TOWARDS A MORE DETAILED DESCRIPTION OF TROPOSPHERIC AQUEOUS PHASE ORGANIC CHEMISTRY: CAPRAM 3.0

H. Herrmann[1]*, A. Tilgner [1], P. Barzaghi [1], Z. Majdik[1], S. Gligorovski 1, L. Poulain [2] and A. Monod [2]

[1]*Leibniz Institut für Troposphärenforschung, Permoserstraße 15, 04318 Leipzig, Germany*

[2]*Laboratoire de Chimie et Environnement, Université de Provence, Place Victor Hugo 3, Marseille cedex 3, France*

*Corresponding author. Leibniz Institut für Troposphärenforschung, Permoserstr. 15, 04318 Leipzig, Germany. Tel.: +49 341 235-2446; fax: +49 341 235-2325

ELECTRONIC SUPPLEMENTAL MATERIAL (ESM)

Table I: Summary of the parameters and reactions included in CAPRAM 3.0

Gas phase initial concentration of organic compounds [ppb]:

Compound	Urban	Remote	Marine	
C_2H_5OCHO	0.02	0.02	0.02	Estimated
$CH_2CH_2CH_2C(O)NCH_3$	0.02	0.02	0.02	Estimated

Initial concentration of organic compounds in the aqueous phase [µM]:

Compound	Urban	Remote	Marine	
$HOOCCH_2COO^-$	1.9	0.22	0.013	Averaged from several aerosol measurements and scaled to the $C_2O_2^{2-}$ concentration
$HOOCC_2H_4COO^-$	0.9	0.12	0.013	At pH_0 most of malonic acid and succinic acid dissociates to the monoanionic form

Phase transfer of organic compounds:

Compound	$K_{H\ 298}$, M atm^{-1}	$-\Delta H$ / R, K	Lit.	α	Lit.	D_g [10^5 m^2 s^{-1}]	Lit.
1-PrOH	135	7500	(Jayne et al., 1991)	0.011	(Jayne et al., 1991)	1,96	(Fuller)
2-PrOH	128	7400	(Jayne et al., 1991)	0.013	(Jayne et al., 1991)	1,96	(Fuller)
1-BuOH	130	7200	(Snider and Dawson, 1985)	0.01		1	
2-BuOH	110	7300	(Snider and Dawson, 1985)	0.01		1	Trend: Smaller α with bigger compounds
CH_3CH_2CHO	13	5700	(Zhou and Mopper, 1990)	0,03	= α(CH_3CHO)	2,02	Fuller, 1986
Butanal	9.6	6200	(Zhou and Mopper, 1990)	0.03		1	= α(Propanal)
Propanoic Acid	5710		(Khan et al., 1995)	0.0322		1	
Butyric Acid	4700		(Khan et al., 1995)	0.03		1	= α(ORA3)
$CH_3C(O)CHO$	1.4		(Betterton and Hoffmann, 1988)	0.03	= α(CH_3CHO)	1.95	(Fuller)
$CH_3C(O)CH_3$	32	5770	(Betterton, 1991)	$5.4 \cdot 10^{-3}$	(Schutze and Herrmann, 2004)	2,02	(Fuller)
$CH_3C(O)CH_2CH_3$	19.8	2184	(Zhou and Mopper, 1990)	$2.1 \cdot 10^{-3}$	(Schutze and Herrmann, 2004)	0.87	(Fuller)

Compound	$K_{H\ 298}$, M atm^{-1}	-ΔH / R, K	Lit.	α	Lit.	D_g [10^5 m^2 s^{-1}]	Lit.
HKET ⇌ $CH_3C(O)CH_2OH$	129		Meylan and Howard, 1991	0.008	= α(Aceton)	1	(Fuller)
DCB ⇌ OHCCH=CHCHO	$3 \cdot 10^5$		Estimated after the effective Henry constant of Glyoxal	0.023	= α(Glyoxal)	1	(Fuller)
$CH_3C(O)CH_2CH(CH_3)_2$	3.91		(Kim et al., 2000)	0.01	Estimated	0.71	(Fuller)
C_2H_5OCHO	2.59		Bocek, 1976	0.01	Estimated	0.93	(Fuller)
$CH_2CH_2CH_2C(O)NCH_3$	$3.13 \cdot 10^5$		(Kim et al., 2000)	0.01	Estimated	0.78	(Fuller)
CH_2OHCH_2OH	$4 \cdot 10^6$		(Bone et al., 1983)	0.04	(Jayne et al., 1991)	1.06	(Fuller)

