}) \rightarrow CO(OH)C(OH)(OH)CO(OH) + O_2^{\bullet-}$					
$CO(OH)C(OH)(OH)C(OH)(OH)(OO^{\bullet}) + OH^{-} \rightarrow CO(OH)C(OH)(OH)CO(OH) + O_2^{\bullet-} + H_2O$	R(567)	$4.0\ 10^{9}$			= k($CH_3CH(OH)(OO^{\bullet})$ + OH^{-})
$CO(OH)C(OH)(OH)C(OH)(OH)(OO^{\bullet}) \rightarrow CO(OH)C(OH)(OH)CO(OH) + HO_2^{\bullet}$	R(568)	$1.0\ 10^{6}$			15
$CO(O^{-})COC(OH)(OH)(OO^{\bullet}) + OH^{-} \rightarrow CO(O^{-})COC(OH)(O^{-})(OO^{\bullet}) + H_2O$		$4.0\ 10^{9}$			
$CO(O^{-})COC(OH)(O^{-})(OO^{\bullet}) \rightarrow CO(OH)COCO(O^{-}) + O_2^{\bullet-}$					9

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CO(O^-)COC(OH)(OH)(OO^\bullet) + OH^- \rightarrow CO(OH)COCO(O^-) + O_2^{\bullet-} + H_2O$	R(569)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^\bullet) + OH^-$)
$CO(O^-)COC(OH)(OH)(OO^\bullet) \rightarrow CO(OH)COCO(O^-) + HO_2^\bullet$	R(570)	$1.0\ 10^6$			15
$CO(O^-)C(OH)(OH)C(OH)(OH)(OO^\bullet) + OH^- \rightarrow CO(O^-)C(OH)(OH)C(OH)(O^-)(OO^\bullet) + H_2O$		$4.0\ 10^9$			
$CO(O^-)C(OH)(OH)C(OH)(O^-)(OO^\bullet) \rightarrow CO(O^-)C(OH)(OH)CO(OH) + O_2^{\bullet-}$					9
$CO(O^-)C(OH)(OH)C(OH)(OH)(OO^\bullet) + OH^- \rightarrow CO(O^-)C(OH)(OH)CO(OH) + O_2^{\bullet-} + H_2O$	R(571)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^\bullet) + OH^-$)
$CO(O^-)C(OH)(OH)C(OH)(OH)(OO^\bullet) \rightarrow CO(O^-)C(OH)(OH)CO(OH) + HO_2^\bullet$	R(572)	$1.0\ 10^6$			15
Oxidation of 3-hydroxypyruvic acid					63
Pathway 1: $CH_2(OH)C(OH)(OH)CO(OH) + HO^\bullet \rightarrow CH_2(OH)C(OH)(O^\bullet)CO(OH) + H_2O$		$2.5\ 10^8$			BR: 48% - 64
$CH_2(OH)C(OH)(O^\bullet)CO(OH) \rightarrow CH_2(OH)CO(OH) + C^\bullet O(OH)$					6 - 7
$C^\bullet O(OH) + O_2 \rightarrow CO(OH)(OO^\bullet)$		$2.0\ 10^9$			5
Pathway 2: $CH_2(OH)C(OH)(OH)CO(OH) + HO^\bullet \rightarrow C^\bullet H(OH)C(OH)(OH)CO(OH) + H_2O$		$1.9\ 10^8$			BR: 36% - 64
$C^\bullet H(OH)C(OH)(OH)CO(OH) + O_2 \rightarrow CH(OH)(OO^\bullet)C(OH)(OH)CO(OH)$		$2.0\ 10^9$			5
Pathway 3: $CH_2(OH)C(OH)(OH)CO(OH) + HO^\bullet \rightarrow CH_2(O^\bullet)C(OH)(OH)CO(OH) + H_2O$		$8.0\ 10^7$			BR: 16% - 64
$CH_2(O^\bullet)C(OH)(OH)CO(OH) \rightarrow CH_2O + C^\bullet(OH)(OH)CO(OH)$					6 - 7
$C^\bullet(OH)(OH)CO(OH) + O_2 \rightarrow CO(OH)C(OH)(OH)(OO^\bullet)$		$2.0\ 10^9$			5
$CH_2(OH)C(OH)(OH)CO(OH) + HO^\bullet \rightarrow 0.36\ CH(OH)(OO^\bullet)C(OH)(OH)CO(OH) + 0.48\ CH_2(OH)CO(OH) + 0.48\ CO(OH)(OO^\bullet) + 0.16\ CH_2O + 0.16\ CO(OH)C(OH)(OH)(OO^\bullet) + H_2O - O_2$	R(573)	$5.2\ 10^8$			13
$CH_2(OH)C(OH)(OH)CO(OH) + NO_3^\bullet \rightarrow C^\bullet H(OH)C(OH)(OH)CO(OH) + NO_3^- + H^+$		$1.1{\cdot}10^6$			BR: 100%
$C^\bullet H(OH)C(OH)(OH)CO(OH) + O_2 \rightarrow CH(OH)(OO^\bullet)C(OH)(OH)CO(OH)$		$2.0\ 10^9$			5
$CH_2(OH)C(OH)(OH)CO(OH) + NO_3^\bullet \rightarrow CH(OH)(OO^\bullet)C(OH)(OH)CO(OH) + NO_3^- + H^+ - O_2$	R(574)	$1.0\ 10^6$			= k(CH(OH)(OH)CO(OH) + $NO_3^\bullet$) - 2
$CH_2(OH)COCO(O^-) + HO^\bullet \rightarrow C^\bullet H(OH)COCO(O^-) + H_2O$		$5.0\ 10^8$			BR: 100% - 65
$C^\bullet H(OH)COCO(O^-) + O_2 \rightarrow CH(OH)(OO^\bullet)COCO(O^-)$		$2.0\ 10^9$			5
$CH_2(OH)COCO(O^-) + HO^\bullet \rightarrow CH(OH)(OO^\bullet)COCO(O^-) + H_2O - O_2$	R(575)	$5.0\ 10^8$			13
$CH_2(OH)COCO(O^-) + NO_3^\bullet \rightarrow C^\bullet H(OH)COCO(O^-) + NO_3^- + H^+$		$3.1{\cdot}10^6$			BR: 100%
$C^\bullet H(OH)COCO(O^-) + O_2 \rightarrow CH(OH)(OO^\bullet)COCO(O^-)$		$2.0\ 10^9$			5
$CH_2(OH)COCO(O^-) + NO_3^\bullet \rightarrow CH(OH)(OO^\bullet)COCO(O^-) + NO_3^- + H^+ - O_2$	R(576)	$3.1{\cdot}10^6$			= k($CH_2(OH)CHO + NO_3^\bullet$)- 2
$CH(OH)(OO^\bullet)C(OH)(OH)CO(OH) + OH^- \rightarrow CH(O^-)(OO^\bullet)C(OH)(OH)CO(OH) + H_2O$		$4.0\ 10^9$			
$CH(O^-)(OO^\bullet)C(OH)(OH)CO(OH) \rightarrow CO(OH)C(OH)(OH)CHO + O_2^{\bullet-}$					9
$CH(OH)(OO^\bullet)C(OH)(OH)CO(OH) + OH^- \rightarrow CO(OH)C(OH)(OH)CHO + O_2^{\bullet-} + H_2O$	R(577)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^\bullet) + OH^-$)
$CH(OH)(OO^\bullet)C(OH)(OH)CO(OH) \rightarrow CO(OH)C(OH)(OH)CHO + HO_2^\bullet$	R(578)	$1.9\ 10^2$			10
$CH(OH)(OO^\bullet)COCO(O^-) + OH^- \rightarrow CH(O^-)(OO^\bullet)COCO(O^-) + H_2O$		$4.0\ 10^9$			
$CH(O^-)(OO^\bullet)COCO(O^-) \rightarrow CO(O^-)COCHO + O_2^{\bullet-}$					9
$CH(OH)(OO^\bullet)COCO(O^-) + OH^- \rightarrow CO(O^-)COCHO + O_2^{\bullet-} + H_2O$	R(579)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^\bullet) + OH^-$)
$CH(OH)(OO^\bullet)COCO(O^-) \rightarrow CO(O^-)COCHO + HO_2^\bullet$	R(580)	$1.9\ 10^2$			10
Oxidation of pyruvic acid					66
$CH_3COCO(OH) + hv \rightarrow CH_3COCO(OH)^*$	R(581)	Calculated		Reed Harris et al., 2014 ; Griffith et al., 2013	
$CH_3COCO(OH)^* + CH_3C(OH)(OH)CO(OH) \rightarrow CH_3C^\bullet(OH)CO(OH) + CH_3C^\bullet(OH)(OH) + CO_2$					67
$CH_3C^\bullet(OH)CO(OH) + O_2 \rightarrow CH_3C(OH)(OO^\bullet)CO(OH)$		$2.0\ 10^9$			5
$CH_3C^\bullet(OH)(OH) + O_2 \rightarrow CH_3C(OH)(OH)(OO^\bullet)$		$2.0\ 10^9$			5
$CH_3COCO(OH)^* + CH_3C(OH)(OH)CO(OH) \rightarrow CH_3C(OH)(OO^\bullet)CO(OH) + CH_3C(OH)(OH)(OO^\bullet) + CO_2 - 2\ O_2$	R(582)	$1.0\ 10^{10}$		Reed Harris et al., 2014 ; Griffith et al., 2013	
$CH_3COCO(O^-)^* + CH_3C(OH)(OH)CO(OH) \rightarrow CH_3C^\bullet(OH)CO(O^-) + CH_3C^\bullet(OH)(OH) + CO_2$					67

