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

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
Oxidation of Succinic Acid					
Pathway 1: $CO(OH)CH_2CH_2CO(OH) + HO^\bullet \rightarrow CO(OH)CH_2C^\bullet HCO(OH) + H_2O$		$1.1\ 10^8$			BR: 100% - 1
$CO(OH)CH_2C^\bullet HCO(OH) + O_2 \rightarrow CO(OH)CH_2CH(OO^\bullet)CO(OH)$		$2.0\ 10^9$			2
$CO(OH)CH_2CH_2CO(OH) + HO^\bullet \rightarrow CO(OH)CH_2CH(OO^\bullet)CO(OH) + H_2O - O_2$	R(1)	$1.1\ 10^8$		Ervens et al., 2003	
Pathway 1: $CO(OH)CH_2CH_2CO(OH) + NO_3^\bullet \rightarrow CO(OH)CH_2C^\bullet HCO(OH) + NO_3^- + H^+$		$5.1\ 10^4$			BR: 100%
$CO(OH)CH_2C^\bullet HCO(OH) + O_2 \rightarrow CO(OH)CH_2CH(OO^\bullet)CO(OH)$		$2.0\ 10^9$			2
$CO(OH)CH_2CH_2CO(OH) + NO_3^\bullet \rightarrow CO(OH)CH_2CH(OO^\bullet)CO(OH) + NO_3^- + H^+ - O_2$	R(2)	$5.1\ 10^4$			= k($CO(OH)CH_2CO(OH)$+ $NO_3^\bullet$) -3
Pathway 1: $CO(OH)CH_2CH_2CO(O^-) + HO^\bullet \rightarrow CO(OH)CH_2CH_2CO(O^\bullet) + OH^-$		$3.4\ 10^8$			BR: 68% - 4
$CO(OH)CH_2CH_2CO(O^\bullet) \rightarrow CO(OH)CH_2C^\bullet H_2 + CO_2$					5 - 6
$CO(OH)CH_2C^\bullet H_2 + O_2 \rightarrow CH_2(OO^\bullet)CH_2CO(OH)$		$2.0\ 10^9$			2
Pathway 2: $CO(OH)CH_2CH_2CO(O^-) + HO^\bullet \rightarrow CO(OH)CH_2C^\bullet HCO(O^-) + H_2O$		$1.6\ 10^8$			BR: 32% - 4
$CO(OH)CH_2C^\bullet HCO(O^-) + O_2 \rightarrow CO(OH)CH_2CH(OO^\bullet)CO(O^-)$		$2.0\ 10^9$			2
$CO(OH)CH_2CH_2CO(O^-) + HO^\bullet \rightarrow 0.68\ CH_2(OO^\bullet)CH_2CO(OH) + 0.32\ CO(OH)CH_2CH(OO^\bullet)CO(O^-) + 0.68\ CO_2 + 0.68\ OH^- + 0.32\ H_2O - O_2$	R(3)	$5.0\ 10^8$		Ervens et al., 2003	
Pathway 1: $CO(OH)CH_2CH_2CO(O^-) + NO_3^\bullet \rightarrow CO(OH)CH_2C^\bullet HCO(O^-) + NO_3^- + H^+$		$5.6{\cdot}10^6$	3369		BR: 100%
$CO(OH)CH_2C^\bullet HCO(O^-) + O_2 \rightarrow CO(OH)CH_2CH(OO^\bullet)CO(O^-)$		$2.0\ 10^9$			2
$CO(OH)CH_2CH_2CO(O^-) + NO_3^\bullet \rightarrow CO(OH)CH_2CH(OO^\bullet)CO(O^-) + NO_3^- + H^+ - O_2$	R(4)	$5.6\ 10^6$	3369		= k($CO(OH)CH_2CO(O^-)$+ $NO_3^\bullet$) - 3
Pathway 1: $CO(O^-)CH_2CH_2CO(O^-) + HO^\bullet \rightarrow CO(O^-)CH_2CH_2CO(O^\bullet) + OH^-$		$5.6\ 10^8$			BR: 55% - [7]
$CO(O^-)CH_2CH_2CO(O^\bullet) \rightarrow CO(O^-)CH_2C^\bullet H_2 + CO_2$					5 - 6
$CO(O^-)CH_2C^\bullet H_2 + O_2 \rightarrow CH_2(OO^\bullet)CH_2CO(O^-)$		$2.0\ 10^9$			2
Pathway 2: $CO(O^-)CH_2CH_2CO(O^-) + HO^\bullet \rightarrow CO(O^-)CH_2C^\bullet HCO(O^-) + H_2O$		$4.6\ 10^8$			BR: 45% - 7
$CO(O^-)CH_2C^\bullet HCO(O^-) + O_2 \rightarrow CO(O^-)CH_2CH(OO^\bullet)CO(O^-)$		$2.0\ 10^9$			2
$CO(O^-)CH_2CH_2CO(O^-) + HO^\bullet \rightarrow 0.55\ CH_2(OO^\bullet)CH_2CO(O^-) + 0.45\ CO(O^-)CH_2CH(OO^\bullet)CO(O^-) + 0.55\ CO_2 + 0.55\ OH^- + 0.45\ H_2O - O_2$	R(5)	$1.0\ 10^9$			8
Pathway 1: $CO(O^-)CH_2CH_2CO(O^-) + NO_3^\bullet \rightarrow CO(O^-)CH_2C^\bullet HCO(O^-) + NO_3^- + H^+$		$2.3{\cdot}10^7$	3008		BR: 100%
$CO(O^-)CH_2C^\bullet HCO(O^-) + O_2 \rightarrow CO(O^-)CH_2CH(OO^\bullet)CO(O^-)$		$2.0\ 10^9$			2
$CO(O^-)CH_2CH_2CO(O^-) + NO_3^\bullet \rightarrow CO(O^-)CH_2CH(OO^\bullet)CO(O^-) + NO_3^- + H^+ - O_2$	R(6)	$2.3\ 10^7$	3008		=k($CO(O^-)CH_2CO(O^-)$+ $NO_3^\bullet$) - 3
Pathway 1: $2\ CO(OH)CH_2CH(OO^\bullet)CO(OH) \rightarrow 2\ CO(OH)CH_2COCO(OH) + H_2O_2$		$2.2\ 10^7$			BR: 30%
Pathway 2: $2\ CO(OH)CH_2CH(OO^\bullet)CO(OH)$ *(+ 2 H_2O)* $\rightarrow 2\ CO(OH)CH_2CHO + 2\ CO_2 + H_2O_2 + 2\ H_2O$		$2.2\ 10^7$			BR: 30%
Pathway 3: $2\ CO(OH)CH_2CH(OO^\bullet)CO(OH) \rightarrow CO(OH)CH_2COCO(OH) + CO(OH)CH_2CH(OH)CO(OH) + O_2$		$2.2\ 10^7$			BR: 30%
Pathway 4: $2\ CO(OH)CH_2CH(OO^\bullet)CO(OH) \rightarrow 2\ CO(OH)CH_2CH(O^\bullet)CO(OH) + O_2$		$9.0\ 10^6$			BR: 10%
$CO(OH)CH_2CH(O^\bullet)CO(OH) \rightarrow CO(OH)CH_2C^\bullet(OH)CO(OH)$					9
$CO(OH)CH_2C^\bullet(OH)CO(OH) + O_2 \rightarrow CO(OH)CH_2C(OH)(OO^\bullet)CO(OH)$		$2.0\ 10^9$			2
$2\ CO(OH)CH_2CH(OO^\bullet)CO(OH) \rightarrow 0.90\ CO(OH)CH_2COCO(OH) + 0.30\ CO(OH)CH_2CH(OH)CO(OH) + 0.20\ CO(OH)CH_2C(OH)(OO^\bullet)CO(OH) + 0.60\ CO(OH)CH_2CHO + 0.60\ CO_2 + 0.60\ H_2O_2 + 0.20\ O_2$	R(7)	$7.5\ 10^7$			= k($2\ CH_2(OO^\bullet)CO(O^-)$) - 10
Pathway 1: $2\ CO(OH)CH_2CH(OO^\bullet)CO(O^-) \rightarrow 2\ CO(OH)CH_2COCO(O^-) + H_2O_2$		$2.2\ 10^7$			BR: 30%
Pathway 2: $2\ CO(OH)CH_2CH(OO^\bullet)CO(O^-)$ *(+ 2 H_2O)* $\rightarrow 2\ CO(OH)CH_2CHO + 2\ CO_2 + H_2O_2 + 2\ OH^-$		$2.2\ 10^7$			BR: 30%
Pathway 3: $2\ CO(OH)CH_2CH(OO^\bullet)CO(O^-) \rightarrow CO(OH)CH_2COCO(O^-) + CO(OH)CH_2CH(OH)CO(O^-) + O_2$		$2.2\ 10^7$			BR: 30%
Pathway 4: $2\ CO(OH)CH_2CH(OO^\bullet)CO(O^-) \rightarrow 2\ CO(OH)CH_2CH(O^\bullet)CO(O^-) + O_2$		$9.0\ 10^6$			BR: 10%
$CO(OH)CH_2CH(O^\bullet)CO(O^-) \rightarrow CO(OH)CH_2C^\bullet(OH)CO(O^-)$					9
$CO(OH)CH_2C^\bullet(OH)CO(O^-) + O_2 \rightarrow CO(OH)CH_2C(OH)(OO^\bullet)CO(O^-)$		$2.0{\cdot}10^9$			2