	Reaction	$k_{298\ K}$ [M^{-1} s^{-1}]	- E_A/R [K]	Comments
	C_2 Compounds			
1	**$OH + CH(OH)_2COO^- \rightarrow H_2O + C(OH)_2COO^-$**	**$2{,}6 \cdot 10^9$**	**4300**	(Ervens et al., 2003)
2	**$NO_3 + CH(OH)_2COO^- \rightarrow C(OH)_2COO^- + NO_3^- + H^+$**	**$1.8 \cdot 10^5$**		**Calculated (Herrmann and Zellner, 1998) BDE's derived after correlation reported in (Gligorovski and Herrmann, 2004)(1)**
3	$C(OH)_2COO^- + O_2 \rightarrow O_2C(OH)_2COO^-$	$2 \cdot 10^9$		Estimated like $CH_2OH + O_2$
4	$2\ O_2C(OH)_2COO^- \rightarrow 2\ CO_2^- + 2\ CO_2 + 2\ H_2O_2$	$2 \cdot 10^7$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
5	$2\ O_2C(OH)_2COO^- \rightarrow 4\ CO_2 + H_2O_2 + 2\ OH^-$	$1.9 \cdot 10^7$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
6	$2\ O_2C(OH)_2COO^- \rightarrow 2\ H_2O + 2\ CO_2^- + 2\ CO_2 + O_2$	$1.9 \cdot 10^7$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
7	$2\ O_2C(OH)_2COO^- \rightarrow 2\ H_2O + CO_2^- + 3\ CO_2 + O_2^-$	$7.5 \cdot 10^6$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
	Oxidation of 1-Propanol			
8	**$OH + C_3H_7OH \rightarrow C_3H_6OH + H_2O$**	**$3{,}2 \cdot 10^9$**	**1000**	(Ervens et al., 2003)

	Reaction	$k_{298\,K}$ [$M^{-1}\,s^{-1}$]	- E_A/R [K]	Comments
9	**$NO_3 + C_3H_7OH \rightarrow C_3H_6OH + NO_3^- + H^+$**	**$3.2 \cdot 10^6$**		**(Herrmann et al., 1994)**
10	$C_3H_6OH + O_2 \rightarrow O_2C_3H_6OH$	$2 \cdot 10^9$		Estimated after (von Sonntag, 1987)
11	$O_2C_3H_6OH + OH^- \rightarrow C_2H_5CH(O) + H_2O + O_2^-$	$4 \cdot 10^9$		Since O_2CH_2OH: $1.6 \cdot 10^{10}$ and $O_2C_2H_4OH$: $8 \cdot 10^9$ C_3-Radical assumedly slower (Factor 2 ??)
12	$O_2C_3H_6OH \rightarrow C_2H_5CH(O) + HO_2$	52		As the C_2-compound
	Oxidation of Propionaldehyde			
13	**$OH + C_2H_5CH(O) \rightarrow C_2H_5C(O) + H_2O$**	**$2.8 \cdot 10^9$**	**1300**	**Hesper and Herrmann, 2003**
14	**$NO_3 + C_2H_5CH(O) \rightarrow C_2H_5C(O) + NO_3^- + H^+$**	**$3.9.10^7$**	**505**	**In CH_3CN (Ito et al., 1989a)**
15	$C_2H_5C(O) + O_2 \rightarrow C_2H_5C(O)O_2$	$2 \cdot 10^9$		Estimated after (von Sonntag, 1987)
16	$2\ C_2H_5C(O)O_2 \rightarrow 2\ C_2H_5C(O)O\cdot + O_2$	$1.5 \cdot 10^8$		Estimated after the ACO_3 recombination, (Herrmann et al., 1999)
17	$C_2H_5C(O)O\cdot \rightarrow C_2H_5\cdot + CO_2$	$2 \cdot 10^9$		(Hilborn and Pincock, 1991)
18	$C_2H_5\cdot + O_2 \rightarrow$ ETHP	$2 \cdot 10^9$		Estimated after (von Sonntag, 1987)
	Oxidation of Propionaldehyde (hydrated form)			
19	**$OH + C_2H_5CH(OH)_2 \rightarrow C_2H_5C(OH)_2 + H_2O$**	**$2.8 \cdot 10^9$**	**1300**	**Hesper and Herrmann, 2003**
20	**$NO_3 + C_2H_5CH(OH)_2 \rightarrow C_2H_5C(OH)_2 + NO_3^- + H^+$**	**$3.9.10^7$**	**505**	**In CH_3CN (Ito et al., 1989a)**
21	$C_2H_5C(OH)_2 + O_2 \rightarrow C_2H_5CO_2\cdot(OH)_2$	$2 \cdot 10^9$		Estimated after (von Sonntag, 1987)
22	$C_2H_5CO_2\cdot(OH)_2 \rightarrow HO_2 + C_2H_5COOH$	1000		Estimated after (von Sonntag, 1987)
	Oxidation of Propanoic acid			
23	**$OH + C_2H_5COOH \rightarrow CH_3CHCOOH + H_2O$**	**$3{,}2 \cdot 10^8$**	**2300**	(Ervens et al., 2003)
24	**$NO_3 + C_2H_5COOH \rightarrow CH_3CHCOOH + NO_3^- + H^+$**	**$4.6 \cdot 10^3$**		**Calculated (Herrmann and Zellner, 1998) BDE's determined with Benson's incremental method[(2)]**
25	$CH_3CHCOOH + O_2 \rightarrow CH_3CH(O_2)COOH$	$2 \cdot 10^9$		Estimated after (von Sonntag, 1987)
26	$2\ CH_3CH(O_2)COOH \rightarrow 2\ CO_2 + 2$ ETHP	$1{,}5 \cdot 10^8$		analog to ACO_3-Rekombination
	Oxidation of Propionate			
27	**$OH + C_2H_5COO^- \rightarrow CH_3CHCOO^- + H_2O$**	**$7{,}3 \cdot 10^8$**	**1800**	(Ervens et al., 2003)
28	**$NO_3 + C_2H_5COO^- \rightarrow CH_3CHCOO^- + NO_3^- + H^+$**	**$3.7 \cdot 10^8$**		**Calculated (Herrmann and Zellner, 1998) BDE's derived after correlation reported in (Gligorovski and Herrmann, 2004)[(1)]**