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CH_3C^{\bullet}(OH)CO(O^-) + O_2 \rightarrow CH_3C(OH)(OO^{\bullet})CO(O^-)$		$2.0\ 10^9$			5
$CH_3C^{\bullet}(OH)(OH) + O_2 \rightarrow CH_3C(OH)(OH)(OO^{\bullet})$		$2.0\ 10^9$			5
$CH_3COCO(OH)^* + CH_3C(OH)(OH)CO(O^-) \rightarrow CH_3C(OH)(OO^{\bullet})CO(O^-) + CH_3C(OH)(OH)(OO^{\bullet}) + CO_2 - 2\ O_2$	R(583)	$1.0\ 10^{10}$		Reed Harris et al., 2014 ; Griffith et al., 2013	
$CH_3COCO(OH) + HO^{\bullet} \rightarrow CO(OH)COCH_2(OO^{\bullet}) + H_2O - O_2$	R(584)	$3.2 \cdot 10^8$	1804	Schaefer et al., 2012	
$CH_3COCO(OH) + NO_3^{\bullet} \rightarrow CO(OH)COCH_2(OO^{\bullet}) + NO_3^- + H^+ - O_2$	R(585)	$2.4 \cdot 10^6$	1804	De Semainville et al., 2007	
$CH_3COCO(OH) + H_2O_2 \rightarrow CH_3CO(OH) + CO_2 + H_2O$	R(586)	$1.2\ 10^{-1}$		Schöne and Herrmann, 2014	
$CH_3COCO(O^-) + hv \rightarrow CH_3COCO(O^-)^*$	R(587)	Calculated		Reed Harris et al., 2014 ; Griffith et al., 2013	
$CH_3COCO(O^-) + HO^{\bullet} \rightarrow CO(O^-)COCH_2(OO^{\bullet}) + H_2O - O_2$	R(588)	$7.1 \cdot 10^8$	3007	Schaefer et al., 2012	
$CH_3COCO(O^-) + NO_3^{\bullet} \rightarrow CO(O^-)COCH_2(OO^{\bullet}) + NO_3^- + H^+ - O_2$	R(589)	$1.9 \cdot 10^7$	2887	De Semainville et al., 2007	
$CH_3COCO(O^-) + H_2O_2 \rightarrow CH_3CO(O^-) + CO_2 + H_2O$	R(590)	$7.5\ 10^{-1}$		Schöne and Herrmann, 2014	
Pathway 1: $2\ CO(OH)COCH_2(OO^{\bullet}) \rightarrow 2\ CO(OH)COCHO + H_2O_2$		$1.8\ 10^8$			BR: 45%
Pathway 2: $2\ CO(OH)COCH_2(OO^{\bullet}) \rightarrow CO(OH)COCHO + CH_2(OH)COCO(OH) + O_2$		$8.0\ 10^7$			BR: 20%
Pathway 3: $2\ CO(OH)COCH_2(OO^{\bullet}) \rightarrow 2\ CO(OH)COCH_2(O^{\bullet}) + O_2$		$1.4\ 10^8$			BR: 35%
$CO(OH)COCH_2(O^{\bullet}) \rightarrow CO(OH)COC^{\bullet}H(OH)$					4
$CO(OH)COC^{\bullet}H(OH) + O_2 \rightarrow CH(OH)(OO^{\bullet})COCO(OH)$		$2.0 \cdot 10^9$			5
$2\ CO(OH)COCH_2(OO^{\bullet}) \rightarrow 1.10\ CO(OH)COCHO + 0.20\ CH_2(OH)COCO(OH) + 0.70\ CH(OH)(OO^{\bullet})COCO(OH) + 0.45\ H_2O_2 - 0.15\ O_2$	R(591)	$4.0\ 10^8$			= k(2 $CH_3COCH_2(OO^{\bullet})$) - 8
Pathway 1: $2\ CO(O^-)COCH_2(OO^{\bullet}) \rightarrow 2\ CO(O^-)COCHO + H_2O_2$		$1.8\ 10^8$			BR: 45%
Pathway 2: $2\ CO(O^-)COCH_2(OO^{\bullet}) \rightarrow CO(O^-)COCHO + CH_2(OH)COCO(O^-) + O_2$		$8.0\ 10^7$			BR: 20%
Pathway 3: $2\ CO(O^-)COCH_2(OO^{\bullet}) \rightarrow 2\ CO(O^-)COCH_2(O^{\bullet}) + O_2$		$1.4\ 10^8$			BR: 35%
$CO(O^-)COCH_2(O^{\bullet}) \rightarrow CO(O^-)COC^{\bullet}H(OH)$					4
$CO(O^-)COC^{\bullet}H(OH) + O_2 \rightarrow CH(OH)(OO^{\bullet})COCO(O^-)$		$2.0 \cdot 10^9$			5
$2\ CO(O^-)COCH_2(OO^{\bullet}) \rightarrow 1.10\ CO(O^-)COCHO + 0.20\ CH_2(OH)COCO(O^-) + 0.70\ CH(OH)(OO^{\bullet})COCO(O^-) + 0.45\ H_2O_2 - 0.15\ O_2$	R(592)	$4.0\ 10^8$			= k(2 $CH_3COCH_2(OO^{\bullet})$) - 8
Pathway 1: $CH_3C(OH)(OH)CO(OH) + HO^{\bullet} \rightarrow CH_3C(OH)(O^{\bullet})CO(OH) + H_2O$		$2.7\ 10^8$			BR: 85% - 68
$CH_3C(OH)(O^{\bullet})CO(OH) \rightarrow CH_3CO(OH) + C^{\bullet}O(OH)$					6 - 7
$C^{\bullet}O(OH) + O_2 \rightarrow CO(OH)(OO^{\bullet})$		$2.0\ 10^9$			5
Pathway 2: $CH_3C(OH)(OH)CO(OH) + HO^{\bullet} \rightarrow C^{\bullet}H_2C(OH)(OH)CO(OH) + H_2O$		$5.0\ 10^7$			BR: 15% - 68
$C^{\bullet}H_2C(OH)(OH)CO(OH) + O_2 \rightarrow CO(OH)C(OH)(OH)CH_2(OO^{\bullet})$		$2.0 \cdot 10^9$			5
$CH_3C(OH)(OH)CO(OH) + HO^{\bullet} \rightarrow 0.15\ CO(OH)C(OH)(OH)CH_2(OO^{\bullet}) + 0.85\ CH_3CO(OH) + 0.85\ CO(OH)(OO^{\bullet}) + H_2O - O_2$	R(593)	$3.2\ 10^8$			13
$CH_3C(OH)(OH)CO(OH) + NO_3^{\bullet} \rightarrow C^{\bullet}H_2C(OH)(OH)CO(OH) + NO_3^- + H^+$		$1.1 \cdot 10^6$			BR: 100%
$C^{\bullet}H_2C(OH)(OH)CO(OH) + O_2 \rightarrow CO(OH)C(OH)(OH)CH_2(OO^{\bullet})$		$2.0 \cdot 10^9$			5
$CH_3C(OH)(OH)CO(OH) + NO_3^{\bullet} \rightarrow CO(OH)C(OH)(OH)CH_2(OO^{\bullet}) + NO_3^- + H^+ - O_2$	R(594)	$1.0 \cdot 10^6$			= k(CH(OH)(OH)CO(OH) + $NO_3^{\bullet}$) - 2
Pathway 1: $2\ CO(OH)C(OH)(OH)CH_2(OO^{\bullet}) \rightarrow 2\ CO(OH)C(OH)(OH)CHO + H_2O_2$		$5.0\ 10^7$			BR: 50%
Pathway 2: $2\ CO(OH)C(OH)(OH)CH_2(OO^{\bullet}) \rightarrow CO(OH)C(OH)(OH)CHO + CH_2(OH)C(OH)(OH)CO(OH) + O_2$		$3.3\ 10^7$			BR: 33%
Pathway 3: $2\ CO(OH)C(OH)(OH)CH_2(OO^{\bullet}) \rightarrow 2\ CH_2(O^{\bullet})C(OH)(OH)CO(OH) + O_2$		$1.7\ 10^7$			BR: 17%
$CH_2(O^{\bullet})C(OH)(OH)CO(OH) \rightarrow CH_2O + C^{\bullet}(OH)(OH)CO(OH)$					6 - 7