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$2\ CO(OH)CH_2CH(OO^{\bullet})CO(O^-) \rightarrow 0.90\ CO(OH)CH_2COCO(O^-) + 0.30\ CO(OH)CH_2CH(OH)CO(O^-) + 0.20\ CO(OH)CH_2C(OH)(OO^{\bullet})CO(O^-) + 0.60\ CO(OH)CH_2CHO + 0.60\ CO_2 + 0.60\ H_2O_2 + 0.60\ OH^- - 0.6\ H_2O + 0.20\ O_2$	R(8)	$7.5\ 10^7$			= k(2 $CH_2(OO^{\bullet})CO(O^-)$) - 10
Pathway 1: $2\ CO(O^-)CH_2CH(OO^{\bullet})CO(OH) \rightarrow 2\ CO(O^-)CH_2COCO(OH) + H_2O_2$		$2.2\ 10^7$			BR: 30%
Pathway 2: $2\ CO(O^-)CH_2CH(OO^{\bullet})CO(OH)\ (+\ 2\ H_2O) \rightarrow 2\ CO(O^-)CH_2CHO + 2\ CO_2 + H_2O_2 + 2\ H_2O$		$2.2\ 10^7$			BR: 30%
Pathway 3: $2\ CO(O^-)CH_2CH(OO^{\bullet})CO(OH) \rightarrow CO(O^-)CH_2COCO(OH) + CO(O^-)CH_2CH(OH)CO(OH) + O_2$		$2.2\ 10^7$			BR: 30%
Pathway 4: $2\ CO(O^-)CH_2CH(OO^{\bullet})CO(OH) \rightarrow 2\ CO(O^-)CH_2CH(O^{\bullet})CO(OH) + O_2$		$9.0\ 10^6$			BR: 10%
$CO(O^-)CH_2CH(O^{\bullet})CO(OH) \rightarrow CO(O^-)CH_2C^{\bullet}(OH)CO(OH)$					9
$CO(O^-)CH_2C^{\bullet}(OH)CO(OH) + O_2 \rightarrow CO(O^-)CH_2C(OH)(OO^{\bullet})CO(OH)$		$2.0\ 10^9$			2
$2\ CO(O^-)CH_2CH(OO^{\bullet})CO(OH) \rightarrow 0.90\ CO(O^-)CH_2COCO(OH) + 0.30\ CO(O^-)CH_2CH(OH)CO(OH) + 0.20\ CO(O^-)CH_2C(OH)(OO^{\bullet})CO(OH) + 0.60\ CO(O^-)CH_2CHO + 0.60\ CO_2 + 0.60\ H_2O_2 + 0.20\ O_2$	R(9)	$7.5\ 10^7$			= k(2 $CH_2(OO^{\bullet})CO(O^-)$) - 10
Pathway 1: $2\ CO(O^-)CH_2CH(OO^{\bullet})CO(O^-) \rightarrow 2\ CO(O^-)CH_2COCO(O^-) + H_2O_2$		$2.2\ 10^7$			BR: 30%
Pathway 2: $2\ CO(O^-)CH_2CH(OO^{\bullet})CO(O^-)\ (+\ 2\ H_2O) \rightarrow 2\ CO(O^-)CH_2CHO + 2\ CO_2 + H_2O_2 + 2\ OH^-$		$2.2\ 10^7$			BR: 30%
Pathway 3: $2\ CO(O^-)CH_2CH(OO^{\bullet})CO(O^-) \rightarrow CO(O^-)CH_2COCO(O^-) + CO(O^-)CH_2CH(OH)CO(O^-) + O_2$		$2.2\ 10^7$			BR: 30%
Pathway 4: $2\ CO(O^-)CH_2CH(OO^{\bullet})CO(O^-) \rightarrow 2\ CO(O^-)CH_2CH(O^{\bullet})CO(O^-) + O_2$		$9.0\ 10^6$			BR: 10%
$CO(O^-)CH_2CH(O^{\bullet})CO(O^-) \rightarrow CO(O^-)CH_2C^{\bullet}(OH)CO(O^-)$					9
$CO(O^-)CH_2C^{\bullet}(OH)CO(O^-) + O_2 \rightarrow CO(O^-)CH_2C(OH)(OO^{\bullet})CO(O^-)$		$2.0\ 10^9$			2
$2\ CO(O^-)CH_2CH(OO^{\bullet})CO(O^-) \rightarrow 0.90\ CO(O^-)CH_2COCO(O^-) + 0.60\ CO(O^-)CH_2CHO + 0.30\ CO(O^-)CH_2CH(OH)CO(O^-) + 0.20\ CO(O^-)CH_2C(OH)(OO^{\bullet})CO(O^-) + 0.60\ CO_2 + 0.60\ H_2O_2 + 0.60\ OH^- - 0.60\ H_2O + 0.20\ O_2$	R(10)	$7.5\ 10^7$			= k(2 $CH_2(OO^{\bullet})CO(O^-)$) - 10
$CO(OH)CH_2C(OH)(OO^{\bullet})CO(OH) + OH^- \rightarrow CO(OH)CH_2C(O^-)(OO^{\bullet})CO(OH) + H_2O$		$4.9\ 10^9$			
$CO(OH)CH_2C(O^-)(OO^{\bullet})CO(OH) \rightarrow CO(OH)CH_2COCO(OH) + O_2^{\bullet-}$					11
$CO(OH)CH_2C(OH)(OO^{\bullet})CO(OH) + OH^- \rightarrow CO(OH)CH_2COCO(OH) + O_2^{\bullet-} + H_2O$	R(11)	$4.9\ 10^9$			= k($CH_3CH(OH)(OO^{\bullet})$ + OH^-)
$CO(OH)CH_2C(OH)(OO^{\bullet})CO(OH) \rightarrow CO(OH)CH_2COCO(OH) + HO_2^{\bullet}$	R(12)	$1.9\ 10^2$			12
$CO(OH)CH_2C(OH)(OO^{\bullet})CO(O^-) + OH^- \rightarrow CO(OH)CH_2C(O^-)(OO^{\bullet})CO(O^-) + H_2O$		$4.9\ 10^9$			
$CO(OH)CH_2C(O^-)(OO^{\bullet})CO(O^-) \rightarrow CO(OH)CH_2COCO(O^-) + O_2^{\bullet-}$					11
$CO(OH)CH_2C(OH)(OO^{\bullet})CO(O^-) + OH^- \rightarrow CO(OH)CH_2COCO(O^-) + O_2^{\bullet-} + H_2O$	R(13)	$4.9\ 10^9$			= k($CH_3CH(OH)(OO^{\bullet})$ + OH^-)
$CO(OH)CH_2C(OH)(OO^{\bullet})CO(O^-) \rightarrow CO(OH)CH_2COCO(O^-) + HO_2^{\bullet}$	R(14)	$1.9\ 10^2$			12
$CO(O^-)CH_2C(OH)(OO^{\bullet})CO(OH) + OH^- \rightarrow CO(O^-)CH_2C(O^-)(OO^{\bullet})CO(OH) + H_2O$		$4.9\ 10^9$			
$CO(O^-)CH_2C(O^-)(OO^{\bullet})CO(OH) \rightarrow CO(O^-)CH_2COCO(OH) + O_2^{\bullet-}$					11
$CO(O^-)CH_2C(OH)(OO^{\bullet})CO(OH) + OH^- \rightarrow CO(O^-)CH_2COCO(OH) + O_2^{\bullet-} + H_2O$	R(15)	$4.9\ 10^9$			= k($CH_3CH(OH)(OO^{\bullet})$ + OH^-)
$CO(O^-)CH_2C(OH)(OO^{\bullet})CO(OH) \rightarrow CO(O^-)CH_2COCO(OH) + HO_2^{\bullet}$	R(16)	$1.9\ 10^2$			12
$CO(O^-)CH_2C(OH)(OO^{\bullet})CO(O^-) + OH^- \rightarrow CO(O^-)CH_2C(O^-)(OO^{\bullet})CO(O^-) + H_2O$		$4.9\ 10^9$			
$CO(O^-)CH_2C(O^-)(OO^{\bullet})CO(O^-) \rightarrow CO(O^-)CH_2COCO(O^-) + O_2^{\bullet-}$					11
$CO(O^-)CH_2C(OH)(OO^{\bullet})CO(O^-) + OH^- \rightarrow CO(O^-)CH_2COCO(O^-) + O_2^{\bullet-} + H_2O$	R(17)	$4.9\ 10^9$			= k($CH_3CH(OH)(OO^{\bullet})$ + OH^-)
$CO(O^-)CH_2C(OH)(OO^{\bullet})CO(O^-) \rightarrow CO(O^-)CH_2COCO(O^-) + HO_2^{\bullet}$	R(18)	$1.9\ 10^2$			12
Oxidation of Oxaloacetic Acid					13
Pathway 1: $CO(OH)CH_2C(OH)(OH)CO(OH) + HO^{\bullet} \rightarrow CO(OH)CH_2C(OH)(O^{\bullet})CO(OH) + H_2O$		$2.6{\cdot}10^8$			BR: 100% - 14
$CO(OH)CH_2C(OH)(O^{\bullet})CO(OH) \rightarrow CO(OH)CH_2CO(OH) + C^{\bullet}O(OH)$					5 - 6
$C^{\bullet}O(OH) + O_2 \rightarrow CO(OH)(OO^{\bullet})$		$2.0{\cdot}10^9$			2
$CO(OH)CH_2C(OH)(OH)CO(OH) + HO^{\bullet} \rightarrow CO(OH)CH_2CO(OH) + CO(OH)(OO^{\bullet}) + H_2O - O_2$	R(19)	$2.6\ 10^8$			8
Pathway 1: $CO(OH)CH_2C(OH)(OH)CO(OH) + NO_3^{\bullet} \rightarrow CO(OH)C^{\bullet}HC(OH)(OH)CO(OH) + NO_3^- + H^+$		$5.1\ 10^4$			BR: 100%
$CO(OH)C^{\bullet}HC(OH)(OH)CO(OH) + O_2 \rightarrow CO(OH)CH(OO^{\bullet})C(OH)(OH)CO(OH)$		$2.0\ 10^9$			2
$CO(OH)CH_2C(OH)(OH)CO(OH) + NO_3^{\bullet} \rightarrow CO(OH)CH(OO^{\bullet})C(OH)(OH)CO(OH) + NO_3^- + H^+ - O_2$	R(20)	$5.1\ 10^4$			= k($CO(OH)CH_2CO(OH) + NO_3^{\bullet}$) - 3
Pathway 1: $CO(OH)CH_2COCO(O^-) + HO^{\bullet} \rightarrow CO(OH)CH_2COCO(O^{\bullet}) + OH^-$		$6.3\ 10^7$			BR: 100% - 15