	Reaction	$k_{298\,K}$ [$M^{-1}\,s^{-1}$]	- E_A/R [K]	Comments
29	$CH_3CHCOO^- + O_2 \rightarrow CH_3CH(O_2)COO^-$	$2\cdot10^9$		Estimated after (von Sonntag, 1987)
30	$2\ CH_3CH(O_2)COO^- \rightarrow 2\ CH_3C(O)COO^- + H_2O_2$	$2\cdot10^7$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
31	$2\ CH_3CH(O_2)COO^- \rightarrow CH_3C(O)COO^- + CH_3CH(OH)COO^- + O_2$	$1{,}9\cdot10^7$		α-Hydroxy-Propanoic acid: No sinks Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
32	$2\ CH_3CH(O_2)COO^- + 2\ H_2O \rightarrow 2\ CH_3CH(O) + 2\ CO_2 + 2\ OH^- + H_2O_2$	$1{,}9\cdot10^7$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
33	$2\ CH_3CH(O_2)COO^- + 2\ OH^- + O_2 \rightarrow 2\ CH_3C(O)COO^- + 2\ H_2O + 2\ O_2^-$	$7{,}5\cdot10^6$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
	Oxidation of 2-Propanol			
34	**$OH + CH_3CH(OH)CH_3 \rightarrow H_2O + CH_3C(OH)CH_3$**	**$2{,}4\cdot10^9$**	**600**	**(Elliot and Simsons, 1984)**
35	**$NO_3 + CH_3CH(OH)CH_3 \rightarrow CH_3C(OH)CH_3 + NO_3^- + H^+$**	**$3.7\cdot10^6$**		**(Herrmann et al., 1994)**
36	$CH_3C(OH)CH_3 + O_2 \rightarrow CH_3C(O_2)(OH)CH_3$	$1{,}6\cdot10^9$		Estimated
37	$CH_3C(O_2)(OH)CH_3 \rightarrow HO_2 + CH_3C(O)CH_3$	665		Estimated after (von Sonntag, 1987)
	Oxidation of Acetone			
38	**$OH + CH_3C(O)CH_3 \rightarrow CH_3C(O)CH_2\cdot + H_2O$**	**$1.7\cdot10^8$**	**1788**	**Average of measurements within the MOST project**
39	**$NO_3 + CH_3C(O)CH_3 \rightarrow CH_3C(O)CH_2\cdot + NO_3^- + H^+$**	**$4.4\cdot10^3$**	**4332**	**(Herrmann et al., 1994)**
40	$CH_3C(O)CH_2\cdot + O_2 \rightarrow CH_3C(O)CH_2OO$	$3{,}1\cdot10^9$		(Zegota et al., 1986)
41	$2\ CH_3C(O)CH_2OO \rightarrow CH_3C(O)CHO + CH_3C(O)CH_2(OH) + O_2$	$6\cdot10^7$		(Zegota et al., 1986) branching ratios after measurements within MOST by Poulain et al.,
42	$2\ CH_3C(O)CH_2OO \rightarrow 2\ CH_3C(O)CH_2O + O_2$	$1.96\cdot10^8$		(Zegota et al., 1986)branching ratios after measurements within MOST by Poulain et al.,
43	$2\ CH_3C(O)CH_2OO \rightarrow 2\ CH_3C(O)CHO + H_2O_2$	$1.2\cdot10^8$		(Zegota et al., 1986)branching ratios after measurements within MOST by Poulain et al.,
44	$CH_3C(O)CH_2O \rightarrow HCHO + CH_3CO$	$1.6\cdot10^6$		Estimated from the gas phase
	Oxidation of Hydroxy Acetone			
45	**$CH_3C(O)CH_2(OH) + OH \rightarrow CH_3C(O)CH(OH) + H_2O$**	**$1.2\cdot10^9$**	**1069**	**Gligorovski and Herrmann (In Preparation)**
46	**$NO_3 + CH_3C(O)CH_2(OH) \rightarrow CH_3C(O)CH(OH) + NO_3^- + H^+$**	**$1.7\cdot10^6$**		**Calculated (Herrmann and Zellner, 1998) BDE's determined with Benson's incremental method[(2)]**
47	$CH_3C(O)CH(OH) + O_2 \rightarrow CH_3C(O)CH(OH)OO$	$2\cdot10^9$		Estimated after (von Sonntag, 1987)