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$C^{\bullet}(OH)(OH)CO(OH) + O_2 \rightarrow CO(OH)C(OH)(OH)(OO^{\bullet})$		$2.0 \cdot 10^9$			5
$2\ CO(OH)C(OH)(OH)CH_2(OO^{\bullet}) \rightarrow 1.33\ CO(OH)C(OH)(OH)CHO + 0.33\ CH_2(OH)C(OH)(OH)CO(OH) + 0.34\ CH_2O + 0.34\ CO(OH)C(OH)(OH)(OO^{\bullet}) + 0.50\ H_2O_2 + 0.16\ O_2$	R(595)	$1.0\ 10^8$			= k(2 $CH_2(OH)CH_2(OO^{\bullet})$) - 8
Oxidation of acrolein (from C4)					69
$CH_2{=}CHCHO + H_2O \rightarrow CH_2(OH)CH_2CHO$	R(596)	$9.4\ 10^{-6}$		Pressman and Lucas, 1942	
$CH_2(OH)CH_2CHO \rightarrow CH_2{=}CHCHO + H_2O$	R(597)	$7.8\ 10^{-7}$		Pressman and Lucas, 1942	
$CH_2{=}CHCHO + HO^{\bullet} \rightarrow CH_2(OH)C^{\bullet}HCHO$		$7.0\ 10^9$			BR: 100% - 70
$CH_2(OH)C^{\bullet}HCHO + O_2 \rightarrow CH_2(OH)CH(OO^{\bullet})CHO$		$2.0\ 10^9$			5
$CH_2{=}CHCHO + HO^{\bullet} \rightarrow CH_2(OH)CH(OO^{\bullet})CHO - O_2$	R(598)	$7.0\ 10^9$		Lilie and Henglein, 1970	
Pathway 1: $2\ CH_2(OH)CH(OO^{\bullet})CHO \rightarrow 2\ CH_2(OH)COCHO + H_2O_2$		$5.0\ 10^7$			BR: 50%
Pathway 2: $2\ CH_2(OH)CH(OO^{\bullet})CHO \rightarrow CH_2(OH)COCHO + CH_2(OH)CH(OH)CHO + O_2$		$3.3\ 10^7$			BR: 33%
Pathway 3: $2\ CH_2(OH)CH(OO^{\bullet})CHO \rightarrow 2\ CH_2(OH)CH(O^{\bullet})CHO + O_2$		$1.7\ 10^7$			BR: 17%
$CH_2(OH)CH(O^{\bullet})CHO \rightarrow 0.50\ C^{\bullet}H_2(OH) + 0.50\ CHOCHO + 0.50\ C^{\bullet}HO + 0.50\ CH_2(OH)CHO$					6 - 7
$C^{\bullet}H_2(OH) + O_2 \rightarrow CH_2(OH)(OO^{\bullet})$		$2.0 \cdot 10^9$			5
$C^{\bullet}HO + O_2 \rightarrow CHO(OO^{\bullet})$		$2.0\ 10^9$			5
$2\ CH_2(OH)CH(OO^{\bullet})CHO \rightarrow 1.33\ CH_2(OH)COCHO + 0.33\ CH_2(OH)CH(OH)CHO + 0.17\ CHOCHO + 0.17\ CH_2(OH)CHO + 0.17\ CH_2(OH)(OO^{\bullet}) + 0.17\ CHO(OO^{\bullet}) + 0.5\ H_2O_2 + 0.16\ O_2$	R(599)	$1.0\ 10^8$			= k(2 $CH_2(OH)CH_2(OO^{\bullet})$) - 8
Pathway 1: $2\ CH_2(OH)CH(OO^{\bullet})CH(OH)(OH) \rightarrow 2\ CH_2(OH)COCH(OH)(OH) + H_2O_2$		$5.0\ 10^7$			BR: 50%
Pathway 2: $2\ CH_2(OH)CH(OO^{\bullet})CH(OH)(OH) \rightarrow CH_2(OH)COCH(OH)(OH) + CH_2(OH)CH(OH)CH(OH)(OH) + O_2$		$3.3\ 10^7$			BR: 33%
Pathway 3: $2\ CH_2(OH)CH(OO^{\bullet})CH(OH)(OH) \rightarrow 2\ CH_2(OH)CH(O^{\bullet})CH(OH)(OH) + O_2$		$1.7\ 10^7$			BR: 17%
$CH_2(OH)CH(O^{\bullet})CH(OH)(OH) \rightarrow 0.50\ C^{\bullet}H_2(OH) + 0.50\ CHOCH(OH)(OH) + 0.50\ C^{\bullet}H(OH)(OH) + 0.50\ CH_2(OH)CHO$					6 - 7
$C^{\bullet}H_2(OH) + O_2 \rightarrow CH_2(OH)(OO^{\bullet})$		$2.0 \cdot 10^9$			5
$C^{\bullet}H(OH)(OH) + O_2 \rightarrow CH(OH)(OH)(OO^{\bullet})$		$2.0\ 10^9$			5
$2\ CH_2(OH)CH(OO^{\bullet})CH(OH)(OH) \rightarrow 1.33\ CH_2(OH)COCH(OH)(OH) + 0.33\ CH_2(OH)CH(OH)CH(OH)(OH) + 0.17\ CHOCH(OH)(OH) + 0.17\ CH_2(OH)CHO + 0.17\ CH_2(OH)(OO^{\bullet}) + 0.17\ CH(OH)(OH)(OO^{\bullet}) + 0.50\ H_2O_2 + 0.16\ O_2$	R(600)	$1.0\ 10^8$			= k(2 $CH_2(OH)CH_2(OO^{\bullet})$) - 8
Oxidation of 2,3-dihydroxypropanal (or glyceraldehyde)					71
Pathway 1: $CH_2(OH)CH(OH)CH(OH)(OH) + HO^{\bullet} \rightarrow C^{\bullet}H(OH)CH(OH)CH(OH)(OH) + H_2O$		$8.3\ 10^8$			BR: 49% - 72
$C^{\bullet}H(OH)CH(OH)CH(OH)(OH) + O_2 \rightarrow CH(OH)(OH)CH(OH)CH(OH)(OO^{\bullet})$		$2.0 \cdot 10^9$			5
Pathway 2: $CH_2(OH)CH(OH)CH(OH)(OH) + HO^{\bullet} \rightarrow CH_2(OH)CH(OH)CH(OH)(O^{\bullet}) + H_2O$		$4.6\ 10^8$			BR: 27% - 72
$CH_2(OH)CH(OH)CH(OH)(O^{\bullet}) \rightarrow CH_2(OH)C^{\bullet}H(OH) + CHO(OH)$					6 - 7
$CH_2(OH)C^{\bullet}H(OH) + O_2 \rightarrow CH_2(OH)CH(OH)(OO^{\bullet})$		$2.0 \cdot 10^9$			5
Pathway 3: $CH_2(OH)CH(OH)CH(OH)(OH) + HO^{\bullet} \rightarrow CH_2(OH)CH(OH)C^{\bullet}(OH)(OH) + H_2O$		$4.1\ 10^8$			BR: 24% - 72
$CH_2(OH)CH(OH)C^{\bullet}(OH)(OH) + O_2 \rightarrow CH_2(OH)CH(OH)C(OH)(OH)(OO^{\bullet})$		$2.0 \cdot 10^9$			5
$CH_2(OH)CH(OH)CH(OH)(OH) + HO^{\bullet} \rightarrow 0.49\ CH(OH)(OH)CH(OH)CH(OH)(OO^{\bullet}) + 0.27\ CHO(OH) + 0.27\ CH_2(OH)CH(OH)(OO^{\bullet}) + 0.24\ CH_2(OH)CH(OH)C(OH)(OH)(OO^{\bullet}) + H_2O - O_2$	R(601)	$1.7\ 10^9$			13
Pathway 1: $CH_2(OH)CH(OH)CH(OH)(OH) + NO_3^{\bullet} \rightarrow C^{\bullet}H(OH)CH(OH)CH(OH)(OH) + NO_3^- + H^+$		$7.4\ 10^5$			BR: 67%
$C^{\bullet}H(OH)CH(OH)CH(OH)(OH) + O_2 \rightarrow CH(OH)(OH)CH(OH)CH(OH)(OO^{\bullet})$		$2.0 \cdot 10^9$			5
Pathway 2: $CH_2(OH)CH(OH)CH(OH)(OH) + NO_3^{\bullet} \rightarrow CH_2(OH)CH(OH)C^{\bullet}(OH)(OH) + NO_3^- + H^+$		$3.6\ 10^5$			BR: 33%
$CH_2(OH)CH(OH)C^{\bullet}(OH)(OH) + O_2 \rightarrow CH_2(OH)CH(OH)C(OH)(OH)(OO^{\bullet})$		$2.0 \cdot 10^9$			5
$CH_2(OH)CH(OH)CH(OH)(OH) + NO_3^{\bullet} \rightarrow 0.67\ CH(OH)(OH)CH(OH)CH(OH)(OO^{\bullet}) + 0.33\ CH_2(OH)CH(OH)C(OH)(OH)(OO^{\bullet}) + NO_3^- + H^+ - O_2$	R(602)	$1.1\ 10^6$			= k($CH_2(OH)CH(OH)(OH)$ + $NO_3^{\bullet}$) - 2
$CH(OH)(OH)CH(OH)CH(OH)(OO^{\bullet}) + OH^- \rightarrow CH(OH)(OH)CH(OH)CH(O^-)(OO^{\bullet}) + H_2O$		$4.0\ 10^9$			
$CH(OH)(OH)CH(OH)CH(O^-)(OO^{\bullet}) \rightarrow CHOCH(OH)CH(OH)(OH) + O_2^{\bullet-}$					9

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CH(OH)(OH)CH(OH)CH(OH)(OO^{\bullet})$ + OH^- → $CHOCH(OH)CH(OH)(OH)$ + $O_2^{\bullet-}$ + H_2O	R(603)	4.0 10^9			= k($CH_3CH(OH)(OO^{\bullet})$ + OH^-)
$CH(OH)(OH)CH(OH)CH(OH)(OO^{\bullet})$ → $CHOCH(OH)CH(OH)(OH)$ + $HO_2^{\bullet}$	R(604)	1.9 10^2			10
$CH_2(OH)CH(OH)C(OH)(OH)(OO^{\bullet})$ + OH^- → $CH_2(OH)CH(OH)C(OH)(O^-)(OO^{\bullet})$ + H_2O		4.0 10^9			
$CH_2(OH)CH(OH)C(OH)(O^-)(OO^{\bullet})$ → $CH_2(OH)CH(OH)CO(OH)$ + $O_2^{\bullet-}$					9
$CH_2(OH)CH(OH)C(OH)(OH)(OO^{\bullet})$ + OH^- → $CH_2(OH)CH(OH)CO(OH)$ + $O_2^{\bullet-}$ + H_2O	R(605)	4.0 10^9			= k($CH_3CH(OH)(OO^{\bullet})$ + OH^-)
$CH_2(OH)CH(OH)C(OH)(OH)(OO^{\bullet})$ → $CH_2(OH)CH(OH)CO(OH)$ + $HO_2^{\bullet}$	R(606)	1.0 10^6			15
Oxidation of hydroxypropanedial					73
Pathway 1: $CH(OH)(OH)CH(OH)CH(OH)(OH)$ + $HO^{\bullet}$ → $CH(OH)(OH)CH(OH)CH(OH)(O^{\bullet})$ + H_2O		8.6 10^8			BR: 54% - 74
$CH(OH)(OH)CH(OH)CH(OH)(O^{\bullet})$ → $CH(OH)(OH)C^{\bullet}H(OH)$ + CHO(OH)					6 - 7
$CH(OH)(OH)C^{\bullet}H(OH)$ + O_2 → $CH(OH)(OO^{\bullet})CH(OH)(OH)$		2.0·10^9			5
Pathway 2: $CH(OH)(OH)CH(OH)CH(OH)(OH)$ + $HO^{\bullet}$ → $CH(OH)(OH)CH(OH)C^{\bullet}(OH)(OH)$ + H_2O		7.4 10^8			BR: 46% - 74
$CH(OH)(OH)CH(OH)C^{\bullet}(OH)(OH)$ + O_2 → $CH(OH)(OH)CH(OH)C(OH)(OH)(OO^{\bullet})$		2.0·10^9			5
$CH(OH)(OH)CH(OH)CH(OH)(OH)$ + $HO^{\bullet}$ → 0.54 CHO(OH) + 0.54 $CH(OH)(OO^{\bullet})CH(OH)(OH)$ + 0.46 $CH(OH)(OH)CH(OH)C(OH)(OH)(OO^{\bullet})$ + H_2O - O_2	R(607)	1.6 10^9			13
$CH(OH)(OH)CH(OH)CH(OH)(OH)$ + $NO_3^{\bullet}$ → $CH(OH)(OH)CH(OH)C^{\bullet}(OH)(OH)$ + NO_3^- + H^+		1.1 10^6			BR: 100%
$CH(OH)(OH)CH(OH)C^{\bullet}(OH)(OH)$ + O_2 → $CH(OH)(OH)CH(OH)C(OH)(OH)(OO^{\bullet})$		2.0·10^9			5
$CH(OH)(OH)CH(OH)CH(OH)(OH)$ + $NO_3^{\bullet}$ → $CH(OH)(OH)CH(OH)C(OH)(OH)(OO^{\bullet})$ + NO_3^- + H^+ - O_2	R(608)	1.1 10^6			= k($CH_2(OH)CH(OH)(OH)$ + $NO_3^{\bullet}$) - 2
$CH(OH)(OH)CH(OH)C(OH)(OH)(OO^{\bullet})$ + OH^- → $CH(OH)(OH)CH(OH)C(OH)(O^-)(OO^{\bullet})$ + H_2O		4.0 10^9			
$CH(OH)(OH)CH(OH)C(OH)(O^-)(OO^{\bullet})$ → $CH(OH)(OH)CH(OH)CO(OH)$ + $O_2^{\bullet-}$					9
$CH(OH)(OH)CH(OH)C(OH)(OH)(OO^{\bullet})$ + OH^- → $CH(OH)(OH)CH(OH)CO(OH)$ + $O_2^{\bullet-}$ + H_2O	R(609)	4.0 10^9			= k($CH_3CH(OH)(OO^{\bullet})$ + OH^-)
$CH(OH)(OH)CH(OH)C(OH)(OH)(OO^{\bullet})$ → $CH(OH)(OH)CH(OH)CO(OH)$ + $HO_2^{\bullet}$	R(610)	1.0 10^6			15

1 - Branching ratios are calculated by the SAR from Monod and Doussin (2013): 16% for CH_3, 16% for CH_2, 65% for $CH_2(OH)$ and 3% for OH. The 3 first pathways are considered corresponding to 97% of the total reactivity. They have been scaled to 15/15/70%.

2 - 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.

3 - We assume the same branching ratio than for the self reaction of $CH_3CH_2(OO^{\bullet})$, *i.e.*, 80/20%. The "alkoxy" pathway (pathway 2) is more likely to occur (80%).

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

5 - 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.

6 - 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.