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CO(OH)CH_2COCO(O^\bullet) \rightarrow CO(OH)CH_2C^\bullet O + CO_2$					5 - 6
$CO(OH)CH_2C^\bullet O + O_2 \rightarrow CO(OH)CH_2CO(OO^\bullet)$		$2.0\ 10^9$			2
$CO(OH)CH_2COCO(O^-) + HO^\bullet \rightarrow CO(OH)CH_2CO(OO^\bullet) + CO_2 + OH^- - O_2$	R(21)	$6.3\ 10^7$			8
Pathway 1: $CO(OH)CH_2COCO(O^-) + NO_3^\bullet \rightarrow CO(OH)C^\bullet HCOCO(O^-) + NO_3^- + H^+$		5.610^6	3369		BR: 100%
$CO(OH)C^\bullet HCOCO(O^-) + O_2 \rightarrow CO(OH)CH(OO^\bullet)COCO(O^-)$		$2.0\ 10^9$			2
$CO(OH)CH_2COCO(O^-) + NO_3^\bullet \rightarrow CO(OH)CH(OO^\bullet)COCO(O^-) + NO_3^- + H^+ - O_2$	R(22)	5.610^6	3369		= k(CO(OH)CH2CO(O-) + NO3•) - 3
Pathway 1: $CO(O^-)CH_2COCO(OH) + HO^\bullet \rightarrow CO(O^\bullet)CH_2COCO(OH) + OH^-$		$2.5\ 10^8$			BR: 100% - 16
$CO(O^\bullet)CH_2COCO(OH) \rightarrow C^\bullet H_2COCO(OH) + CO_2$					5 - 6
$C^\bullet H_2COCO(OH) + O_2 \rightarrow CO(OH)COCH_2(OO^\bullet)$		$2.0\ 10^9$			2
$CO(O^-)CH_2COCO(OH) + HO^\bullet \rightarrow CO(OH)COCH_2(OO^\bullet) + CO_2 + OH^- - O_2$	R(23)	$2.5\ 10^8$			8
Pathway 1: $CO(O^-)CH_2COCO(OH) + NO_3^\bullet \rightarrow CO(O^-)C^\bullet HCOCO(OH) + NO_3^- + H^+$		$5.6\ 10^6$	3369		BR: 100%
$CO(O^-)C^\bullet HCOCO(OH) + O_2 \rightarrow CO(O^-)CH(OO^\bullet)COCO(OH)$		$2.0\ 10^9$			2
$CO(O^-)CH_2COCO(OH) + NO_3^\bullet \rightarrow CO(O^-)CH(OO^\bullet)COCO(OH) + NO_3^- + H^+ - O_2$	R(24)	$5.6\ 10^6$	3369		= k(CO(OH)CH2CO(O-) + NO3•) - 3
Pathway 1: $CO(O^-)CH_2C(OH)(OH)CO(OH) + HO^\bullet \rightarrow CO(O^\bullet)CH_2C(OH)(OH)CO(OH) + OH^-$		$2.7\ 10^8$			BR: 50% - 17
$CO(O^\bullet)CH_2C(OH)(OH)CO(OH) \rightarrow C^\bullet H_2C(OH)(OH)CO(OH) + CO_2$					5 - 6
$C^\bullet H_2C(OH)(OH)CO(OH) + O_2 \rightarrow CH_2(OO^\bullet)C(OH)(OH)CO(OH)$		$2.0\ 10^9$			2
Pathway 2: $CO(O^-)CH_2C(OH)(OH)CO(OH) + HO^\bullet \rightarrow CO(O^-)CH_2C(OH)(O^\bullet)CO(OH) + H_2O$		$2.7\ 10^8$			BR: 50% - 17
$CO(O^-)CH_2C(OH)(O^\bullet)CO(OH) \rightarrow CO(O^-)CH_2CO(OH) + C^\bullet O(OH)$					5 - 6
$C^\bullet O(OH) + O_2 \rightarrow CO(OH)(OO^\bullet)$		$2.0\ 10^9$			2
$CO(O^-)CH_2C(OH)(OH)CO(OH) + HO^\bullet \rightarrow 0.50\ CO(OH)C(OH)(OH)CH_2(OO^\bullet) + 0.50\ CO(OH)CH_2CO(O^-) + 0.50\ CO(OH)(OO^\bullet) + 0.50\ CO_2 + 0.50\ OH^- + 0.50\ H_2O - O_2$	R(25)	$5.4\ 10^8$			8
Pathway 1: $CO(O^-)CH_2C(OH)(OH)CO(OH) + NO_3^\bullet \rightarrow CO(O^-)C^\bullet HC(OH)(OH)CO(OH) + NO_3^- + H^+$		$5.6\ 10^6$	3369		BR: 100%
$CO(O^-)C^\bullet HC(OH)(OH)CO(OH) + O_2 \rightarrow CO(O^-)CH(OO^\bullet)C(OH)(OH)CO(OH)$		$2.0\ 10^9$			2
$CO(O^-)CH_2C(OH)(OH)CO(OH) + NO_3^\bullet \rightarrow CO(O^-)CH(OO^\bullet)C(OH)(OH)CO(OH) + NO_3^- + H^+ - O_2$	R(26)	$5.6\ 10^6$	3369		= k(CO(OH)CH2CO(O-) + NO3•) - 3
Pathway 1: $CO(O^-)CH_2COCO(O^-) + HO^\bullet \rightarrow CO(O^\bullet)CH_2COCO(O^-) + OH^-$		$2.6\ 10^8$			BR: 82% - 18
$CO(O^\bullet)CH_2COCO(O^-) \rightarrow C^\bullet H_2COCO(O^-) + CO_2$					5 - 6
$C^\bullet H_2COCO(O^-) + O_2 \rightarrow CH_2(OO^\bullet)COCO(O^-)$		$2.0\ 10^9$			2
Pathway 2: $CO(O^-)CH_2COCO(O^-) + HO^\bullet \rightarrow CO(O^-)CH_2COCO(O^\bullet) + OH^-$		$5.8\ 10^7$			BR: 18% - 18
$CO(O^-)CH_2COCO(O^\bullet) \rightarrow CO(O^-)CH_2C^\bullet O + CO_2$					5 - 6
$CO(O^-)CH_2C^\bullet O + O_2 \rightarrow CO(O^-)CH_2CO(OO^\bullet)$		$2.0\ 10^9$			2
$CO(O^-)CH_2COCO(O^-) + HO^\bullet \rightarrow 0.82\ CH_2(OO^\bullet)COCO(O^-) + 0.18\ CO(O^-)CH_2CO(OO^\bullet) + CO_2 + OH^- - O_2$	R(27)	$3.2\ 10^8$			8
Pathway 1: $CO(O^-)CH_2COCO(O^-) + NO_3^\bullet \rightarrow CO(O^-)C^\bullet HCOCO(O^-) + NO_3^- + H^+$		$2.3\ 10^7$	3008		BR: 100%
$CO(O^-)C^\bullet HCOCO(O^-) + O_2 \rightarrow CO(O^-)CH(OO^\bullet)COCO(O^-)$		$2.0\ 10^9$			2
$CO(O^-)CH_2COCO(O^-) + NO_3^\bullet \rightarrow CO(O^-)CH(OO^\bullet)COCO(O^-) + NO_3^- + H^+ - O_2$	R(28)	$2.3\ 10^7$	3008		= k(CO(O-)CH2CO(O-) + NO3•) - 3
Pathway 1: $2\ CO(OH)CH(OO^\bullet)C(OH)(OH)CO(OH) \rightarrow 2\ CO(OH)COC(OH)(OH)CO(OH) + H_2O_2$		$2.2\ 10^7$			BR: 30%
Pathway 2: $2\ CO(OH)CH(OO^\bullet)C(OH)(OH)CO(OH)$ *(+ 2 H_2O)* $\rightarrow 2\ CHOC(OH)(OH)CO(OH) + 2\ CO_2 + H_2O_2 + 2\ H_2O$		$2.2\ 10^7$			BR: 30%
Pathway 3: $2\ CO(OH)CH(OO^\bullet)C(OH)(OH)CO(OH) \rightarrow CO(OH)CH(OH)C(OH)(OH)CO(OH) + CO(OH)COC(OH)(OH)CO(OH) + O_2$		$2.2\ 10^7$			BR: 30%
Pathway 4: $2\ CO(OH)CH(OO^\bullet)C(OH)(OH)CO(OH) \rightarrow 2\ CO(OH)CH(O^\bullet)C(OH)(OH)CO(OH) + O_2$		$9.0\ 10^6$			BR: 10%
$CO(OH)CH(O^\bullet)C(OH)(OH)CO(OH) \rightarrow CO(OH)C^\bullet(OH)C(OH)(OH)CO(OH)$					9
$CO(OH)C^\bullet(OH)C(OH)(OH)CO(OH) + O_2 \rightarrow CO(OH)C(OH)(OO^\bullet)C(OH)(OH)CO(OH)$		$2.0\ 10^9$			2
$2\ CO(OH)CH(OO^\bullet)C(OH)(OH)CO(OH) \rightarrow 0.90\ CO(OH)COC(OH)(OH)CO(OH) + 0.60\ CO(OH)C(OH)(OH)CHO + 0.30\ CO(OH)CH(OH)C(OH)(OH)CO(OH) + 0.20\ CO(OH)C(OH)(OO^\bullet)C(OH)(OH)CO(OH) + 0.60\ CO_2 + 0.60\ H_2O_2 + 0.20\ O_2$	R(29)	$7.5\ 10^7$			= k(2 CH2(OO•)CO(O-)) - 10
Pathway 1: $2\ CO(OH)CH(OO^\bullet)COCO(O^-) \rightarrow 2\ CO(OH)COCOCO(O^-) + H_2O_2$		$2.2\ 10^7$			BR: 30%
Pathway 2: $2\ CO(OH)CH(OO^\bullet)COCO(O^-)$ *(+ 2 H_2O)* $\rightarrow 2\ CHOCOCO(O^-) + 2\ CO_2 + H_2O_2 + 2\ H_2O$		$2.2\ 10^7$			BR: 30%
Pathway 3: $2\ CO(OH)CH(OO^\bullet)COCO(O^-) \rightarrow CO(OH)CH(OH)COCO(O^-) + CO(OH)COCOCO(O^-) + O_2$		$2.2\ 10^7$			BR: 30%