	Reaction	$k_{298\,K}$ [$M^{-1}\,s^{-1}$]	- E_A/R [K]	Comments
48	$CH_3C(O)CH(OH)OO \rightarrow CH_3C(O)CHO + HO_2$	$2.1\cdot10^2$	4990	Estimated after $OOCHOHCHOHCH_2OH$, (Bothe et al., 1978)
49	$2\ CH_3C(O)CH(OH)OO \rightarrow H_2O_2 + 2\ CH_3C(O)COOH$	$3.5\cdot10^8$		Estimated after the decay of $CH_3CH(OH)OO$, (Bothe et al., 1983)
	Oxidation of Methylglyoxal (hydrated form)			
50	**$CH_3C(O)CH(OH)_2 + OH \rightarrow CH_3C(O)C(OH)_2 + H_2O$**	**$7.9\cdot10^8$**	**1589**	**Average of measurements within the MOST project**
51	**$NO_3 + CH_3C(O)CH(OH)_2 \rightarrow CH_3C(O)C(OH)_2 + NO_3^- + H^+$**	**$6.3\cdot10^7$**		**Estimated**
52	$CH_3C(O)C(OH)_2 + O_2 \rightarrow CH_3C(O)C(OH)_2OO$	$2\cdot10^9$		Estimated after (von Sonntag, 1987)
53	$CH_3C(O)C(OH)_2OO \rightarrow CH_3C(O)COOH + HO_2$	$1\cdot10^7$		In analogy with glyoxal, (Buxton et al., 1997)(approximation)
	Oxidation of Malonic acid			
54	**$OH + CH_2(COOH)_2 \rightarrow H_2O + HOOCCHCOOH$**	**$1.6\cdot10^7$**		**(Walling and Eltaliaw.Gm, 1973)**
55	**$NO_3 + CH_2(COOH)_2 \rightarrow HOOCCHCOOH + NO_3^- + H^+$**	**$1.2\cdot10^5$**		**Calculated (Herrmann and Zellner, 1998) BDE's derived after correlation reported in (Gligorovski and Herrmann, 2004)(1)**
56	$HOOCCHCOOH + O_2 \rightarrow HOOCCHO_2COOH$	$2\cdot10^9$		Estimated after (von Sonntag, 1987)
57	$2\ HOOCCHO_2COOH \rightarrow HOOCC(O)COOH + HOOCCH(OH)COOH + O_2$	$1{,}9\cdot10^7$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
58	$2\ HOOCCHO_2COOH \rightarrow 2\ HOOCC(O)COOH + H_2O_2$	$2\cdot10^7$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
59	$2\ HOOCCHO_2COOH + 2\ H_2O \rightarrow 2\ CH(OH)_2COOH + 2\ CO_2 + H_2O_2$	$1{,}9\cdot10^7$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
60	$2\ HOOCCHO_2COOH + 2\ OH^- + O_2 \rightarrow 2\ HOOCC(O)COOH + 2\ O_2^- + 2\ H_2O$	$7{,}5\cdot10^6$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
	Oxidation of Malonate (dianion)			
61	**$OH + CH_2(COO^-)_2 \rightarrow H_2O + {}^-OOCCHCOO^-$**	**$2{,}4\cdot10^8$**		**(Logan, 1989)**
62	**$NO_3 + CH_2(COO^-)_2 \rightarrow {}^-OOCCHCOO^- + NO_3^- + H^+$**	**$1.1\cdot10^6$**		**Calculated (Herrmann and Zellner, 1998) BDE's derived after correlation reported in (Gligorovski and Herrmann, 2004)(1)**
63	${}^-OOCCHCOO^- + O_2 \rightarrow {}^-OOCCH(O_2)COO^-$	$2\cdot10^9$		Estimated after (von Sonntag, 1987)