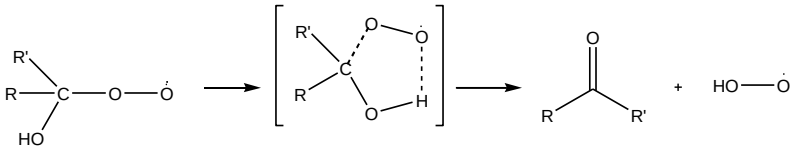
7 - For alkoxyl radical, we assume an electron transfer reaction. When an oxygenated functional group is in β-position, we assume a fragmentation of the corresponding c-c bond. When there are two oxygenated function in β-position, we assume that the fragmentation occurs in priority on the C-CO(OH) bond.

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

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

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

10 - 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}.

11 - The hydration constant is calculated with the GROMHE method; K_h = 2.49. We consider the reactivity of the hydrated and non-hydrated forms since the hydrated form represents 71% of the total species.

12 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 60% for CHO, 36% for $CH_2(OH)$, 2% for (OH) and 2% for CH_2. The 2 first pathways are considered corresponding to 96% of the total reactivity. They have been scaled to 62/38%.

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

14 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 27% for H on CH(OH)(OH), 55% for CH_2 on $CH_2(OH)$, 3% for (OH) on $CH_2(OH)$, 2% for CH_2 and 13% for OH on CH(OH)(OH). The 2 first pathways are considered corresponding to 82% of the total reactivity. They have been scaled to 33/67%.

15 - 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}.

16 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 42% for CH_2, 38% for CH on CH(OH), 10% for CH_3, 5% for OH on CH2(OH) and 5% for OH on CH(OH). The 2 first pathways are considered corresponding to 80% of the total reactivity. They have been scaled to 60/40%.

17 - The hydration constant is calculated with the GROMHE method; K_h = 6.1. We only consider the reactivity of the hydrated form since the hydrated form represents 86% of the total species.

18 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 29% for OH on CH(OH)(OH), 28% for CH on CH(OH)(OH), 22% for CH on CH(OH), 14% for CH_3 and 7% for OH on CH(OH). The 3 first pathways are considered corresponding to 79% of the total reactivity. They have been scaled to 37/35/28%.

19 - The hydration constant is calculated with the GROMHE method. The K_h for the mono-hydrated and the di-hydrated form is equal to 22 and 100, respectively. The di-hydrated form represent 81% of the total species. We only consider the reactivity of di-hydrated form.

20 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 32% for OH on CH(OH)(OH), 66% for CH on CH(OH)(OH), 2% for CH_2. The 2 first pathways are considered corresponding to 98% of the total reactivity. They have been scaled to 33/67%.

21 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 91% for CH_2 on $CH_2(OH)$, 7% for on OH $CH_2(OH)$ and 2% for CH_2.The first pathway is considered corresponding to 91% of the total reactivity. It has been scaled to 100%.

22 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 82% for CH_2 on $CH_2(OH)$, 4% for OH on $CH_2(OH)$, 3% for CH_2 and 11% 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%.

23 - Branching ratios are determined by Padmaja and Huie (1993): 87% for CH on CH(OH) and 13% for CH_3. Branching ratios calculated by the SAR from Doussin and Monod (2013) are close: 78% for CH on CH(OH) and 18% for CH_3, and 4% for OH on CH(OH). 4%).

24 - The hydration constant is equal to 0.87. The hydrated form represents 47% of the total species. We consider the reactivity of the hydrated and non-hydrated forms.

25 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 82% for CHO, 12% for CH_3, 6% for CH_2. The 2 first pathways are considered corresponding to 94% of the total reactivity. They have been scaled to 87/13%.

26 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 47% for CH on CH(OH)(OH), 23% for CH_3, 21% for OH on CH(OH)(OH), 9% for CH_2. The 3 first pathways are considered corresponding to 91% of the total reactivity. They have been scaled to 52/25/23%.

27 - The mono-hydrated form $CH_3COCH(OH)(OH)$ and the di-hydrated form represent respectively 66% and 32% of the total species (the non-hydrated + the two mono-hydrated + the di-hydrated forms). We only consider the reactivity of this mono-hydrated form and of the di-hydrated form.

28 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 57% for OH on CH(OH)(OH), 29% for CH on CH(OH)(OH), 14% for CH_3.The 3 pathways are considered corresponding to 100% of the total reactivity.
29 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 41% for OH on C(OH)(OH), 37% for OH on CH(OH)(OH), 15% for CH on CH(OH)(OH) and 7% for CH_3.The 2 first pathways are considered corresponding to 78% of the total reactivity. They have been scaled to 53/47%
30 - The non-hydrated form and the mono-hydrated form on the ketone function are negligible. The mono-hydrated form $CH_2(OH)COCH(OH)(OH)$ and the di-hydrated form $CH_2(OH)C(OH)(OH)CH(OH)(OH)$ are the main forms (respectively 18% and 81% of the total species). The reactivity of these two forms are considered.
31 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 37% for OH on CH(OH)(OH), 36% for CH_2 on $CH_2(OH)$, 18% for CH on CH(OH)(OH), 9% for (OH) on $CH_2(OH)$. The 3 first pathways are considered corresponding to 91% of the total reactivity. They have been scaled to 41/40/19%.
32 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 31% for OH on C(OH)(OH), 29% for OH on CH(OH)(OH), 22% for CH_2 on $CH_2(OH)$, 11% for CH on CH(OH)(OH) and 7% for OH on $CH_2(OH)$. The 3 first pathways are considered corresponding to 82% of the total reactivity. They have been scaled to 38/35/27%.
33 - The tri-hydrated form is dominant (97%). We only consider its reactivity. This compound is also produced under its mono-hydrated form in the oxidation of methyl glyoxal and 2-oxo,3-hydroxy propanal.
34 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 54% for OH on CH(OH)(OH), 27% for OH on C(OH)(OH), 19% for CH on CH(OH)(OH). The 2 first pathways are considered corresponding to 81% of the total reactivity. They have been scaled to 67/33%.
35 - $K_h = 2.0\ 10^{-3}$ (Bell, 1966). The hydrated form is not significant. Only the reactivity of the non-hydrated is considered. The equilibrium is not considered because the hydrated form cannot be produced through reactivity.
36 - $K_h = 7.0\ 10^{-2}$ estimated by GROMHE. The hydrated form is not significant. Only the reactivity of the non-hydrated is considered. The equilibrium is not considered because the hydrated form cannot be produced through reactivity.
37 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 16% for CH_3, 69% for CH_2 on $CH_2(OH)$, 15% for OH on $CH_2(OH)$. The 3 first pathways are considered corresponding to 100% of the total reactivity.
38 - $K_h = 0.32$ estimated by GROMHE. The hydrated form represent 24% of the total species. Only the reactivity of the non-hydrated is considered.
39 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 81% for CH_2, 19% for OH on $CH_2(OH)$. The first pathway is considered corresponding to 81% of the total reactivity. The branching ratio is scaled to 100%.
40 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 17% for CH_2, 83% for CH_3. The two pathways are considered corresponding to 100% of the total reactivity.
41 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 28% for CH_2, 72% for CH_3. The two pathways are considered corresponding to 100% of the total reactivity.
42 - The hydration constant of the acid form $CO(OH)CH_2CHO$ is equal to 10 by GROMHE. The hydrated form represents 91% of the total species. We only consider the reactivity of the hydrated form.
For $CO(O^-)CH_2CHO$, the hydration constant is 1.4 estimated by GROMHE. The hydrated form represents 58% of the total species. We consider the reactivity of the hydrated and non-hydrated forms.
43 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 57% for CH on CH(OH)(OH), 42% for OH on CH(OH)(OH) and 1% for CH_2. The two pathways are considered corresponding to 99% of the total reactivity. They have been scaled to 58/42%.
44 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 59% for CH on CH(OH)(OH), 25% for OH on CH(OH)(OH), 16% for the electron-transfer on $CO(O^-)$. The 3 pathways are considered corresponding to 100% of the total reactivity.
45 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 91% for CHO, 8% for the electron-transfer on $CO(O^-)$, 1% for CH_2. The first pathway is considered corresponding to 91% of the total reactivity.
46 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 6% for CH_2 and 94% for the electron-transfer on $CO(O^-)$. The 2 pathways are considered corresponding to 100% of the total reactivity.
47 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 6% for CH_2 and 94% for the electron-transfer on $CO(O^-)$. The 2 pathways are considered corresponding to 100% of the total reactivity.
48 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 11% for CH on CH(OH) and 89% for OH on CH(OH). The 2 pathways are considered corresponding to 100% of the total reactivity.
49 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 11% for CH on CH(OH), 43% for OH on CH(OH) and 46% for the electron-transfer on $CO(O^-)$. The 3 pathways are considered corresponding to 100% of the total reactivity.
50 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 13% for CH on CH(OH), 27% for OH on CH(OH) and 60% for the electron-transfer on $CO(O^-)$. The 3 pathways are considered corresponding to 100% of the total reactivity.
51 - The hydration constant of the acid form CO(OH)COCO(OH) is measured at 100 by Le Henaff (1968). We only consider the reactivity of the hydrated form. For the mono-anion $CO(OH)COCO(O^-)$, the hydration constant is equal to 2.4; the hydrated form represents 71% of the total species. Therefore, we consider the reactivity of the hydrated and non-hydrated forms. For the di-anion $CO(O^-)COCO(O^-)$, the hydration constant is low and estimated at $1.6\ 10^{-2}$ by GROMHE. We only consider the reactivity of the non-hydrated form.
52 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 34% for CH on CH(OH), 44% for CH_3 and 22% for OH on CH(OH). The 3 pathways are considered corresponding to 100% of the total reactivity.
53 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 42% for CH on CH(OH), 28% for CH_3, 14% for OH on CH(OH) and 16% for the electron-transfer on $CO(O^-)$. The 4 pathways are considered corresponding to 100% of the total reactivity.
54 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 72% for CH_2, 13% for OH on $CH_2(OH)$, 9% for OH on CH(OH) and 6% for CH on CH(OH). The two pathways are considered corresponding to 85% of the total reactivity. They have been scaled to 85/15%.
55 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 66% for CH_2, 10% for CH on CH(OH), 9% for the electron-transfer on $CO(O^-)$, 8% for OH on CH(OH) and 7% OH on $CH_2(OH)$. The two pathways are considered corresponding to 76% of the total reactivity. They have been scaled to 87/13%.