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
Pathway 4: 2 $CO(OH)CH(OO^{\bullet})COCO(O^-)$ → 2 $CO(OH)CH(O^{\bullet})COCO(O^-)$ + O_2		9.0 10^6			BR: 10%
$CO(OH)CH(O^{\bullet})COCO(O^-)$ → $CO(OH)C^{\bullet}(OH)COCO(O^-)$					9
$CO(OH)C^{\bullet}(OH)COCO(O^-)$ + O_2 → $CO(OH)C(OH)(OO^{\bullet})COCO(O^-)$		2.0 10^9			2
2 $CO(OH)CH(OO^{\bullet})COCO(O^-)$ → 0.90 $CO(OH)COCOCO(O^-)$ + 0.60 $CO(O^-)COCHO$ + 0.30 $CO(OH)CH(OH)COCO(O^-)$ + 0.20 $CO(OH)C(OH)(OO^{\bullet})COCO(O^-)$ + 0.60 CO_2 + 0.60 H_2O_2 + 0.20 O_2	R(30)	7.5 10^7			= k(2 $CH_2(OO^{\bullet})CO(O^-)$) - 10
Pathway 1: 2 $CO(O^-)CH(OO^{\bullet})COCO(OH)$ → 2 $CO(O^-)COCOCO(OH)$ + H_2O_2		2.2 10^7			BR: 30%
Pathway 2: 2 $CO(O^-)CH(OO^{\bullet})COCO(OH)$ *(+ 2 H_2O)* → 2 $CHOCOCO(OH)$ + 2 CO_2 + H_2O_2 + 2 OH^-		2.2 10^7			BR: 30%
Pathway 3: 2 $CO(O^-)CH(OO^{\bullet})COCO(OH)$ → $CO(O^-)CH(OH)COCO(OH)$ + $CO(O^-)COCOCO(OH)$ + O_2		2.2 10^7			BR: 30%
Pathway 4: 2 $CO(O^-)CH(OO^{\bullet})COCO(OH)$ → 2 $CO(O^-)CH(O^{\bullet})COCO(OH)$ + O_2		9.0 10^6			BR: 10%
$CO(O^-)CH(O^{\bullet})COCO(OH)$ → $CO(O^-)C^{\bullet}(OH)COCO(OH)$					9
$CO(O^-)C^{\bullet}(OH)COCO(OH)$ + O_2 → $CO(O^-)C(OH)(OO^{\bullet})COCO(OH)$		2.0 10^9			2
2 $CO(O^-)CH(OO^{\bullet})COCO(OH)$ → 0.90 $CO(OH)COCOCO(O^-)$ + 0.60 $CO(OH)COCHO$ + 0.30 $CO(O^-)CH(OH)COCO(OH)$ + 0.20 $CO(O^-)C(OH)(OO^{\bullet})COCO(OH)$ + 0.60 CO_2 + 0.60 H_2O_2 + 0.60 OH^- - 0.60 H_2O + 0.20 O_2	R(31)	7.5 10^7			= k(2 $CH_2(OO^{\bullet})CO(O^-)$) - 10
Pathway 1: 2 $CO(O^-)CH(OO^{\bullet})C(OH)(OH)CO(OH)$ → 2 $CO(O^-)COC(OH)(OH)CO(OH)$ + H_2O_2		2.2 10^7			BR: 30%
Pathway 2: 2 $CO(O^-)CH(OO^{\bullet})C(OH)(OH)CO(OH)$ *(+ 2 H_2O)* → 2 $CHOC(OH)(OH)CO(OH)$ + 2 CO_2 + H_2O_2 + 2 OH^-		2.2 10^7			BR: 30%
Pathway 3: 2 $CO(O^-)CH(OO^{\bullet})C(OH)(OH)CO(OH)$ → $CO(O^-)CH(OH)C(OH)(OH)CO(OH)$ + $CO(O^-)COC(OH)(OH)CO(OH)$ + O_2		2.2 10^7			BR: 30%
Pathway 4: 2 $CO(O^-)CH(OO^{\bullet})C(OH)(OH)CO(OH)$ → 2 $CO(O^-)CH(O^{\bullet})C(OH)(OH)CO(OH)$ + O_2		9.0 10^6			BR: 10%
$CO(O^-)CH(O^{\bullet})C(OH)(OH)CO(OH)$ → $CO(O^-)C^{\bullet}(OH)C(OH)(OH)CO(OH)$					9
$CO(O^-)C^{\bullet}(OH)C(OH)(OH)CO(OH)$ + O_2 → $CO(O^-)C(OH)(OO^{\bullet})C(OH)(OH)CO(OH)$		2.0 10^9			2
2 $CO(O^-)CH(OO^{\bullet})C(OH)(OH)CO(OH)$ → 0.90 $CO(OH)COC(OH)(OH)CO(O^-)$ + 0.60 $CO(OH)C(OH)(OH)CHO$ + 0.30 $CO(O^-)CH(OH)C(OH)(OH)CO(OH)$ + 0.20 $CO(O^-)C(OH)(OO^{\bullet})C(OH)(OH)CO(OH)$ + 0.60 CO_2 + 0.60 H_2O_2 + 0.60 OH^- - 0.60 H_2O + 0.20 O_2	R(32)	7.5 10^7			= k(2 $CH_2(OO^{\bullet})CO(O^-)$) - 10
Pathway 1: 2 $CO(O^-)CH(OO^{\bullet})COCO(O^-)$ → 2 $CO(O^-)COCOCO(O^-)$ + H_2O_2		2.2 10^7			BR: 30%
Pathway 2: 2 $CO(O^-)CH(OO^{\bullet})COCO(O^-)$ *(+ 2 H_2O)* → 2 $CHOCOCO(O^-)$ + 2 CO_2 + H_2O_2 + 2 OH^-		2.2 10^7			BR: 30%
Pathway 3: 2 $CO(O^-)CH(OO^{\bullet})COCO(O^-)$ → $CO(O^-)CH(OH)COCO(O^-)$ + $CO(O^-)COCOCO(O^-)$ + O_2		2.2 10^7			BR: 30%
Pathway 4: 2 $CO(O^-)CH(OO^{\bullet})COCO(O^-)$ → 2 $CO(O^-)CH(O^{\bullet})COCO(O^-)$ + O_2		9.0 10^6			BR: 10%
$CO(O^-)CH(O^{\bullet})COCO(O^-)$ → $CO(O^-)C^{\bullet}(OH)COCO(O^-)$					9
$CO(O^-)C^{\bullet}(OH)COCO(O^-)$ + O_2 → $CO(O^-)C(OH)(OO^{\bullet})COCO(O^-)$		2.0 10^9			2
2 $CO(O^-)CH(OO^{\bullet})COCO(O^-)$ → 0.90 $CO(O^-)COCOCO(O^-)$ + 0.60 $CO(O^-)COCHO$+ 0.30 $CO(O^-)CH(OH)COCO(O^-)$ + 0.20 $CO(O^-)C(OH)(OO^{\bullet})COCO(O^-)$ + 0.60 CO_2 + 0.60 H_2O_2 + 0.60 OH^- - 0.60 H_2O + 0.20 O_2	R(33)	7.5 10^7			= k(2 $CH_2(OO^{\bullet})CO(O^-)$) - 10
Oxidation of Malic Acid					
Pathway 1: $CO(OH)CH_2CH(OH)CO(OH)$ + $HO^{\bullet}$ → $CO(OH)CH_2CH(O^{\bullet})CO(OH)$ + H_2O		1.8 10^8			BR: 50% - 19
$CO(OH)CH_2CH(O^{\bullet})CO(OH)$ → $CO(OH)CH_2CHO$ + $C^{\bullet}O(OH)$					5 - 6
$C^{\bullet}O(OH)$ + O_2 → $CO(OH)(OO^{\bullet})$		2.0 10^9			2
Pathway 2: $CO(OH)CH_2CH(OH)CO(OH)$ + $HO^{\bullet}$ → $CO(OH)CH_2C^{\bullet}(OH)CO(OH)$ + H_2O		1.8 10^8			BR: 50% - 19
$CO(OH)CH_2C^{\bullet}(OH)CO(OH)$ + O_2 → $CO(OH)CH_2C(OH)(OO^{\bullet})CO(OH)$		2.0 10^9			2
$CO(OH)CH_2CH(OH)CO(OH)$ + $HO^{\bullet}$ → 0.50 $CO(OH)CH_2CHO$ + 0.50 $CO(OH)(OO^{\bullet})$ + 0.50 $CO(OH)CH_2C(OH)(OO^{\bullet})CO(OH)$ + H_2O - O_2	R(34)	3.6 10^8		Herrmann et al., 2010	
Pathway 1: $CO(OH)CH_2CH(OH)CO(OH)$ + $NO_3^{\bullet}$ → $CO(OH)CH_2C^{\bullet}(OH)CO(OH)$ + NO_3^- + H^+		5.1 10^4			BR: 100%
$CO(OH)CH_2C^{\bullet}(OH)CO(OH)$ + O_2 → $CO(OH)CH_2C(OH)(OO^{\bullet})CO(OH)$		2.0 10^9			2
$CO(OH)CH_2CH(OH)CO(OH)$ + $NO_3^{\bullet}$ → $CO(OH)CH_2C(OH)(OO^{\bullet})CO(OH)$ + NO_3^- + H^+ - O_2	R(35)	5.1 10^4			= k($CO(OH)CH(OH)CO(OH)$ + $NO_3^{\bullet}$) - 3
Pathway 1: $CO(OH)CH_2CH(OH)CO(O^-)$ + $HO^{\bullet}$ → $CO(OH)CH_2C^{\bullet}(OH)CO(O^-)$ + H_2O		2.1 10^8			BR: 48% - 20
$CO(OH)CH_2C^{\bullet}(OH)CO(O^-)$ + O_2 → $CO(OH)CH_2C(OH)(OO^{\bullet})CO(O^-)$		2.0 10^9			2
Pathway 2: $CO(OH)CH_2CH(OH)CO(O^-)$ + $HO^{\bullet}$ → $CO(OH)CH_2CH(OH)CO(O^{\bullet})$ + OH^-		1.2 10^8			BR: 27% - 20