	Reaction	$k_{298\,K}$ [$M^{-1}\,s^{-1}$]	- E_A/R [K]	Comments
64	2 $^-OOCCH(O_2)COO^-$ → $^-OOCC(O)COO^-$ + $^-OOCCH(OH)COO^-$ + O_2	$1{,}9\cdot10^7$		No sinks for mesoxalate and tartronate Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
65	2 $^-OOCCH(O_2)COO^-$ → 2 $^-OOCC(O)COO^-$ + H_2O_2	$2\cdot10^7$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
66	2 $^-OOCCH(O_2)COO^-$ + 4 H_2O→ 2 $CH(OH)_2COO^-$ + 2 CO_2 + H_2O_2 + 2 OH^-	$1{,}9\cdot10^7$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
67	2 $^-OOCCH(O_2)COO^-$ + 2 OH^- + O_2 → 2 $^-OOCC(O)COO^-$ + 2 O_2^- + 2 H_2O	$7{,}5\cdot10^6$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
	Oxidation of Malonate (monoanion)			
68	**OH + $^-OOCCH_2COOH$ → H_2O + $^-OOCCHCOOH$**	**$3{,}6\cdot10^8$**	**1300**	**(Ervens et al., 2003)**
69	**NO_3 + $^-OOCCH_2COOH$ → $^-OOCCHCOOH$ + NO_3^- + H^+**	**$1.1\cdot10^6$**		**Calculated (Herrmann and Zellner, 1998) BDE's derived after correlation reported in (Gligorovski and Herrmann, 2004)(1)**
70	$^-OOCCHCOOH$ + O_2→ $^-OOCCH(O_2)COOH$	$2\cdot10^9$		Estimated after (von Sonntag, 1987)
71	2 $^-OOCCH(O_2)COOH$ → $^-OOCC(O)COOH$ + $^-OOCCH(OH)COOH$ + O_2	$1.9\cdot10^7$		No sinks for mesoxalate and tartronate Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
72	2 $^-OOCCH(O_2)COOH$ → 2 $^-OOCC(O)COOH$ + H_2O_2	$2\cdot10^7$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
73	2 $^-OOCCH(O_2)COOH$ + 4 H_2O→ 2 $CH(OH)_2COOH$ + 2 CO_2 + H_2O_2 + 2 OH^-	$1{,}9\cdot10^7$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
74	2 $^-OOCCH(O_2)COOH$ + 2 OH^- + O_2 → 2 $^-OOCC(O)COOH$ + 2 O_2^- + 2 H_2O	$7{,}5\cdot10^6$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
	Oxidation of Pyruvic acid			
75	**OH + $CH_3C(O)COOH$ → $CH_2C(O)COOH$ + H_2O**	**$1{,}2\cdot10^8$**	**2800**	**(Ervens et al., 2003)**
76	**NO_3 + $CH_3C(O)COOH$ → $CH_2C(O)COOH$ + NO_3^- + H^+**	**$4.8\cdot10^6$**		**Calculated (Herrmann and Zellner, 1998) BDE's determined with Benson's incremental method(2)**
77	$CH_2C(O)COOH$ + O_2 → $O_2CH_2C(O)COOH$	$2\cdot10^9$		Estimated after (von Sonntag, 1987)
78	2 $O_2CH_2C(O)COOH$ → $OCHC(O)COOH$ + $HOCH_2C(O)COOH$ + O_2	$1.9\cdot10^7$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
79	2 $O_2CH_2C(O)COOH$ → 2 $OCHC(O)COOH$ + H_2O_2	$2\cdot10^7$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
80	2 $O_2CH_2C(O)COOH$ + 2 H_2O → 2 CH_3CHO + H_2O_2 + 2 CO_2 + 2 O_2	$1.9\cdot10^7$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)