56 - K_h= 46 for the acid form CHOCH(OH)CO(OH) estimated by GROMHE. The hydrated form represent 98% of the total species. Only the reactivity of the hydrated form is considered. K_h = 6.1 for the anion CHOCH(OH)CO(O-) estimated by GROMHE. The hydrated form represent 86% of the total species. Only the reactivity of the hydrated is considered.
57 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 57% for OH on CH(OH)(OH), 33% for CH on CH(OH)(OH), 8% for OH on CH(OH), 2% for CH on CH(OH). The two pathways are considered corresponding to 90% of the total reactivity. They have been scaled to 63/37%.
58 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 37% for OH on CH(OH)(OH), 38% for CH on CH(OH)(OH), 10% for the electron-transfer on $CO(O^-)$, 10% for OH on CH(OH), 5% for CH on CH(OH). The two pathways are considered corresponding to 75% of the total reactivity. They have been scaled to 49/51%.
59 - For the acid form, the di-hydrate is the main form (99%) due to its high K_h ($1.3\ 10^5$ calculated with GROMHE). Only the reactivity of the di-hydrated form is considered. For the anionic form, the mono-hydrate $CO(O^-)$COCH(OH)(OH) is dominant (49%) together with the di-hydrated form (49%). Only the reactivity of the di-hydrated form and of one of the mono-hydrated form ($CO(O^-)$COCH(OH)(OH)) is considered.
60 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 52% for OH on CH(OH)(OH), 35% for OH on C(OH)(OH), 13% for CH on CH(OH)(OH). The three pathways are considered corresponding to 100% of the total reactivity.
61 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 60% for OH on CH(OH)(OH), 32% for CH on CH(OH)(OH), 8% for the electron-transfer on $CO(O^-)$. The two pathways are considered corresponding to 92% of the total reactivity. They have been scaled to 65/35%.
62 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 37% for OH on CH(OH)(OH), 43% for OH on C(OH)(OH), 16% for CH on CH(OH)(OH) and 4% for the electron-transfer on $CO(O^-)$. The three first pathways are considered corresponding to 96% of the total reactivity. They have been scaled to 39/45/16%.
63 - For the acid form, the hydrated form is the main form (92%) due to its high K_h (10.8 calculated with GROMHE). Only the reactivity of the hydrated form is considered. For the anionic form, the hydrated form is negligible (7%). Only the reactivity of the non-hydrated form is considered.
64 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 48% for OH on C(OH)(OH), 36% for CH_2 on CH_2(OH), 16% for OH on CH_2(OH). The three pathways are considered corresponding to 100% of the total reactivity.
65 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 75% for CH_2 on CH_2(OH), 15% for OH on CH_2(OH) and 10% for the electron-transfer on $CO(O^-)$. The first pathway is considered corresponding to 75% of the total reactivity. This has been scaled to 100%.
66 - For the acid form, K_h = 1.5 following Poker et al. (1969). The hydrated form represents 60% of the total species. We consider the reactivity of the hydrated and non-hydrated forms. For the anion, $K_h = 5.7\ 10^{-2}$ from Poker et al. (1969). Therefore, we only consider the reactivity of the non-hydrated form.
67 - We suppose this reaction to be non limiting.
68 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 85% for OH on C(OH)(OH), 15% for CH_3. The two pathways are considered corresponding to 100% of the total reactivity.
69 - Acrolein establishes a very slow equilibrium with 3-hydroxypropionaldehyde following Pressmann and Lucas (1942).
70 - The addition of OH on the internal carbon of the C=C bond is highly favored (>80%). Von Sonntag et Schuchmann (1997) have shown that for ethene, this pathway is the most efficient.
71 - K_h = 11.2 estimated by GROMHE. The hydrated form represent the main form of the total species. Only the reactivity of the hydrated form is considered.
72 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 41% for CH_2, 22% for OH on CH(OH)(OH), 20% for CH on CH(OH)(OH), 7% for CH on CH(OH), 5% for OH on CH_2(OH) and 5% for OH on CH(OH). The three first pathways are considered corresponding to 83% of the total reactivity. They have been scaled to 49/27/24%.
73 - The hydration constant is calculated with the GROMHE method. The K_h for the mono-hydrated and the di-hydrated form is equal to 98 and $2.0\ 10^3$, respectively. The di-hydrated form represent 95% of the total species. We only consider the reactivity of di-hydrated form.
74 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 49% for OH on CH(OH)(OH), 42% for CH on CH(OH)(OH), 5% for OH on CH(OH), 3% for CH on CH(OH). The two first pathways are considered corresponding to 91% of the total reactivity. They have been scaled to 54/46%.

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Equilibria

Species		K_a or K_h	-ΔH/R (K)	References	Notes
C3 compounds					
3-hydroxypropionaldehyde					
$CH_2(OH)CH_2CHO + H_2O \leftrightarrow CH_2(OH)CH_2CH(OH)(OH)$	T(48)	2.5		Estimated with GROMHE	
$CH_2(OH)CH_2CO(OO^\bullet) + H_2O \leftrightarrow CH_2(OH)CH_2C(OH)(OH)(OO^\bullet)$	T(49)	2.5			1 = $K_h(CH_2(OH)CH_2CHO/CH_2(OH)CH_2CH(OH)(OH))$
$CHOCH_2CH(OH)(OO^\bullet) + H_2O \leftrightarrow CH(OH)(OH)CH_2CH(OH)(OO^\bullet)$	T(50)	2.5			1 = $K_h(CH_2(OH)CH_2CHO/CH_2(OH)CH_2CH(OH)(OH))$
2-hydroxypropionaldehyde					
$CH_3CH(OH)CHO + H_2O \leftrightarrow CH_3CH(OH)CH(OH)(OH)$	T(51)	6.1		Estimated with GROMHE	
$CH_3CH(OH)CO(OO^\bullet) + H_2O \leftrightarrow CH_3CH(OH)C(OH)(OH)(OO^\bullet)$	T(52)	$1.0\ 10^{-3}$			2
$CH_3C(OH)(OO^\bullet)CHO + H_2O \leftrightarrow CH_3C(OH)(OO^\bullet)CH(OH)(OH)$	T(53)	6.1			1 = $K_h(CH_3CH(OH)CHO/CH_3CH(OH)CH(OH)(OH))$
Propanedial					
$CHOCH_2CHO + H_2O \leftrightarrow CHOCH_2CH(OH)(OH)$	T(54)	$2.2\ 10^{1}$		Estimated with GROMHE	
$CHOCH_2CHO + 2\ H_2O \leftrightarrow CH(OH)(OH)CH_2CH(OH)(OH)$	T(55)	$1.0\ 10^{2}$		Estimated with GROMHE	
$CHOCH_2CO(OO^\bullet) + H_2O \leftrightarrow CHOCH_2C(OH)(OH)(OO^\bullet)$	T(56)	$1.0\ 10^{-3}$			2
$CHOCH_2CO(OO^\bullet) + H_2O \leftrightarrow CH(OH)(OH)CH_2CO(OO^\bullet)$	T(57)	$2.2\ 10^{1}$			1 = $K_h(CHOCH_2CHO/CHOCH_2CH(OH)(OH)) - 3$
$CHOCH_2CO(OO^\bullet) + 2\ H_2O \leftrightarrow CH(OH)(OH)CH_2C(OH)(OH)(OO^\bullet)$	T(58)	$1.0\ 10^{2}$			1 = $K_h(CHOCH_2CHO/CH(OH)(OH)CH_2CH(OH)(OH))$
3-hydroxypropionic acid					
$CH_2(OH)CH_2CO(OH) \leftrightarrow CH_2(OH)CH_2CO(O^-) + H^+$	T(59)	$3.1\ 10^{-5}$		Lide, 2005	
$CH(OH)(OO^\bullet)CH_2CO(OH) \leftrightarrow CH(OH)(OO^\bullet)CH_2CO(O^-) + H^+$	T(60)	$3.1\ 10^{-5}$			4 = $K_a(CH_2(OH)CH_2CO(OH)/CH_2(OH)CH_2CO(O^-))$
Propionaldehyde					
$CH_3CH_2CHO + H_2O \leftrightarrow CH_3CH_2CH(OH)(OH)$	T(61)	0.87	2715	Socrates, 1969	
$CH_3CH_2CO(OO^\bullet) + H_2O \leftrightarrow CH_3CH_2C(OH)(OH)(OO^\bullet)$	T(62)	0.87			1 = $K_h(CH_3CH_2CHO/CH_3CH_2CH(OH)(OH))$
$CHOCH_2CH_2(OO^\bullet) + H_2O \leftrightarrow CH(OH)(OH)CH_2CH_2(OO^\bullet)$	T(63)	0.87			1 = $K_h(CH_3CH_2CHO/CH_3CH_2CH(OH)(OH))$
Methylglyoxal					
$CH_3COCHO + H_2O \leftrightarrow CH_3COCH(OH)(OH)$	T(64)	$1.8\ 10^{3}$		Wasa and Musha, 1970	5
$CH_3COCHO + H_2O \leftrightarrow CH_3C(OH)(OH)CHO$	T(65)	$5.4\ 10^{1}$		Wasa and Musha, 1970	5
$CH_3COCHO + 2\ H_2O \leftrightarrow CH_3C(OH)(OH)CH(OH)(OH)$	T(66)	$8.7\ 10^{2}$		Wasa and Musha, 1970	5