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CO(OH)CH_2CH(OH)CO(O^•) \rightarrow CO(OH)CH_2C^•H(OH) + CO_2$					5 - 6
$CO(OH)CH_2C^•H(OH) + O_2 \rightarrow CO(OH)CH_2CH(OH)(OO^•)$		$2.0\ 10^9$			2
Pathway 3: $CO(OH)CH_2CH(OH)CO(O^-) + HO^• \rightarrow CO(OH)CH_2CH(O^•)CO(O^-) + H_2O$		$1.1\ 10^8$			BR: 25% - 20
$CO(OH)CH_2CH(O^•)CO(O^-) \rightarrow CO(OH)CH_2CHO + C^•O(O^-)$					5 - 6
$C^•O(O^-) + O_2 \rightarrow CO(O^-)(OO^•)$		$2.0\ 10^9$			2
$CO(OH)CH_2CH(OH)CO(O^-) + HO^• \rightarrow 0.48\ CO(OH)CH_2C(OH)(OO^•)CO(O^-) + 0.27\ CH(OH)(OO^•)CH_2CO(OH) + 0.25\ CO(OH)CH_2CHO + 0.25\ CO(O^-)(OO^•) + 0.27\ CO_2 + 0.27\ OH^- + 0.73\ H_2O - O_2$	R(36)	$4.8\ 10^9$		Herrmann et al., 2010	21
Pathway 1: $CO(OH)CH_2CH(OH)CO(O^-) + NO_3^• \rightarrow CO(OH)CH_2C^•(OH)CO(O^-) + NO_3^- + H^+$		$5.6\ 10^6$	3369		BR: 100%
$CO(OH)CH_2C^•(OH)CO(O^-) + O_2 \rightarrow CO(OH)CH_2C(OH)(OO^•)CO(O^-)$		$2.0\ 10^9$			2
$CO(OH)CH_2CH(OH)CO(O^-) + NO_3^• \rightarrow CO(OH)CH_2C(OH)(OO^•)CO(O^-) + NO_3^- + H^+ - O_2$	R(37)	$5.6\ 10^6$	3369		= k(CO(OH)CH(OH)CO(O^-) + $NO_3^•$) - 3
Pathway 1: $CO(O^-)CH_2CH(OH)CO(OH) + HO^• \rightarrow CO(O^•)CH_2CH(OH)CO(OH) + OH^-$		$3.5\ 10^8$			BR: 73% - 22
$CO(O^•)CH_2CH(OH)CO(OH) \rightarrow C^•H_2CH(OH)CO(OH) + CO_2$					5 - 6
$C^•H_2CH(OH)CO(OH) + O_2 \rightarrow CH_2(OO^•)CH(OH)CO(OH)$		$2.0\cdot 10^9$			2
Pathway 2: $CO(O^-)CH_2CH(OH)CO(OH) + HO^• \rightarrow CO(O^-)CH_2C^•(OH)CO(OH) + H_2O$		$1.3\ 10^8$			BR: 27% - 22
$CO(O^-)CH_2C^•(OH)CO(OH) + O_2 \rightarrow CO(O^-)CH_2C(OH)(OO^•)CO(OH)$		$2.0\ 10^9$			2
$CO(O^-)CH_2CH(OH)CO(OH) + HO^• \rightarrow 0.27\ CO(O^-)CH_2C(OH)(OO^•)CO(OH) + 0.73\ CH_2(OO^•)CH(OH)CO(OH) + 0.73\ CO_2 + 0.73\ OH^- + 0.27\ H_2O - O_2$	R(38)	$4.8\ 10^9$		Herrmann et al., 2010	21
Pathway 1: $CO(O^-)CH_2CH(OH)CO(OH) + NO_3^• \rightarrow CO(O^-)CH_2C^•(OH)CO(OH) + NO_3^- + H^+$		$5.1\ 10^4$			BR: 100%
$CO(O^-)CH_2C^•(OH)CO(OH) + O_2 \rightarrow CO(O^-)CH_2C(OH)(OO^•)CO(OH)$		$2.0\ 10^9$			2
$CO(O^-)CH_2CH(OH)CO(OH) + NO_3^• \rightarrow CO(O^-)CH_2C(OH)(OO^•)CO(OH) + NO_3^- + H^+ - O_2$	R(39)	$5.1\ 10^4$			= k(CO(OH)CH(OH)CO(OH) + $NO_3^•$) - 3
Pathway 1: $CO(O^-)CH_2CH(OH)CO(O^-) + HO^• \rightarrow CO(O^-)CH_2C^•(OH)CO(O^-) + H_2O$		$4.5\ 10^8$			BR: 48% - 23
$CO(O^-)CH_2C^•(OH)CO(O^-) + O_2 \rightarrow CO(O^-)CH_2C(OH)(OO^•)CO(O^-)$		$2.0\ 10^9$			2
Pathway 2: $CO(O^-)CH_2CH(OH)CO(O^-) + HO^• \rightarrow CO(O^•)CH_2CH(OH)CO(O^-) + OH^-$		$3.4\ 10^8$			BR: 37% - 23
$CO(O^•)CH_2CH(OH)CO(O^-) \rightarrow C^•H_2CH(OH)CO(O^-) + CO_2$					5 - 6
$C^•H_2CH(OH)CO(O^-) + O_2 \rightarrow CH_2(OO^•)CH(OH)CO(O^-)$		$2.0\ 10^9$			2
Pathway 3: $CO(O^-)CH_2CH(OH)CO(O^-) + HO^• \rightarrow CO(O^-)CH_2CH(OH)CO(O^•) + OH^-$		$1.4\ 10^8$			BR: 15% - 23
$CO(O^-)CH_2CH(OH)CO(O^•) \rightarrow CO(O^-)CH_2C^•H(OH) + CO_2$					5 - 6
$CO(O^-)CH_2C^•H(OH) + O_2 \rightarrow CO(O^-)CH_2CH(OH)(OO^•)$		$2.0\ 10^9$			2
$CO(O^-)CH_2CH(OH)CO(O^-) + HO^• \rightarrow 0.48\ CO(O^-)CH_2C(OH)(OO^•)CO(O^-) + 0.37\ CH_2(OO^•)CH(OH)CO(O^-) + 0.15\ CH(OH)(OO^•)CH_2CO(O^-) + 0.52\ CO_2 + 0.52\ OH^- + 0.48\ H_2O - O_2$	R(40)	$8.5\ 10^8$		Herrmann et al., 2010	
Pathway 1: $CO(O^-)CH_2CH(OH)CO(O^-) + NO_3^• \rightarrow CO(O^-)CH_2C^•(OH)CO(O^-) + NO_3^- + H^+$		$5.6\ 10^6$	3369		BR: 100%
$CO(O^-)CH_2C^•(OH)CO(O^-) + O_2 \rightarrow CO(O^-)CH_2C(OH)(OO^•)CO(O^-)$		$2.0\ 10^9$			2
$CO(O^-)CH_2CH(OH)CO(O^-) + NO_3^• \rightarrow CO(O^-)CH_2C(OH)(OO^•)CO(O^-) + NO_3^- + H^+ - O_2$	R(41)	$5.6\ 10^6$	3369		= k(CO(OH)CH(OH)CO(O^-) + $NO_3^•$) - 3
Oxidation of Tartric Acid					
Pathway 1: $CO(OH)CH(OH)CH(OH)CO(OH) + HO^• \rightarrow CO(OH)CH(O^•)CH(OH)CO(OH) + H_2O$		$1.1\ 10^8$			BR: 70% - 24
$CO(OH)CH(O^•)CH(OH)CO(OH) \rightarrow C^•O(OH) + CHOCH(OH)CO(OH)$					5 - 6
$C^•O(OH) + O_2 \rightarrow CO(OH)(OO^•)$		$2.0\ 10^9$			2
Pathway 2: $CO(OH)CH(OH)CH(OH)CO(OH) + HO^• \rightarrow CO(OH)C^•(OH)CH(OH)CO(OH) + H_2O$		$5.0\ 10^7$			BR: 30% - 24
$CO(OH)C^•(OH)CH(OH)CO(OH) + O_2 \rightarrow CO(OH)C(OH)(OO^•)CH(OH)CO(OH)$		$2.0\cdot 10^9$			2
$CO(OH)CH(OH)CH(OH)CO(OH) + HO^• \rightarrow 0.70\ CHOCH(OH)CO(OH) + 0.70\ CO(OH)(OO^•) + 0.30\ CO(OH)CH(OH)C(OH)(OO^•)CO(OH) + H_2O - O_2$	R(42)	$1.6\ 10^8$			8
Pathway 1: $CO(OH)CH(OH)CH(OH)CO(OH) + NO_3^• \rightarrow CO(OH)C^•(OH)CH(OH)CO(OH) + NO_3^- + H^+$		$5.1\ 10^4$			BR: 100%