	Reaction	$k_{298\,K}$ [M^{-1} s^{-1}]	- E_A/R [K]	Comments
81	$2\ O_2CH_2C(O)COOH + 2\ OH^- + O_2 \rightarrow 2\ OHCC(O)COOH + 2\ O_2^- + 2\ H_2O$	$7.5 \cdot 10^6$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
	Oxidation of Pyruvate			
82	**$CH_3C(O)COO^- + OH \rightarrow CH_2C(O)COO^- + H_2O$**	**$7 \cdot 10^8$**	**2285**	**(Ervens et al., 2003)**
83	**$NO_3 + CH_3C(O)COO^- \rightarrow CH_2C(O)COO^- + NO_3^- + H^+$**	**$1.9 \cdot 10^8$**		**Calculated (Herrmann and Zellner, 1998) BDE's derived after correlation reported in (Gligorovski and Herrmann, 2004)(1)**
84	$CH_2C(O)COO^- + O_2 \rightarrow OOCH_2C(O)COO^-$	$2 \cdot 10^9$		Estimated after (von Sonntag, 1987)
85	$2\ OOCH_2C(O)COO^- \rightarrow O_2 + OCHC(O)COO^- + HOCH_2C(O)COO^-$	$1.9 \cdot 10^7$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
86	$2\ OOCH_2C(O)COO^- \rightarrow H_2O_2 + 2\ OCHC(O)COO^-$	$2 \cdot 10^7$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
87	$2\ OOCH_2C(O)COO^- + 4\ H_2O \rightarrow 2\ CH_3CHO + 2\ CO_2 + 2O_2 + H_2O_2 + 2\ OH^-$	$1.9 \cdot 10^7$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
88	$2\ OOCH_2C(O)COO^- + 2\ OH^- + O_2 \rightarrow 2\ O_2^- + 2\ OCHC(O)COO^- + 2\ H_2O$	$7.5 \cdot 10^6$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
	Oxidation of Succinic acid			
89	**$OH + CH_2CH_2(COOH)_2 \rightarrow CHCH_2(COOH)_2 + H_2O$**	**$1{,}1 \cdot 10^8$**	**1300**	**(Ervens et al., 2003)**
90	**$NO_3 + CH_2CH_2(COOH)_2 \rightarrow CHCH_2(COOH)_2 + NO_3^- + H^+$**	**$2.3 \cdot 10^5$**		**Calculated (Herrmann and Zellner, 1998) BDE's determined with Benson's incremental method(2)**
91	$CHCH_2(COOH)_2 + O_2 \rightarrow O_2CHCH_2(COOH)_2$	$2 \cdot 10^9$		Estimated after (von Sonntag, 1987)
92	$2\ O_2CHCH_2(COOH)_2 \rightarrow HOOCC(O)CH_2COOH + HOOCCH(OH)CH_2COOH + O_2$	$1.9 \cdot 10^7$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
93	$2\ O_2CHCH_2(COOH)_2 \rightarrow 2\ HOOCC(O)CH_2COOH + H_2O_2$	$2 \cdot 10^7$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
94	$2\ O_2CHCH_2(COOH)_2 \rightarrow 2\ CH(O)CH_2COOH + 2\ CO_2 + H_2O_2$	$1.9 \cdot 10^7$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
95	$2\ O_2CHCH_2(COOH)_2 + 2\ OH^- + O_2 \rightarrow 2\ O_2^- + 2\ HOOCC(O)CH_2COOH + 2\ H_2O$	$7.5 \cdot 10^6$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
96	**$OH + CH(OH)_2CH_2COOH \rightarrow C(OH)_2CH_2COOH + H_2O$**	**$5.4 \cdot 10^8$**		**Estimated after Glycolic acid**
97	**$NO_3 + CH(OH)_2CH_2COOH \rightarrow C(OH)_2CH_2COOH + NO_3^- + H^+$**	**$3 \cdot 10^6$**		**Estimated after Glycolic acid**
98	$C(OH)_2CH_2COOH + O_2 \rightarrow CH(OH)_2O_2CH_2COOH$	$2 \cdot 10^9$		Estimated after (von Sonntag, 1987)
99	$CH(OH)_2O_2CH_2COOH \rightarrow HOOCCH_2COOH + HO_2$	1000		Estimated after (von Sonntag, 1987)
	Oxidation of Succinate (dianion)			
100	**$OH + CH_2CH_2(COO^-)_2 \rightarrow CHCH_2(COO^-)_2 + H_2O$**	**$5 \cdot 10^8$**	**1300**	**(Ervens et al., 2003)**