Species		K_a or K_h	-ΔH/R (K)	References	Notes
$CH_3COCO(OO^\bullet) + H_2O \leftrightarrow CH_3COC(OH)(OH)(OO^\bullet)$	T(67)	$1.0\ 10^{-3}$			2
$CH_3COCO(OO^\bullet) + H_2O \leftrightarrow CH_3C(OH)(OH)CO(OO^\bullet)$	T(68)	$5.4\ 10^{1}$			1 = $K_h(CH_3COCHO/CH_3C(OH)(OH)CHO)$
$CH_3COCO(OO^\bullet) + 2\ H_2O \leftrightarrow CH_3C(OH)(OH)C(OH)(OH)(OO^\bullet)$	T(69)	$8.7\ 10^{2}$			1 = $K_h(CH_3COCHO/CH_3C(OH)(OH)CH(OH)(OH))$
$CHOCOCH_2(OO^\bullet) + H_2O \leftrightarrow CH(OH)(OH)COCH_2(OO^\bullet)$	T(70)	$1.8\ 10^{3}$			1 = $K_h(CH_3COCHO/CH_3COCH(OH)(OH))$
$CHOCOCH_2(OO^\bullet) + H_2O \leftrightarrow CHOC(OH)(OH)CH_2(OO^\bullet)$	T(71)	$5.4\ 10^{1}$			1 = $K_h([CH_3COCHO/CH_3C(OH)(OH)CHO])$
$CHOCOCH_2(OO^\bullet) + 2\ H_2O \leftrightarrow CH(OH)(OH)C(OH)(OH)CH_2(OO^\bullet)$	T(72)	$8.7\ 10^{2}$			1 = $K_h([CH_3COCHO/CH_3C(OH)(OH)CH(OH)(OH)])$
2-oxo, 3-hydroxypropanal					
$CH_2(OH)COCHO + H_2O \leftrightarrow CH_2(OH)COCH(OH)(OH)$	T(73)	$2.0\ 10^{2}$		Estimated with GROMHE	
$CH_2(OH)COCHO + H_2O \leftrightarrow CH_2(OH)C(OH)(OH)CHO$	T(74)	$1.3\ 10^{1}$		Estimated with GROMHE	
$CH_2(OH)COCHO + 2\ H_2O \leftrightarrow CH_2(OH)C(OH)(OH)CH(OH)(OH)$	T(75)	$9.2\ 10^{2}$		Estimated with GROMHE	
$CH_2(OH)COCO(OO^\bullet) + H_2O \leftrightarrow CH_2(OH)COC(OH)(OH)(OO^\bullet)$	T(76)	$1.0\ 10^{-3}$			2
$CH_2(OH)COCO(OO^\bullet) + H_2O \leftrightarrow CH_2(OH)C(OH)(OH)CO(OO^\bullet)$	T(77)	$1.3\ 10^{1}$			1 = $K_h(CH_2(OH)COCHO/CH_2(OH)C(OH)(OH)CHO)$
$CH_2(OH)COCO(OO^\bullet) + 2\ H_2O \leftrightarrow CH_2(OH)C(OH)(OH)C(OH)(OH)(OO^\bullet)$	T(78)	$9.2\ 10^{2}$			1 = $K_h(CH_2(OH)COCHO/CH_2(OH)C(OH)(OH)CH(OH)(OH))$
$CHOCOCH(OH)(OO^\bullet) + H_2O \leftrightarrow CH(OH)(OH)COCH(OH)(OO^\bullet)$	T(79)	$2.0\ 10^{2}$			1 = $K_h(CH_2(OH)COCHO/CH_2(OH)COCH(OH)(OH))$
$CHOCOCH(OH)(OO^\bullet) + H_2O \leftrightarrow CHOC(OH)(OH)CH(OH)(OO^\bullet)$	T(80)	$1.3\ 10^{1}$			1 = $K_h(CH_2(OH)COCHO/CH_2(OH)C(OH)(OH)CHO)$
$CHOCOCH(OH)(OO^\bullet) + 2\ H_2O \leftrightarrow CH(OH)(OH)C(OH)(OH)CH(OH)(OO^\bullet)$	T(81)	$9.2\ 10^{2}$			1 = $K_h(CH_2(OH)COCHO/CH_2(OH)C(OH)(OH)CH(OH)(OH))$
Oxopropanedial					
$CHOCOCHO + H_2O \leftrightarrow CHOCOCH(OH)(OH)$	T(82)	$1.7\ 10^{3}$		Estimated with GROMHE	
$CHOCOCHO + H_2O \leftrightarrow CHOC(OH)(OH)CHO$	T(83)	$5.1\ 10^{2}$		Estimated with GROMHE	
$CHOCOCHO + 2\ H_2O \leftrightarrow CH(OH)(OH)COCH(OH)(OH)$	T(84)	$6.3\ 10^{5}$		Estimated with GROMHE	
$CHOCOCHO + 2\ H_2O \leftrightarrow CHOC(OH)(OH)CH(OH)(OH)$	T(85)	$3.3\ 10^{5}$		Estimated with GROMHE	
$CHOCOCHO + 3\ H_2O \leftrightarrow CH(OH)(OH)C(OH)(OH)CH(OH)(OH)$	T(86)	$3.4\ 10^{7}$		Estimated with GROMHE	
$CHOCOCO(OO^\bullet) + H_2O \leftrightarrow CHOCOC(OH)(OH)(OO^\bullet)$	T(87)	$1.0\ 10^{-3}$			2

Species		K_a or K_h	-ΔH/R (K)	References	Notes
$CHOCOCO(OO^{\bullet}) + H_2O \leftrightarrow CHOC(OH)(OH)CO(OO^{\bullet})$	T(88)	$5.1\ 10^{2}$			1 = K_h(CHOCOCHO/CHOC(OH)(OH)CHO)
$CHOCOCO(OO^{\bullet}) + 2\ H_2O \leftrightarrow CH(OH)(OH)COC(OH)(OH)(OO^{\bullet})$	T(89)	$6.3\ 10^{5}$			1 = K_h(CHOCOCHO/CH(OH)(OH)COCH(OH)(OH))
$CHOCOCO(OO^{\bullet}) + 2\ H_2O \leftrightarrow CHOC(OH)(OH)C(OH)(OH)(OO^{\bullet})$	T(90)	$3.3\ 10^{5}$			1 = K_h(CHOCOCHO/CHOC(OH)(OH)CH(OH)(OH))
$CHOCOCO(OO^{\bullet}) + 2\ H_2O \leftrightarrow CH(OH)(OH)C(OH)(OH)CO(OO^{\bullet})$	T(91)	$3.3\ 10^{5}$			1 = K_h(CHOCOCHO/CHOC(OH)(OH)CH(OH)(OH))
$CHOCOCO(OO^{\bullet}) + 3\ H_2O \leftrightarrow CH(OH)(OH)C(OH)(OH)C(OH)(OH)(OO^{\bullet})$	T(92)	$3.4\ 10^{7}$			1 = K_h(CHOCOCHO/CH(OH)(OH)C(OH)(OH)CH(OH)(OH))
Dihydroxyacetone					
$CH_2(OH)COCH_2(OH) + H_2O \leftrightarrow CH_2(OH)C(OH)(OH)CH_2(OH)$	T(93)	$3.2\ 10^{-1}$		Estimated with GROMHE	
$CH_2(OH)COCH(OH)(OO^{\bullet}) + H_2O \leftrightarrow CH_2(OH)C(OH)(OH)CH(OH)(OO^{\bullet})$	T(94)	$3.2\ 10^{-1}$			1 = K_h($CH_2(OH)COCH_2(OH)$/$CH_2(OH)C(OH)(OH)CH_2(OH)$
Propionic acid					
$CH_3CH_2CO(OH) \leftrightarrow CH_3CH_2CO(O^-) + H^+$	T(95)	$1.3{\cdot}10^{-5}$		Lide, 2005	
$CH_3CH(OO^{\bullet})CO(OH) \leftrightarrow CH_3CH(OO^{\bullet})CO(O^-) + H^+$	T(96)	$1.3{\cdot}10^{-5}$			4 = K_a($CH_3CH_2CO(OH)$/$CH_3CH_2CO(O^-)$)
$CH_2(OO^{\bullet})CH_2CO(OH) \leftrightarrow CH_2(OO^{\bullet})CH_2CO(O^-) + H^+$	T(97)	$1.3{\cdot}10^{-5}$			4 = K_a($CH_3CH_2CO(OH)$/$CH_3CH_2CO(O^-)$)
3-oxopropionic acid					
$CO(OH)CH_2CHO \leftrightarrow CO(O^-)CH_2CHO + H^+$	T(98)	$1.3{\cdot}10^{-5}$			= K_a($CH_3CH_2CO(OH)$/$CH_3CH_2CO(O^-)$)
$CO(OH)CH_2CHO + H_2O \leftrightarrow CO(OH)CH_2CH(OH)(OH)$	T(99)	$1.0\ 10^{1}$		Estimated with GROMHE	
$CO(O^-)CH_2CHO + H_2O \leftrightarrow CO(O^-)CH_2CH(OH)(OH)$	T(100)	1.4		Estimated with GROMHE	
$CO(OH)CH_2C(OH)(OH)(OO^{\bullet}) \leftrightarrow CO(O^-)CH_2C(OH)(OH)(OO^{\bullet}) + H^+$	T(101)	$1.3{\cdot}10^{-5}$			4 = K_a($CO(OH)CH_2CHO$/$CO(O^-)CH_2CHO$)
$CO(OH)CH_2CO(OO^{\bullet}) + H_2O \leftrightarrow CO(OH)CH_2C(OH)(OH)(OO^{\bullet})$	T(102)	$1.0\ 10^{-3}$			2
$CO(O^-)CH_2CO(OO^{\bullet}) + H_2O \leftrightarrow CO(O^-)CH_2C(OH)(OH)(OO^{\bullet})$	T(103)	$1.0\ 10^{-3}$			2
Malonic acid					
$CO(OH)CH_2CO(OH) \leftrightarrow CO(OH)CH_2CO(O^-) + H^+$	T(104)	$1.4{\cdot}10^{-3}$		Lide, 2005	
$CO(OH)CH_2CO(O^-) \leftrightarrow CO(O^-)CH_2CO(O^-) + H^+$	T(105)	$2.0{\cdot}10^{-6}$		Lide, 2005	
$CO(OH)CH(OO^{\bullet})CO(OH) \leftrightarrow CO(OH)CH(OO^{\bullet})CO(O^-) + H^+$	T(106)	$1.4{\cdot}10^{-3}$			4 = K_a($CO(OH)CH_2CO(OH)$/$CO(OH)CH_2CO(O^-)$)
$CO(OH)CH(OO^{\bullet})CO(O^-) \leftrightarrow CO(O^-)CH(OO^{\bullet})CO(O^-) + H^+$	T(107)	$2.0{\cdot}10^{-6}$			4 = K_a($CO(OH)CH_2CO(O^-)$/$[CO(O^-)CH_2CO(O^-)$)
Tartronic acid					
$CO(OH)CH(OH)CO(OH) \leftrightarrow CO(OH)CH(OH)CO(O^-) + H^+$	T(108)	$3.8{\cdot}10^{-3}$		Lide, 2005	
$CO(OH)CH(OH)CO(O^-) \leftrightarrow CO(O^-)CH(OH)CO(O^-) + H^+$	T(109)	$2.9{\cdot}10^{-5}$		Lide, 2005	