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CO(OH)C^{\bullet}(OH)CH(OH)CO(OH) + O_2 \rightarrow CO(OH)C(OH)(OO^{\bullet})CH(OH)CO(OH)$		$2.0\ 10^9$			2
$CO(OH)CH(OH)CH(OH)CO(OH) + NO_3^{\bullet} \rightarrow CO(OH)CH(OH)C(OH)(OO^{\bullet})CO(OH) + NO_3^- + H^+ - O_2$	R(43)	$5.1\ 10^4$			=k(CO(OH)CH(OH)CO(OH) + $NO_3^{\bullet}$) - 3
Pathway 1: $CO(OH)CH(OH)CH(OH)CO(O^-) + HO^{\bullet} \rightarrow CO(OH)CH(OH)CH(OH)CO(O^{\bullet}) + OH^-$		$1.4\ 10^8$			BR: 37% - 25
$CO(OH)CH(OH)CH(OH)CO(O^{\bullet}) \rightarrow CO(OH)CH(OH)C^{\bullet}H(OH) + CO_2$					5 - 6
$CO(OH)CH(OH)C^{\bullet}H(OH) + O_2 \rightarrow CO(OH)CH(OH)CH(OH)(OO^{\bullet})$		$2.0\ 10^9$			2
Pathway 2: $CO(OH)CH(OH)CH(OH)CO(O^-) + HO^{\bullet} \rightarrow CO(OH)CH(OH)CH(O^{\bullet})CO(O^-) + H_2O$		$1.4\ 10^8$			BR: 35% - 25
$CO(OH)CH(OH)CH(O^{\bullet})CO(O^-) \rightarrow CO(OH)CH(OH)CHO + C^{\bullet}O(O^-)$					5 - 6
$C^{\bullet}O(O^-) + O_2 \rightarrow CO(O^-)(OO^{\bullet})$		$2.0\ 10^9$			2
Pathway 3: $CO(OH)CH(OH)CH(OH)CO(O^-) + HO^{\bullet} \rightarrow CO(OH)CH(OH)C^{\bullet}(OH)CO(O^-) + H_2O$		$1.1\ 10^8$			BR: 28% - 25
$CO(OH)CH(OH)C^{\bullet}(OH)CO(O^-) + O_2 \rightarrow CO(OH)CH(OH)C(OH)(OO^{\bullet})CO(O^-)$		$2.0\ 10^9$			2
$CO(OH)CH(OH)CH(OH)CO(O^-) + HO^{\bullet} \rightarrow 0.37\ CH(OH)(OO^{\bullet})CH(OH)CO(OH) + 0.35\ CHOCH(OH)CO(OH) + 0.35\ CO(O^-)(OO^{\bullet}) + 0.28\ CO(OH)CH(OH)C(OH)(OO^{\bullet})CO(O^-) + 0.37\ CO_2 + 0.37\ OH^- + 0.63\ H_2O - O_2$	R(44)	$3.9\ 10^8$			8
Pathway 1: $CO(OH)CH(OH)CH(OH)CO(O^-) + NO_3^{\bullet} \rightarrow CO(OH)CH(OH)C^{\bullet}(OH)CO(O^-) + NO_3^- + H^+$		$5.6\ 10^6$	3369		BR: 100%
$CO(OH)CH(OH)C^{\bullet}(OH)CO(O^-) + O_2 \rightarrow CO(OH)CH(OH)C(OH)(OO^{\bullet})CO(O^-)$					
$CO(OH)CH(OH)CH(OH)CO(O^-) + NO_3^{\bullet} \rightarrow CO(OH)CH(OH)C(OH)(OO^{\bullet})CO(O^-) + NO_3^- + H^+ - O_2$	R(45)	$5.6\ 10^6$	3369		=k(CO(OH)CH(OH)CO(O^-) + $NO_3^{\bullet}$) - 3
Pathway 1: $CO(O^-)CH(OH)CH(OH)CO(O^-) + HO^{\bullet} \rightarrow CO(O^-)CH(OH)C^{\bullet}(OH)CO(O^-) + H_2O$		$2.9\ 10^8$			BR: 41% - 26
$CO(O^-)CH(OH)C^{\bullet}(OH)CO(O^-) + O_2 \rightarrow CO(O^-)CH(OH)C(OH)(OO^{\bullet})CO(O^-)$		$2.0\ 10^9$			2
Pathway 2: $CO(O^-)CH(OH)CH(OH)CO(O^-) + HO^{\bullet} \rightarrow CO(O^-)CH(OH)CH(OH)CO(O^{\bullet}) + OH^-$		$2.1\ 10^8$			BR: 31% - 26
$CO(O^-)CH(OH)CH(OH)CO(O^{\bullet}) \rightarrow CO(O^-)CH(OH)C^{\bullet}H(OH) + CO_2$					5 - 6
$CO(O^-)CH(OH)C^{\bullet}H(OH) + O_2 \rightarrow CO(O^-)CH(OH)CH(OH)(OO^{\bullet})$		$2.0\ 10^9$			2
Pathway 3: $CO(O^-)CH(OH)CH(OH)CO(O^-) + HO^{\bullet} \rightarrow CO(O^-)CH(OH)CH(O^{\bullet})CO(O^-) + H_2O$		$2.0\ 10^8$			BR: 28% - 26
$CO(O^-)CH(OH)CH(O^{\bullet})CO(O^-) \rightarrow CO(O^-)CH(OH)CHO + C^{\bullet}O(O^-)$					5 - 6
$C^{\bullet}O(O^-) + O_2 \rightarrow CO(O^-)(OO^{\bullet})$		$2.0\ 10^9$			2
$CO(O^-)CH(OH)CH(OH)CO(O^-) + HO^{\bullet} \rightarrow 0.41\ CO(O^-)CH(OH)C(OH)(OO^{\bullet})CO(O^-) + 0.31\ CO(O^-)CH(OH)CH(OH)(OO^{\bullet}) + 0.28\ CO(O^-)CH(OH)CHO + 0.28\ CO(O^-)(OO^{\bullet}) + 0.31\ CO_2 + 0.31\ OH^- + 0.69\ H_2O - O_2$	R(46)	$7.0\ 10^8$			8
Pathway 1: $CO(O^-)CH(OH)CH(OH)CO(O^-) + NO_3^{\bullet} \rightarrow CO(O^-)CH(OH)C^{\bullet}(OH)CO(O^-) + NO_3^- + H^+$		$5.6\ 10^6$	3369		BR: 100%
$CO(O^-)CH(OH)C^{\bullet}(OH)CO(O^-) + O_2 \rightarrow CO(O^-)CH(OH)C(OH)(OO^{\bullet})CO(O^-)$		$2.0\ 10^9$			2
$CO(O^-)CH(OH)CH(OH)CO(O^-) + NO_3^{\bullet} \rightarrow CO(O^-)CH(OH)C(OH)(OO^{\bullet})CO(O^-) + NO_3^- + H^+$	R(47)	$5.6\ 10^6$	3369		=k(CO(OH)CH(OH)CO(O^-) + $NO_3^{\bullet}$) - 3
$CO(OH)C(OH)(OO^{\bullet})CH(OH)CO(OH) + OH^- \rightarrow CO(OH)C(O^-)(OO^{\bullet})CH(OH)CO(OH) + H_2O$		$4.0\ 10^9$			
$CO(OH)C(O^-)(OO^{\bullet})CH(OH)CO(OH) \rightarrow CO(OH)COCH(OH)CO(OH) + O_2^{\bullet-}$					11
$CO(OH)C(OH)(OO^{\bullet})CH(OH)CO(OH) + OH^- \rightarrow CO(OH)CH(OH)COCO(OH) + O_2^{\bullet-} + H_2O$	R(48)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^{\bullet})$ + OH^-)
$CO(OH)C(OH)(OO^{\bullet})CH(OH)CO(OH) \rightarrow CO(OH)CH(OH)COCO(OH) + HO_2^{\bullet}$	R(49)	$1.9\ 10^2$			12
$CO(OH)CH(OH)C(OH)(OO^{\bullet})CO(O^-) + OH^- \rightarrow CO(OH)CH(OH)C(O^-)(OO^{\bullet})CO(O^-) + H_2O$		$4.0\ 10^9$			
$CO(OH)CH(OH)C(O^-)(OO^{\bullet})CO(O^-) \rightarrow CO(OH)CH(OH)COCO(O^-) + O_2^{\bullet-}$					11
$CO(OH)CH(OH)C(OH)(OO^{\bullet})CO(O^-) + OH^- \rightarrow CO(OH)CH(OH)COCO(O^-) + O_2^{\bullet-} + H_2O$	R(50)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^{\bullet})$ + OH^-)
$CO(OH)CH(OH)C(OH)(OO^{\bullet})CO(O^-) \rightarrow CO(OH)CH(OH)COCO(O^-) + HO_2^{\bullet}$	R(51)	$1.9\ 10^2$			12
$CO(O^-)CH(OH)C(OH)(OO^{\bullet})CO(OH) + OH^- \rightarrow CO(O^-)CH(OH)C(O^-)(OO^{\bullet})CO(OH) + H_2O$		$4.0\ 10^9$			
$CO(O^-)CH(OH)C(O^-)(OO^{\bullet})CO(OH) \rightarrow CO(O^-)CH(OH)COCO(OH) + O_2^{\bullet-}$					11
$CO(O^-)CH(OH)C(OH)(OO^{\bullet})CO(OH) + OH^- \rightarrow CO(O^-)CH(OH)COCO(OH) + O_2^{\bullet-} + H_2O$	R(52)	$4.0\ 10^9$			= k($CH_3CH(OH)(OO^{\bullet})$ + OH^-)
$CO(O^-)CH(OH)C(OH)(OO^{\bullet})CO(OH) \rightarrow CO(O^-)CH(OH)COCO(OH) + HO_2^{\bullet}$	R(53)	$1.9\ 10^2$			12
$CO(O^-)CH(OH)C(OH)(OO^{\bullet})CO(O^-) + OH^- \rightarrow CO(O^-)CH(OH)C(O^-)(OO^{\bullet})CO(O^-) + H_2O$		$4.0\ 10^9$			
$CO(O^-)CH(OH)C(O^-)(OO^{\bullet})CO(O^-) \rightarrow CO(O^-)CH(OH)COCO(O^-) + O_2^{\bullet-}$					11