	Reaction	$k_{298\,K}$ [M^{-1} s^{-1}]	- E_A/R [K]	Comments
101	**$NO_3 + CH_2CH_2(COO^-)_2 \rightarrow CHCH_2(COO^-)_2 + NO_3^- + H^+$**	**$5.5 \cdot 10^7$**		**Calculated (Herrmann and Zellner, 1998) BDE's derived after correlation reported in (Gligorovski and Herrmann, 2004)[(1)]**
102	$CHCH_2(COO^-)_2 + O_2 \rightarrow O_2CHCH_2(COO^-)_2$	$2 \cdot 10^9$		Estimated after (von Sonntag, 1987)
103	$2\ O_2CHCH_2(COO^-)_2 \rightarrow {}^-OOCC(O)CH_2COO^- + {}^-OOCCH(OH)CH_2COO^- + O_2$	$1.9 \cdot 10^7$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
104	$2\ O_2CHCH_2(COO^-)_2 \rightarrow 2\ {}^-OOCC(O)CH_2COO^- + H_2O_2$	$2 \cdot 10^7$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
105	$2\ O_2CHCH_2(COO^-)_2 + 2H_2O \rightarrow 2\ CH(O)CH_2COO^- + 2\ CO_2 + H_2O_2 + 2\ OH^-$	$1{,}9 \cdot 10^7$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
106	$2\ O_2CHCH_2(COO^-)_2 + O_2 + 2\ OH^- \rightarrow 2\ {}^-OOCC(O)CH_2COO^- + 2\ O_2^- + 2\ H_2O$	$7{,}5 \cdot 10^6$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
107	**$OH + CH(OH)_2CH_2COO^- \rightarrow C(OH)_2CH_2COO^- + H_2O$**	**$1.2 \cdot 10^9$**		**Estimated after Glycolate**
108	**$NO_3 + CH(OH)_2CH_2COO^- \rightarrow C(OH)_2CH_2COO^- + NO_3^- + H^+$**	**$1.1 \cdot 10^9$**		**Estimated after Glycolate**
109	$C(OH)_2CH_2COO^- + O_2 \rightarrow CH(OH)_2O_2CH_2COO^-$	$2 \cdot 10^9$		Estimated after (von Sonntag, 1987)
110	$CH(OH)_2O_2CH_2COO^- \rightarrow HOOCCH_2COO^- + HO_2$	1000		Estimated after (von Sonntag, 1987)
	Oxidation of Succinate (monoanion)			
111	**$OH + HOOCCH_2CH_2COO^- \rightarrow HOOCCHCH_2COO^- + H_2O$**	**$5 \cdot 10^8$**	**1300**	**estimated: $k_{Dianion} = k_{Monoanion}$**
112	**$NO_3 + HOOCCH_2CH_2COO^- \rightarrow HOOCCHCH_2COO^- + NO_3^- + H^+$**	**$5.5 \cdot 10^7$**		**Calculated (Herrmann and Zellner, 1998) BDE's derived after correlation reported in (Gligorovski and Herrmann, 2004)[(1)]**
113	$HOOCCHCH_2COO^- + O_2 \rightarrow HOOCCH(O_2)CH_2COO^-$	$2 \cdot 10^9$		Estimated after (von Sonntag, 1987)
114	$2\ HOOCCH(O_2)CH_2COO^- \rightarrow HOOCC(O)CH_2COO^- + HOOCCH(OH)CH_2COO^- + O_2$	$2 \cdot 10^7$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
115	$2\ HOOCCH(O_2)CH_2COO^- \rightarrow 2\ HOOCC(O)CH_2COO^- + H_2O_2$	$1{,}9 \cdot 10^7$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
116	$2\ HOOCCH(O_2)CH_2COO^- + 2\ H_2O \rightarrow 2\ CH(O)CH_2COOH + 2\ CO_2 + H_2O_2 + 2\ OH^-$	$1{,}9 \cdot 10^7$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
117	$2\ HOOCCH(O_2)CH_2COO^- + 2OH^- + O_2 \rightarrow 2\ HOOCC(O)CH_2COO^- + 2\ O_2^- + 2\ H_2O$	$7{,}5 \cdot 10^6$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
	Oxidation of Lactic acid			
118	**$OH + CH_3CHOHCOOH \rightarrow CH_3COHCOOH + H_2O$**	**$4{,}3 \cdot 10^8$**		**(Adams et al., 1965)**