Species		K_a or K_h	-ΔH/R (K)	References	Notes
$CO(OH)C(OH)(OO^{\bullet})CO(OH) \leftrightarrow CO(OH)C(OH)(OO^{\bullet})CO(O^-) + H^+$	T(110)	$3.8 \cdot 10^{-3}$			4 = $K_a(CO(OH)CH(OH)CO(OH)/CO(OH)CH(OH)CO(O^-))$
$CO(OH)C(OH)(OO^{\bullet})CO(O^-) \leftrightarrow CO(O^-)C(OH)(OO^{\bullet})CO(O^-) + H^+$	T(111)	$2.9 \cdot 10^{-5}$			4 = $K_a(CO(OH)CH(OH)CO(O^-)/CO(O^-)CH(OH)CO(O^-))$
Mesoxalic acid					
$CO(OH)C(OH)(OH)CO(OH) \leftrightarrow CO(OH)C(OH)(OH)CO(O^-) + H^+$	T(112)	$3.2 \cdot 10^{-3}$		Albalat et al., 1989	
$CO(OH)C(OH)(OH)CO(O^-) \leftrightarrow CO(O^-)C(OH)(OH)CO(O^-) + H^+$	T(113)	$1.3 \cdot 10^{-4}$		Albalat et al., 1989	
$CO(OH)COCO(OH) + H_2O \leftrightarrow CO(OH)C(OH)(OH)CO(OH)$	T(114)	$1.0\ 10^{2}$		Le Henaff, 1968	
$CO(OH)COCO(O^-) + H_2O \leftrightarrow CO(OH)C(OH)(OH)CO(O^-)$	T(115)	2.4		Estimated with GROMHE	
$CO(O^-)COCO(O^-) + H_2O \leftrightarrow CO(O^-)C(OH)(OH)CO(O^-)$	T(116)	$1.6\ 10^{-2}$		Estimated with GROMHE	
Lactic acid					
$CH_3CH(OH)CO(OH) \leftrightarrow CH_3CH(OH)CO(O^-) + H^+$	T(117)	$1.4 \cdot 10^{-4}$		Lide, 2005	
$CH_3C(OH)(OO^{\bullet})CO(OH) \leftrightarrow CH_3C(OH)(OO^{\bullet})CO(O^-) + H^+$	T(118)	$1.4 \cdot 10^{-4}$			4 = $K_a(CH_3CH(OH)CO(OH)/CH_3CH(OH)CO(O^-))$
$CH_2(OO^{\bullet})CH(OH)CO(OH) \leftrightarrow CH_2(OO^{\bullet})CH(OH)CO(O^-) + H^+$	T(119)	$1.4 \cdot 10^{-4}$			4 = $K_a(CH_3CH(OH)CO(OH)/CH_3CH(OH)CO(O^-))$
2,3-dihydroxypropanoic acid - glyceric acid					
$CH_2(OH)CH(OH)CO(OH) \leftrightarrow CH_2(OH)CH(OH)CO(O^-) + H^+$	T(120)	$3.0 \cdot 10^{-4}$		Lide, 2005	
$CH(OH)(OO^{\bullet})CH(OH)CO(OH) \leftrightarrow CH(OH)(OO^{\bullet})CH(OH)CO(O^-) + H^+$	T(121)	$3.0 \cdot 10^{-4}$			4 = $K_a(CH_2(OH)CH(OH)CO(OH)/CH_2(OH)CH(OH)CO(O^-))$
$CH_2(OH)C(OH)(OO^{\bullet})CO(OH) \leftrightarrow CH_2(OH)C(OH)(OO^{\bullet})CO(O^-) + H^+$	T(122)	$3.0 \cdot 10^{-4}$			4 = $K_a(CH_2(OH)CH(OH)CO(OH)/CH_2(OH)CH(OH)CO(O^-))$
2-hydroxy, 3-oxopropanoïc acid					
$CHOCH(OH)CO(OH) \leftrightarrow CHOCH(OH)CO(O^-) + H^+$	T(123)	$3.0 \cdot 10^{-4}$			= $K_a(CH_2(OH)CH(OH)CO(OH)/CH_2(OH)CH(OH)CO(O^-))$
$CHOCH(OH)CO(OH) + H_2O \leftrightarrow CH(OH)(OH)CH(OH)CO(OH)$	T(124)	$4.6\ 10^{1}$		Estimated with GROMHE	
$CHOCH(OH)CO(O^-) + H_2O \leftrightarrow CH(OH)(OH)CH(OH)CO(O^-)$	T(125)	6.1		Estimated with GROMHE	
$CO(OH)CH(OH)C(OH)(OH)(OO^{\bullet}) \leftrightarrow CO(O^-)CH(OH)C(OH)(OH)(OO^{\bullet}) + H^+$	T(126)	$3.0 \cdot 10^{-4}$			4 = $K_a(CHOCH(OH)CO(OH)/CHOCH(OH)CO(O^-))$
$CO(OH)CH(OH)CO(OO^{\bullet}) + H_2O \leftrightarrow CO(OH)CH(OH)C(OH)(OH)(OO^{\bullet})$	T(127)	$1.0\ 10^{-3}$			2
$CO(O^-)CH(OH)CO(OO^{\bullet}) + H_2O \leftrightarrow CO(O^-)CH(OH)C(OH)(OH)(OO^{\bullet})$	T(128)	$1.0\ 10^{-3}$			2
3-oxopyruvic acid					
$CO(OH)COCHO \leftrightarrow CO(O^-)COCHO + H^+$	T(129)	$4.1 \cdot 10^{-3}$			= $K_a(CH_3COCO(OH)/CH_3COCO(O^-))$
$CO(OH)COCHO + H_2O \leftrightarrow CO(OH)COCH(OH)(OH)$	T(130)	$8.1\ 10^{2}$		Estimated with GROMHE	
$CO(OH)COCHO + H_2O \leftrightarrow CO(OH)C(OH)(OH)CHO$	T(131)	$4.4\ 10^{2}$		Estimated with GROMHE	

Species		K_a or K_h	-ΔH/R (K)	References	Notes
$CO(OH)COCHO + 2\ H_2O \leftrightarrow CO(OH)C(OH)(OH)CH(OH)(OH)$	T(132)	$1.3\ 10^{5}$		Estimated with GROMHE	
$CO(O^-)COCHO + H_2O \leftrightarrow CO(O^-)COCH(OH)(OH)$	T(133)	$1.1\ 10^{2}$		Estimated with GROMHE	
$CO(O^-)COCHO + H_2O \leftrightarrow CO(O^-)C(OH)(OH)CHO$	T(134)	2.8		Estimated with GROMHE	
$CO(O^-)COCHO + 2\ H_2O \leftrightarrow CO(O^-)C(OH)(OH)CH(OH)(OH)$	T(135)	$1.1\ 10^{2}$		Estimated with GROMHE	
$CO(OH)C(OH)(OH)C(OH)(OH)(OO^\bullet) \leftrightarrow CO(O^-)C(OH)(OH)C(OH)(OH)(OO^\bullet) + H^+$	T(136)	$4.1{\cdot}10^{-3}$			4 = K_a(CO(OH)COCHO/CO(O⁻)COCHO)
$CO(OH)COCO(OO^\bullet) + H_2O \leftrightarrow CO(OH)COC(OH)(OH)(OO^\bullet)$	T(137)	$1.0\ 10^{-3}$			2
$CO(OH)COCO(OO^\bullet) + H_2O \leftrightarrow CO(OH)C(OH)(OH)CO(OO^\bullet)$	T(138)	$4.4\ 10^{2}$			1 = K_h(CO(OH)COCHO/CO(OH)C(OH)(OH)CHO)
$CO(OH)COCO(OO^\bullet) + 2\ H_2O \leftrightarrow CO(OH)C(OH)(OH)C(OH)(OH)(OO^\bullet)$	T(139)	$1.3\ 10^{5}$			1 = K_h(CO(OH)COCHO/CO(OH)C(OH)(OH)CH(OH)(OH))
$CO(O^-)COCO(OO^\bullet) + H_2O \leftrightarrow CO(O^-)COC(OH)(OH)(OO^\bullet)$	T(140)	$1.0\ 10^{-3}$			2
$CO(O^-)COCO(OO^\bullet) + H_2O \leftrightarrow CO(O^-)C(OH)(OH)CO(OO^\bullet)$	T(141)	2.8			1 = K_h(CO(O⁻)COCHO/CO(O⁻)C(OH)(OH)CHO)
$CO(O^-)COCO(OO^\bullet) + 2\ H_2O \leftrightarrow CO(O^-)C(OH)(OH)C(OH)(OH)(OO^\bullet)$	T(142)	$1.1\ 10^{2}$			1 = K_h(CO(O⁻)COCHO/CO(O⁻)C(OH)(OH)CH(OH)(OH))
3-hydroxypyruvic acid					
$CH_2(OH)COCO(OH) \leftrightarrow CH_2(OH)COCO(O^-) + H^+$	T(143)	$4.1{\cdot}10^{-3}$			= K_a(CH₃COCO(OH)/CH₃COCO(O⁻))
$CH_2(OH)COCO(OH) + H_2O \leftrightarrow CH_2(OH)C(OH)(OH)CO(OH)$	T(144)	$1.1\ 10^{1}$		Estimated with GROMHE	
$CH_2(OH)COCO(O^-) + H_2O \leftrightarrow CH_2(OH)C(OH)(OH)CO(O^-)$	T(145)	$7.0\ 10^{-2}$		Estimated with GROMHE	
$CH(OH)(OO^\bullet)COCO(OH) \leftrightarrow CH(OH)(OO^\bullet)COCO(O^-) + H^+$	T(146)	$4.1{\cdot}10^{-3}$			4 = K_a(CH₃COCO(OH)/CH₃COCO(O⁻))
$CH(OH)(OO^\bullet)COCO(OH) + H_2O \leftrightarrow CH(OH)(OO^\bullet)C(OH)(OH)CO(OH)$	T(147)	$1.1\ 10^{1}$			1 = K_h(CH₂(OH)COCO(OH)/CH₂(OH)C(OH)(OH)CO(OH))
$CH(OH)(OO^\bullet)COCO(O^-) + H_2O \leftrightarrow CH(OH)(OO^\bullet)C(OH)(OH)CO(O^-)$	T(148)	$7.0\ 10^{-2}$			1 = K_h(CH₂(OH)COCO(O⁻)/CH₂(OH)C(OH)(OH)CO(O⁻))
Pyruvic acid					
$CH_3COCO(OH) \leftrightarrow CH_3COCO(O^-) + H^+$	T(149)	$4.1{\cdot}10^{-3}$		Lide, 2005	
$CH_3COCO(OH) + H_2O \leftrightarrow CH_3C(OH)(OH)CO(OH)$	T(150)	1.5		Pocker et al., 1969	
$CH_3COCO(O^-) + H_2O \leftrightarrow CH_3C(OH)(OH)CO(O^-)$	T(151)	$5.7\ 10^{-2}$		Pocker et al., 1969	
$CO(OH)COCH_2(OO^\bullet) \leftrightarrow CO(O^-)COCH_2(OO^\bullet) + H^+$	T(152)	$4.1{\cdot}10^{-3}$			4 = K_a(CH₃COCO(OH)/CH₃COCO(O⁻))
$CO(OH)COCH_2(OO^\bullet) + H_2O \leftrightarrow CO(OH)C(OH)(OH)CH_2(OO^\bullet)$	T(153)	1.5			1 = K_h(CH₃COCO(OH)/CH₃C(OH)(OH)CO(OH))
$CO(O^-)COCH_2(OO^\bullet) + H_2O \leftrightarrow CO(O^-)C(OH)(OH)CH_2(OO^\bullet)$	T(154)	$5.7\ 10^{-2}$			1 = K_h(CH₃COCO(O⁻)/CH₃C(OH)(OH)CO(O⁻))

Species		K_a or K_h	-ΔH/R (K)	References	Notes
Acroleine					
$CH_2(OH)CH(OO^\bullet)CHO + H_2O \leftrightarrow CH_2(OH)CH(OO^\bullet)CH(OH)(OH)$	T(155)	$1.1\ 10^1$			1 = $K_h(CH_2(OH)CH(OH)CHO/CH_2(OH)CH(OH)CH(OH)(OH))$
2,3 dihydroxypropanal - glyceraldehyde					
$CH_2(OH)CH(OH)CHO + H_2O \leftrightarrow CH_2(OH)CH(OH)CH(OH)(OH)$	T(156)	$1.1\ 10^1$		Estimated with GROMHE	
$CHOCH(OH)CH(OH)(OO^\bullet) + H_2O \leftrightarrow CH(OH)(OH)CH(OH)CH(OH)(OO^\bullet)$	T(157)	$1.1\ 10^1$			1 = $K_h(CH_2(OH)CH(OH)CHO/CH_2(OH)CH(OH)CH(OH)(OH))$
$CH_2(OH)CH(OH)CO(OO^\bullet) + H_2O \leftrightarrow CH_2(OH)CH(OH)C(OH)(OH)(OO^\bullet)$	T(158)	$1.0\ 10^{-3}$			2
Hydroxypropanedial					
$CHOCH(OH)CHO + H_2O \leftrightarrow CHOCH(OH)CH(OH)(OH)$	T(159)	$9.8\ 10^1$		Estimated with GROMHE	
$CHOCH(OH)CHO + 2\ H_2O \leftrightarrow CH(OH)(OH)CH(OH)CH(OH)(OH)$	T(160)	$2.0\ 10^3$		Estimated with GROMHE	
$CHOCH(OH)CO(OO^\bullet) + H_2O \leftrightarrow CHOCH(OH)C(OH)(OH)(OO^\bullet)$	T(161)	$1.0\ 10^{-3}$			2
$CHOCH(OH)CO(OO^\bullet) + 2\ H_2O \leftrightarrow CH(OH)(OH)CH(OH)C(OH)(OH)(OO^\bullet)$	T(162)	$2.0\ 10^3$			1 = $K_h(CHOCH(OH)CHO/CH(OH)(OH)CH(OH)CH(OH)(OH))$

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

2 - For acyl peroxyl radicals, we assumed that hydration is not favored on the –$CO(OO^\bullet)$ 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 ($K_h = 10^{-3}$) to the hydration constant of these species.