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CO(O^-)CH(OH)C(OH)(OO^\bullet)CO(O^-) + OH^- \rightarrow CO(O^-)CH(OH)COCO(O^-) + O_2^{\bullet-} + H_2O$	R(54)	$4.0\ 10^9$			$= k(CH_3CH(OH)(OO^\bullet) + OH^-)$
$CO(O^-)CH(OH)C(OH)(OO^\bullet)CO(O^-) \rightarrow CO(O^-)CH(OH)COCO(O^-) + HO_2^\bullet$	R(55)	$1.9\ 10^2$			12
Oxidation of fumaric Acid					
$CO(OH)CH=CHCO(OH) + HO^\bullet \rightarrow CO(OH)CH(OH)C^\bullet HCO(OH)$		$6.0\ 10^9$			BR: 100% - 27
$CO(OH)CH(OH)C^\bullet HCO(OH) + O_2 \rightarrow CO(OH)CH(OH)CH(OO^\bullet)CO(OH)$		$2.0\ 10^9$			2
$Cis\text{-}CO(OH)CH=CHCO(OH) + HO^\bullet \rightarrow CO(OH)CH(OH)CH(OO^\bullet)CO(OH) + H_2O - O_2$	R(56)	$5.9\ 10^9$			28
$CO(O^-)CH=CHCO(OH) + HO^\bullet \rightarrow 0.50\ CO(O^-)CH(OH)C^\bullet HCO(OH) + 0.50\ CO(O^-)C^\bullet HCH(OH)CO(OH)$		$6.1\ 10^9$			BR: 100% - 29
$CO(O^-)CH(OH)C^\bullet HCO(OH) + O_2 \rightarrow CO(O^-)CH(OH)CH(OO^\bullet)CO(OH)$		$2.0\ 10^9$			2
$CO(O^-)C^\bullet HCH(OH)CO(OH) + O_2 \rightarrow CO(OH)CH(OH)CH(OO^\bullet)CO(O^-)$		$2.0\ 10^9$			2
$Cis\text{-}CO(O^-)CH=CHCO(OH) + HO^\bullet \rightarrow 0.50\ CO(O^-)CH(OH)CH(OO^\bullet)CO(OH) + 0.50\ CO(OH)CH(OH)CH(OO^\bullet)CO(O^-) + H_2O - O_2$	R(57)	$6.1\ 10^9$			28
$CO(O^-)CH=CHCO(O^-) + HO^\bullet \rightarrow CO(O^-)CH(OH)C^\bullet HCO(O^-)$		$6.3\ 10^9$			BR: 100% - 30
$CO(O^-)CH(OH)C^\bullet HCO(O^-) + O_2 \rightarrow CO(O^-)CH(OH)CH(OO^\bullet)CO(O^-)$		$2.0\ 10^9$			2
$Cis\text{-}CO(O^-)CH=CHCO(O^-) + HO^\bullet \rightarrow CO(O^-)CH(OH)CH(OO^\bullet)CO(O^-) + H_2O - O_2$	R(58)	$6.3\ 10^9$			28
Pathway 1: $2\ CO(OH)CH(OH)CH(OO^\bullet)CO(OH) \rightarrow CO(OH)CH(OH)COCO(OH) + H_2O_2$		$2.2\ 10^7$			BR: 30%
Pathway 2: $2\ CO(OH)CH(OH)CH(OO^\bullet)CO(OH)\ (+\ 2\ H_2O) \rightarrow CHOCH(OH)CO(OH) + 2\ CO_2 + H_2O_2 + 2\ H_2O$		$2.2\ 10^7$			BR: 30%
Pathway 3: $2\ CO(OH)CH(OH)CH(OO^\bullet)CO(OH) \rightarrow CO(OH)CH(OH)CHOCO(OH) + CO(OH)CH(OH)CH(OH)CO(OH) + O_2$		$2.2\ 10^7$			BR: 30%
Pathway 4: $2\ CO(OH)CH(OH)CH(OO^\bullet)CO(OH) \rightarrow CO(OH)CH(OH)CH(O^\bullet)CO(OH) + O_2$		$9.0\ 10^6$			BR: 10%
$CO(OH)CH(OH)CH(O^\bullet)CO(OH) \rightarrow CO(OH)CH(OH)C^\bullet(OH)CO(OH)$					9
$CO(OH)CH(OH)C^\bullet(OH)CO(OH) \rightarrow CO(OH)CH(OH)C(OH)(OO^\bullet)CO(OH)$		$2.0\ 10^9$			2
$2\ CO(OH)CH(OH)CH(OO^\bullet)CO(OH) \rightarrow 0.90\ CO(OH)CH(OH)COCO(OH) + 0.30\ CO(OH)CH(OH)CH(OH)CO(OH) + 0.20\ CO(OH)CH(OH)C(OH)(OO^\bullet)CO(OH) + 0.60\ CHOCH(OH)CO(OH) + 0.60\ CO_2 + 0.60\ H_2O_2 + 0.20\ O_2$	R(59)	$7.5\ 10^7$			$= k(2\ CH_2(OO^\bullet)CO(O^-)) - 10$
Pathway 1: $2\ CO(O^-)CH(OH)CH(OO^\bullet)CO(OH) \rightarrow CO(O^-)CH(OH)COCO(OH) + H_2O_2$		$2.2\ 10^7$			BR: 30%
Pathway 2: $2\ CO(O^-)CH(OH)CH(OO^\bullet)CO(OH)\ (+\ 2\ H_2O) \rightarrow CHOCH(OH)CO(O^-) + 2\ CO_2 + H_2O_2 + 2\ H_2O$		$2.2\ 10^7$			BR: 30%
Pathway 3: $2\ CO(O^-)CH(OH)CH(OO^\bullet)CO(OH) \rightarrow CO(O^-)CH(OH)CHOCO(OH) + CO(OH)CH(OH)CH(OH)CO(O^-) + O_2$		$2.2\ 10^7$			BR: 30%
Pathway 4: $2\ CO(O^-)CH(OH)CH(OO^\bullet)CO(OH) \rightarrow CO(O^-)CH(OH)CH(O^\bullet)CO(OH) + O_2$		$9.0\ 10^6$			BR: 10%
$CO(O^-)CH(OH)CH(O^\bullet)CO(OH) \rightarrow CO(O^-)CH(OH)C^\bullet(OH)CO(OH)$					9
$CO(O^-)CH(OH)C^\bullet(OH)CO(OH) \rightarrow CO(O^-)CH(OH)C(OH)(OO^\bullet)CO(OH)$		$2.0\ 10^9$			2
$2\ CO(O^-)CH(OH)CH(OO^\bullet)CO(OH) \rightarrow 0.90\ CO(O^-)CH(OH)COCO(OH) + 0.30\ CO(OH)CH(OH)CH(OH)CO(O^-) + 0.20\ CO(O^-)CH(OH)C(OH)(OO^\bullet)CO(OH) + 0.60\ CHOCH(OH)CO(O^-) + 0.60\ CO_2 + 0.60\ H_2O_2 + 0.20\ O_2$	R(60)	$7.5\ 10^7$			$= k(2\ CH_2(OO^\bullet)CO(O^-)) - 10$
Pathway 1: $2\ CO(OH)CH(OH)CH(OO^\bullet)CO(O^-) \rightarrow CO(OH)CH(OH)COCO(O^-) + H_2O_2$		$2.2\ 10^7$			BR: 30%
Pathway 2: $2\ CO(OH)CH(OH)CH(OO^\bullet)CO(O^-)\ (+\ 2\ H_2O) \rightarrow CO(OH)CH(OH)CHO + 2\ CO_2 + H_2O_2 + 2\ OH^-$		$2.2\ 10^7$			BR: 30%
Pathway 3: $2\ CO(OH)CH(OH)CH(OO^\bullet)CO(O^-) \rightarrow CO(OH)CH(OH)CHOCO(O^-) + CO(OH)CH(OH)CH(OH)CO(O^-) + O_2$		$2.2\ 10^7$			BR: 30%
Pathway 4: $2\ CO(OH)CH(OH)CH(OO^\bullet)CO(O^-) \rightarrow CO(OH)CH(OH)CH(O^\bullet)CO(O^-) + O_2$		$9.0\ 10^6$			BR: 10%
$CO(OH)CH(OH)CH(O^\bullet)CO(O^-) \rightarrow CO(OH)CH(OH)C^\bullet(OH)CO(O^-)$					9
$CO(OH)CH(OH)C^\bullet(OH)CO(O^-) \rightarrow CO(OH)CH(OH)C(OH)(OO^\bullet)CO(O^-)$		$2.0\ 10^9$			2
$2\ CO(OH)CH(OH)CH(OO^\bullet)CO(O^-) \rightarrow 0.90\ CO(OH)CH(OH)COCO(O^-) + 0.30\ CO(OH)CH(OH)CH(OH)CO(O^-) + 0.20\ CO(OH)CH(OH)C(OH)(OO^\bullet)CO(O^-) + 0.60\ CO(OH)CH(OH)CHO + 0.60\ CO_2 + 0.60\ H_2O_2 + 0.60\ OH^- - 0.6\ H_2O + 0.20\ O_2$	R(61)	$7.5\ 10^7$			$= k(2\ CH_2(OO^\bullet)CO(O^-)) - 10$
Pathway 1: $2\ CO(O^-)CH(OH)CH(OO^\bullet)CO(O^-) \rightarrow CO(O^-)CH(OH)COCO(O^-) + H_2O_2$		$2.2\ 10^7$			BR: 30%
Pathway 2: $2\ CO(O^-)CH(OH)CH(OO^\bullet)CO(O^-)\ (+\ 2\ H_2O) \rightarrow CHOCH(OH)CO(O^-) + 2\ CO_2 + H_2O_2 + 2\ OH^-$		$2.2\ 10^7$			BR: 30%
Pathway 3: $2\ CO(O^-)CH(OH)CH(OO^\bullet)CO(O^-) \rightarrow CO(O^-)CH(OH)CHOCO(O^-) + CO(O^-)CH(OH)CH(OH)CO(O^-) + O_2$		$2.2\ 10^7$			BR: 30%
Pathway 4: $2\ CO(O^-)CH(OH)CH(OO^\bullet)CO(O^-) \rightarrow CO(O^-)CH(OH)CH(O^\bullet)CO(O^-) + O_2$		$9.0\ 10^6$			BR: 10%
$CO(O^-)CH(OH)CH(O^\bullet)CO(O^-) \rightarrow CO(O^-)CH(OH)C^\bullet(OH)CO(O^-)$					9

Reactions		k_{298} (M^{-n+1} s^{-1})	Ea/R (K)	References	Notes
$CO(O^-)CH(OH)C^\bullet(OH)CO(O^-)$ → $CO(O^-)CH(OH)C(OH)(OO^\bullet)CO(O^-)$		$2.0\ 10^9$			2
2 $CO(O^-)CH(OH)CH(OO^\bullet)CO(O^-)$ → 0.90 $CO(O^-)CH(OH)COCO(O^-)$ + 0.30 $CO(O^-)CH(OH)CH(OH)CO(O^-)$ + 0.20 $CO(O^-)CH(OH)C(OH)(OO^\bullet)CO(O^-)$ + 0.60 $CHOCH(OH)CO(O^-)$ + 0.60 CO_2 + 0.60 H_2O_2 + 0.60 OH^- - 0.6 H_2O + 0.20 O_2	R(62)	$7.5\ 10^7$			= k(2 $CH_2(OO^\bullet)CO(O^-)$) - 10
Oxidation of maleic Acid					
$CO(OH)CH=CHCO(OH)$ + $HO^\bullet$ → $CO(OH)CH(OH)C^\bullet HCO(OH)$		$3.4\ 10^9$			BR: 100% - 31
$CO(OH)CH(OH)C^\bullet HCO(OH)$ + O_2 → $CO(OH)CH(OH)CH(OO^\bullet)CO(OH)$		$2.0\ 10^9$			2
Trans-$CO(OH)CH=CHCO(OH)$ + $HO^\bullet$ → $CO(OH)CH(OH)CH(OO^\bullet)CO(OH)$ + H_2O - O_2	R(63)	$3.4\ 10^9$			28
$CO(O^-)CH=CHCO(OH)$ + $HO^\bullet$ → 0.50 $CO(O^-)CH(OH)C^\bullet HCO(OH)$ + 0.50 $CO(O^-)C^\bullet HCH(OH)CO(OH)$		$3.5\ 10^9$			BR: 100% - 32
$CO(O^-)CH(OH)C^\bullet HCO(OH)$ + O_2 → $CO(O^-)CH(OH)CH(OO^\bullet)CO(OH)$		$2.0\ 10^9$			2
$CO(O^-)C^\bullet HCH(OH)CO(OH)$ + O_2 → $CO(O^-)CH(OO^\bullet)CH(OH)CO(OH)$		$2.0\ 10^9$			2
Trans-$CO(O^-)CH=CHCO(OH)$ + $HO^\bullet$ → 0.50 $CO(O^-)CH(OH)CH(OO^\bullet)CO(OH)$ + 0.50 $CO(O^-)CH(OO^\bullet)CH(OH)CO(OH)$ + H_2O - O_2	R(64)	$3.5\ 10^9$			28
$CO(O^-)CH=CHCO(O^-)$ + $HO^\bullet$ → $CO(O^-)CH(OH)C^\bullet HCO(O^-)$		$3.7\ 10^9$			BR: 100% - 33
$CO(O^-)CH(OH)C^\bullet HCO(O^-)$ + O_2 → $CO(O^-)CH(OH)CH(OO^\bullet)CO(O^-)$		$2.0\ 10^9$			2
Trans-$CO(O^-)CH=CHCO(O^-)$ + $HO^\bullet$ → $CO(O^-)CH(OH)CH(OO^\bullet)CO(O^-)$ + H_2O - O_2	R(65)	$3.7\ 10^9$			28

1 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 100% for CH_2.

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

3 - The oxidation by the radicals ($NO_3^\bullet$, $SO_4^{\bullet-}$, $Cl^\bullet$, $Cl_2^{\bullet-}$, $CO_3^{\bullet-}$) 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.

4 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 58% for the electron transfer, 28% for CH_2 on $CH_2CO(O^-)$, 14% for CH_2 on $CH_2CO(OH)$. The first two pathways are considered corresponding to 86% of the total reactivity. They have been scaled to 68/32%.

5 - 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.

6 - 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.

7 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 55% for the electron transfer and 45% on CH_2. The first two pathways are considered corresponding to 100% of the total reactivity.

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

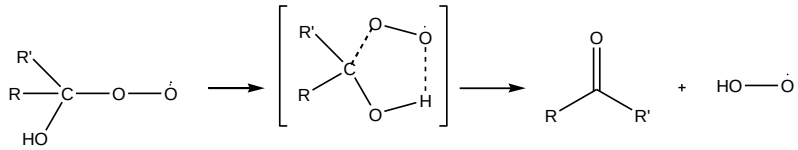
9 - DeCosta and Pincock (1989) showed that electron transfer proceeds with a rate constant around $1.0\ 10^{10}$ s^{-1}. We assumed that the electron transfer is non limiting.

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

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

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

12 - 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

13 - Oxaloacetic acid hydration is estimated to K_h = 18. The hydrate represents 95% of the total species. Therefore only the reactivity of the hydrate is considered. The first oxaloacetate monoanion ($CO(OH)CH_2COCO(O^-)$) hydration is estimated to K_h = 0.12. The hydrate represents 11% of the total species. Therefore only the reactivity of the hydrated form is considered. The second oxaloacetate monoanion ($CO(O^-)CH_2COCO(OH)$) hydration is estimated to K_h = 2.4. The hydrate represents 70% of the total species. Therefore the reactivity of both hydrated and non hydrated ions is considered. The oxaloacetate dianion hydration is estimated to K_h = 0.02. The hydrate represents 2% of the total species. Therefore only the reactivity of the non hydrated form is considered.

14 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 98% for OH on C(OH)(OH) and 2% on CH_2. The first pathway is considered corresponding to 98% of the total reactivity. It has been scaled to 100%.

15 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 80% for the electron transfer and 20% on CH_2. The first pathway is considered corresponding to 80% of the total reactivity. It has been scaled to 100%.

16 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 90% for the electron transfer and 10% on CH_2. The first pathway is considered corresponding to 90% of the total reactivity. It has been scaled to 100%.

17 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 48% for the electron transfer, 48% for OH on C(OH)(OH) and 2% on CH_2. The first two pathways are considered corresponding to 96% of the total reactivity. They have been scaled to 50/50%.

18 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 71% for the electron transfer on $CH_2CO(O^-)$, 16% for the electron transfer on $COCO(O^-)$ and 13% on CH_2. The first two pathways are considered corresponding to 87% of the total reactivity. They have been scaled to 82/18%.

19 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 44% for OH on CH(OH), 44% for on CH on CH(OH) and 12% on CH_2. The first two pathways are considered corresponding to 88% of the total reactivity. They have been scaled to 50/50%.

20 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 45% for CH on CH(OH), 25% for the electron transfer, 23% for OH on CH(OH) and 7% on CH_2. The first three pathways are considered corresponding to 93% of the total reactivity. They have been scaled to 48/27/25%.

21 - The global rate constant of both monoanions with HO is calculated by Gligoroski et al. (2009) for pH=4.3. The two mono-anions are supposed to be equally distributed because they have the same pKa. Therefore, the global rate constant is divided by two and applied to both monoanions.

22 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 56% for the electron transfer, 21% for CH on CH(OH), 12% for OH on CH(OH) and 11% on CH_2. The first two pathways are considered corresponding to 93% of the total reactivity. They have been scaled to 73/27%.

23 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 38% for CH on CH(OH), 29% for the electron transfer on $CH_2CO(O^-)$, 12% for the electron transfer on $CH(OH)CO(O^-)$, 11% for OH and 10% on CH_2. The first three pathways are considered corresponding to 79% of the total reactivity. They have been scaled to 48/37/15%.

24 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 70% for OH on CH(OH) and 30% for CH. The first two pathways are considered corresponding to 100% of the total reactivity.

25 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 28% for the electron transfer, 26% for OH on $CH(OH)CO(O^-)$, 21% for CH on $CH(OH)CO(O^-)$, 14% for OH on CH(OH)CO(OH) and 11% for CH on CH(OH)CO(OH. The first three pathways are considered corresponding to 75% of the total reactivity. They have been scaled to 37/35/28%.

26 - Branching ratios are calculated by the SAR from Doussin and Monod (2013) : 41% for CH, 31% for the electron transfer and 28% for OH. The first three pathways are considered corresponding to 100% of the total reactivity.

27 - For fumaric acid, we suppose that the addition on the external double bonded carbon is the main oxidation pathway. The SAR from Minakata et al. (2009) estimates a 95% branching ratio for this external addition on fumaric acid. This SAR estimates k_{global} equal to 5.91 10^9 M^{-1} s^{-1} with k_{abs} = 2.02 10^8 M^{-1} s^{-1} and k_{add} = 5.71 10^9 M^{-1} s^{-1}. The global rate constant is similar to the measured value (6.0 10^9 M^{-1} s^{-1}) from Cabelli and Bielski (1985).

28 - Rate constant calculated from Minakata et al. (2009).

29 - For fumarate monoanion, we suppose that the addition on the external double bonded carbon is the main oxidation pathway. The SAR from Minakata et al. (2009) estimates a 94% branching ratio for this external addition on fumaric acid. This SAR estimates k_{global} equal to 6.12 10^9 M^{-1} s^{-1} with k_{abs} = 2.02 10^8 M^{-1} s^{-1} , k_{add} = 5.71 10^9 M^{-1} s^{-1} and $k_{electron\ transfert}$ = 2.1 10^8 M^{-1} s^{-1}. Two different radicals are formed $CO(O^-)CH(OH)C^{\bullet}HCO(OH)$ and $CO(O^-)C^{\bullet}HCH(OH)CO(OH)$ with equal probability (50/50).

30 - For fumarate dianion, we suppose that the addition on the external double bonded carbon is the main oxidation pathway. The SAR from Minakata et al. (2009) estimates a 90% branching ratio for this external addition on fumaric acid. This SAR estimates k_{global} equal to 6.33 10^9 M^{-1} s^{-1} with k_{abs} = 2.02 10^8 M^{-1} s^{-1} , k_{add} = 5.71 10^9 M^{-1} s^{-1} and $k_{electron\ transfert}$ = 2 × 2.1 10^8 M^{-1} s^{-1}.

31 - For maleic acid, we suppose that the addition on the external double bonded carbon is the main oxidation pathway. The SAR from Minakata et al. (2009) estimates a 97% branching ratio for this external addition on fumaric acid. This SAR estimates k_{global} equal to 3.4 10^9 M^{-1} s^{-1} with k_{abs} = 1.02 10^8 M^{-1} s^{-1} and k_{add} = 3.3 10^9 M^{-1} s^{-1}.

32 - For maleate monoanion, we suppose that the addition on the external double bonded carbon is the main oxidation pathway. The SAR from Minakata et al. (2009) estimates a 94% branching ratio for this external addition on fumaric acid. This SAR estimates k_{global} equal to 3.51 10^9 M^{-1} s^{-1} with k_{abs} = 1.02 10^8 M^{-1} s^{-1}, k_{add} = 3.3 10^9 M^{-1} s^{-1} and $k_{electron\ transfert}$ = 2.1 10^8 M^{-1} s^{-1}. Two different radicals are formed $CO(O^-)CH(OH)C^{\bullet}HCO(OH)$ and $CO(O^-)C^{\bullet}HCH(OH)CO(OH)$ with equal probability (50/50).

33 - For maleate dianion, we suppose that the addition on the external double bonded carbon is the main oxidation pathway. The SAR from Minakata et al. (2009) estimates a 89% branching ratio for this external addition on fumaric acid. This SAR estimates k_{global} equal to 3.73 10^9 M^{-1} s^{-1} with k_{abs} = 2.02 10^8 M^{-1} s^{-1}, k_{add} = 5.71 10^9 M^{-1} s^{-1} and $k_{electron\ transfert}$ = 2 × 2.1 10^8 M^{-1} s^{-1}.

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