3 - The parent species is symetrical whereas the corresponding $R(OO^\bullet)$ is asymetrical. We assume that hydration occurs mainly on the $CO(OO^\bullet)$ function.

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

5 - For methylglyoxal, Wasa and Musha (1970) measured the total hydratation constant. Each fractional hydration constant is calculated from the measured total hydration constant weighted by the relative contribution of each hydrate estimated with GROMHE.

References:

Wasa, T., and Musha, S.: Polarographic behavior of glyoxal and its related compounds, Bull. Univ. Osaka Pref. A, Eng. Nat. Sci., 19, 169-180, 1970.

Henry's law constants

Species		H (298K) ($M\ atm^{-1}$)	-ΔH/R (K)	References	Notes
C3 compounds					
1-propanol					
$CH_3CH_2CH_2(OH)$	T(42)	$1.3\ 10^2$	7470	Sander, 2015	
3-hydroxypropionaldehyde					
$CH_2(OH)CH_2CHO$	T(43)	$2.3\ 10^3$	6014	Estimated	1 - 2 - 3
Propane-1,2-diol					
$CH_3CH(OH)CH_2(OH)$	T(44)	$3.0\ 10^6$	6014	Estimated	3 - 4
2-hydroxypropionaldehyde					
$CH_3CH(OH)CHO$	T(45)	$2.2\ 10^3$	6014	Estimated	1 - 2 - 3
Propanedial					
$CHOCH_2CHO$	T(46)	$3.3\ 10^4$	6014	Estimated	1 - 2 - 3
3-hydroxypropionic acid					
$CH_2(OH)CH_2CO(OH)$	T(47)	$2.0\ 10^5$	6014	Estimated	1 - 3
2-propanol					
$CH_3CH(OH)CH_3$	T(48)	$1.3\ 10^2$	7470	Sander, 2015	
Propionaldehyde					
CH_3CH_2CHO	T(49)	$1.0\ 10^1$	4330	Sander, 2015	2
Methylglyoxal					
CH_3COCHO	T(50)	$3.7\ 10^3$	7540	Betterton and Hoffmann, 1988	2
2-oxo, 3-hydroxypropanal					
$CH_2(OH)COCHO$	T(51)	$1.3\ 10^7$	6014	Estimated	1 - 2 - 3
Oxopropanedial					
$CHOCOCHO$	T(52)	$9.8\ 10^{10}$	6014	Estimated	1 - 2 - 3
Acetone					
CH_3COCH_3	T(53)	$2.8\ 10^1$	5050	Sander, 2015	2
Hydroxyacetone					
$CH_3COCH_2(OH)$	T(54)	$1.6\ 10^3$	6014	Estimated	1 - 2 - 3
Dihydroxyacetone					
$CH_2(OH)COCH_2(OH)$	T(55)	$1.1\ 10^7$	6014	Estimated	1 - 2 - 3
Propionic acid					
$CH_3CH_2CO(OH)$	T(56)	$5.7\ 10^3$		Khan et al., 1995	
3-oxopropionic acid					
$CO(OH)CH_2CHO$	T(57)	$9.0\ 10^5$	6014	Estimated	1 - 2 - 3

Species		H (298K) (M atm^{-1})	-ΔH/R (K)	References	Notes
Malonic acid					
$CO(OH)CH_2CO(OH)$	T(58)	$3.9\ 10^{10}$	11000	Compernolle and Müller, 2014	
Tartronic acid					
$CO(OH)CH(OH)CO(OH)$	T(59)	$1.0\ 10^{7}$	6014	Estimated	1 - 3
Mesoxalic acid					
$CO(OH)COCO(OH)$	T(60)	$2.7\ 10^{10}$	6014	Estimated	1 - 2 - 3
Lactic acid					
$CH_3CH(OH)CO(OH)$	T(61)	$9.6\ 10^{4}$	6014	Estimated	1 - 3
2,3-dihydroxypropanoic acid					
$CH_2(OH)CH(OH)CO(OH)$	T(62)	$8.1\ 10^{7}$	6014	Estimated	1 - 3
2-hydroxy, 3-oxopropanoic acid					
$CHOCH(OH)CO(OH)$	T(63)	$1.6\ 10^{6}$	6014	Estimated	1 - 2 - 3
3-oxopyruvic acid					
$CO(OH)COCHO$	T(64)	$1.2\ 10^{11}$	6014	Estimated	1 - 2 - 3
3-hydroxypyruvic acid					
$CH_2(OH)COCO(OH)$	T(65)	$4.3\ 10^{7}$	6014	Estimated	1 - 2 - 3
Pyruvic acid					
$CH_3COCO(OH)$	T(66)	$3.1\ 10^{5}$	5090	Sander, 2015	
Acrolein					
$CH_2=CHCHO$	T(67)	7.4	5100	Snider and Dawson, 1985	
2,3-dihydroxypropanal - glyceraldehyde					
$CH_2(OH)CH(OH)CHO$	T(68)	$3.2\ 10^{5}$	6014	Estimated	1 - 2 - 3
Hydroxypropanedial					
$CHOCH(OH)CHO$	T(69)	$2.3\ 10^{5}$	6014	Estimated	1 - 2 - 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.
4 - Saxena and Hildemann (1996) estimated the Henry's law constant between 10^5 and $6.0\ 10^6$ M atm^{-1}. We suppose the Henry's law constant equal to $3.0\ 10^6$ M atm^{-1}.

References:

Raventos-Duran, T., Camredon, M., Valorso, R., Mouchel-Vallon, C., and Aumont, B.: Structure-activity relationships to estimate the effective Henry's law constants of organics of atmospheric interest, Atmos. Chem. Phys., 10, 7643-7654, 2010.
Saxena, P., and Hildemann, L. M.: Water-soluble organics in atmospheric particles: A critical review of the literature and application of thermodynamics to identify candidate compounds, J. Atmos. Chem., 24, 57-109, 1996.

Accommodation coefficients

Species		α (298K)	-ΔH (J/mol)	-ΔS (J/mol/K)	References	Notes
C3 compounds		1				
1-propanol						
$CH_3CH_2CH_2(OH)$	T(42)	$6.0\ 10^{-3}$	$3.8\ 10^{4}$	$1.7\ 10^{2}$	Davidovits et al., 2011	
3-hydroxypropionaldehyde						
$CH_2(OH)CH_2CHO$	T(43)	$5.0\ 10^{-2}$			Estimated	2
Propane-1,2-diol						
$CH_3CH(OH)CH_2(OH)$	T(44)	$5.0\ 10^{-2}$			Estimated	2
2-hydroxypropionaldehyde						
$CH_3CH(OH)CHO$	T(45)	$5.0\ 10^{-2}$			Estimated	2
Propanedial						
$CHOCH_2CHO$	T(46)	$5.0\ 10^{-2}$			Estimated	2
3-hydroxypropionic acid						
$CH_2(OH)CH_2CO(OH)$	T(47)	$5.0\ 10^{-2}$			Estimated	2
2-propanol						
$CH_3CH(OH)CH_3$	T(48)	$7.0\ 10^{-3}$	$4.1\ 10^{4}$	$1.8\ 10^{2}$	Davidovits et al., 2011	
Propionaldehyde						
CH_3CH_2CHO	T(49)	$5.0\ 10^{-2}$			Estimated	2
Methylglyoxal						
CH_3COCHO	T(50)	$1.0\ 10^{-4}$			Sander, 2015	
2-oxo, 3-hydroxypropanal						
$CH_2(OH)COCHO$	T(51)	$5.0\ 10^{-2}$			Estimated	2
Oxopropanedial						
$CHOCOCHO$	T(52)	$5.0\ 10^{-2}$			Estimated	2
Acetone						
CH_3COCH_3	T(53)	$4.0\ 10^{-3}$	$5.3\ 10^{4}$	$2.2\ 10^{2}$	Davidovits et al., 2011	
Hydroxyacetone						
$CH_3COCH_2(OH)$	T(54)	$5.0\ 10^{-2}$			Estimated	2
Dihydroxyacetone						
$CH_2(OH)COCH_2(OH)$	T(55)	$5.0\ 10^{-2}$			Estimated	2
Propionic acid						
$CH_3CH_2CO(OH)$	T(56)	$5.0\ 10^{-2}$			Estimated	2
3-oxopropionic acid						
$CO(OH)CH_2CHO$	T(57)	$5.0\ 10^{-2}$			Estimated	2
Malonic acid						
$CO(OH)CH_2CO(OH)$	T(58)	$5.0\ 10^{-2}$			Estimated	2

Species		α (298K)	-ΔH (J/mol)	-ΔS (J/mol/K)	References	Notes
Tartronic acid						
$CO(OH)CH(OH)CO(OH)$	T(59)	$5.0\ 10^{-2}$			Estimated	2
Mesoxalic acid						
$CO(OH)COCO(OH)$	T(60)	$5.0\ 10^{-2}$			Estimated	2
Lactic acid						
$CH_3CH(OH)CO(OH)$	T(61)	$5.0\ 10^{-2}$			Estimated	2
2,3-dihydroxypropanoic acid						
$CH_2(OH)CH(OH)CO(OH)$	T(62)	$5.0\ 10^{-2}$			Estimated	2
2-hydroxy, 3-oxopropanoic acid						
$CHOCH(OH)CO(OH)$	T(63)	$5.0\ 10^{-2}$			Estimated	2
3-oxopyruvic acid						
$CO(OH)COCHO$	T(64)	$5.0\ 10^{-2}$			Estimated	2
3-hydroxypyruvic acid						
$CH_2(OH)COCO(OH)$	T(65)	$5.0\ 10^{-2}$			Estimated	2
Pyruvic acid						
$CH_3COCO(OH)$	T(66)	$5.0\ 10^{-2}$			Estimated	2
Acrolein						
$CH_2=CHCHO$	T(67)	$5.0\ 10^{-2}$			Estimated	2
2,3-dihydroxypropanal - glyceraldehyde						
$CH_2(OH)CH(OH)CHO$	T(68)	$5.0\ 10^{-2}$			Estimated	2
Hydroxypropanedial						
$CHOCH(OH)CHO$	T(69)	$5.0\ 10^{-2}$			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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