	Reaction	$k_{298\,K}$ [$M^{-1}\,s^{-1}$]	- E_A/R [K]	Comments
119	**$NO_3 + CH_3CHOHCOOH \rightarrow CH_3COHCOOH + NO_3^- + H^+$**	**$3\cdot10^6$**		**Calculated (Herrmann and Zellner, 1998) BDE's determined with Benson's incremental method[(2)]**
120	$CH_3COHCOOH + O_2 \rightarrow CH_3CO_2OHCOOH$	$2\cdot10^9$		Estimated after (von Sonntag, 1987)
121	$CH_3CO_2OHCOOH \rightarrow CH_3C(O)COOH + HO_2$	665		Estimated after Isopropanol (von Sonntag, 1987)
	Oxidation of Lactate			
122	**$OH + CH_3CHOHCOO^- \rightarrow CH_3COHCOO^- + H_2O$**	**$1.2\cdot10^9$**		**(Logan, 1989)**
123	**$NO_3 + CH_3CHOHCOO^- \rightarrow CH_3COHCOO^- + NO_3^- + H^+$**	**$5.4\cdot10^9$**		**Calculated (Herrmann and Zellner, 1998) BDE's derived after correlation reported in (Gligorovski and Herrmann, 2004)[(1)]**
124	$CH_3COHCOO^- + O_2 \rightarrow CH_3CO_2OHCOO^-$	$2\cdot10^9$		Estimated after (von Sonntag, 1987)
125	$CH_3CO_2OHCOO^- \rightarrow CH_3C(O)COO^- + HO_2$	665		Estimated after Isopropanol (von Sonntag, 1987)
	Oxidation of Glycolic acid			
126	**$CH_2OHCOOH + OH \rightarrow CHOHCOOH + H_2O$**	**$5.4\cdot10^8$**		**(Scholes and Willson, 1967)**
127	**$NO_3 + CH_2OHCOOH \rightarrow CHOHCOOH + NO_3^- + H^+$**	**$3\cdot10^6$**		**Calculated (Herrmann and Zellner, 1998) BDE's determined with Benson's incremental method[(2)]**
128	$CHOHCOOH + O_2 \rightarrow O_2CHOHCOOH$	$2\cdot10^9$		Estimated after (von Sonntag, 1987)
129	$O_2CHOHCOOH + H_2O \rightarrow HO_2 + CH(OH)_2COOH$	52		Estimated after Ethanol, (von Sonntag, 1987)
	Oxidation of Glycolate			
130	**$CH_2OHCOO^- + OH \rightarrow CHOHCOO^- + H_2O$**	**$1.2\cdot10^9$**		**(Logan, 1989)**
131	**$NO_3 + CH_2OHCOO^- \rightarrow CHOHCOO^- + NO_3^- + H^+$**	**$1.1\cdot10^9$**		**Calculated (Herrmann and Zellner, 1998) BDE's derived after correlation reported in (Gligorovski and Herrmann, 2004)[(1)]**
132	$CHOHCOO^- + O_2 \rightarrow O_2CHOHCOO^-$	$2\cdot10^9$		Estimated after (von Sonntag, 1987)
133	$O_2CHOHCOO^- + H_2O \rightarrow HO_2 + CH(OH)_2COO^-$	52		Estimated after Ethanol, (von Sonntag, 1987)
	Reactions of the peroxyl radical formed from acetic acid			
134	$O_2CH_2COOH + HO_2 \rightarrow HO_2CH_2COOH + O_2$	$8.3\cdot10^5$	2720	= k ($HO_2 + HO_2$) (Bielski et al., 1985)

	Reaction	$k_{298\,K}$ [$M^{-1}\,s^{-1}$]	- E_A/R [K]	Comments
135	$O_2CH_2COOH + O_2^- + H^+ \rightarrow HO_2CH_2COOH + O_2$	$9.7\cdot10^7$	1060	= k ($HO_2 + O_2^-$) (Bielski et al., 1985)
136	$O_2CH_2COOH + HSO_3^- \rightarrow HO_2CH_2COOH + SO_3^-$	$5\cdot10^5$		= k ($CH_3O_2 + HSO_3^-$) (Herrmann et al., 1999)
137	$O_2CH_2COO^- + HO_2 \rightarrow HO_2CH_2COO^- + O_2$	$8.3\cdot10^5$	2720	= k($HO_2 + O_2^-$) (Bielski et al., 1985)
138	$O_2CH_2COO^- + O_2^- + H^+ \rightarrow HO_2CH_2COO^- + O_2$	$9.7\cdot10^7$	1060	= k ($HO_2 + O_2^-$) (Bielski et al., 1985)
139	$O_2CH_2COO^- + HSO_3^- \rightarrow HO_2CH_2COO^- + SO_3^-$	$5\cdot10^5$		= k ($CH_3O_2 + HSO_3^-$) (Herrmann et al., 1999)
	Oxidation of Acetic acid hydroxyperoxide			
140	**$HO_2CH_2COOH + OH \rightarrow O_2CH_2COOH + H_2O$**	**$3\cdot10^7$**		**= k ($OH + H_2O_2$)**
141	**$NO_3 + HO_2CH_2COOH \rightarrow HO_2CHCOOH + NO_3^- + H^+$**	**$1.7\cdot10^6$**		**Calculated (Herrmann and Zellner, 1998) BDE's determined with Benson's incremental method(2)**
142	$HO_2CH_2COOH + Fe^{2+} + H_2O \rightarrow Fe^{3+} + CH_2(OH)COOH + OH + OH^-$	50		= k ($Fe^{2+} + H_2O_2$)
	Oxidation of acetate hydroxyperoxide			
143	**$HO_2CH_2COO^- + OH \rightarrow O_2CH_2COO^- + H_2O$**	**$3\cdot10^7$**		**= k ($OH + H_2O_2$)**
144	**$NO_3 + HO_2CH_2COO^- \rightarrow O_2CH_2COO^-\ NO_3^- + H^+$**	**$7.1\cdot10^6$**		**= k ($NO_3 + H_2O_2$)**
145	$HO_2CH_2COO^- + Fe^{2+} \rightarrow Fe^{3+} + CH_2(OH)COO^- + OH + OH^-$	50		= k ($Fe^{2+} + H_2O_2$)
	Oxidation of 1-Butanol			
146	**$OH + CH_3CH_2CH_2CH_2OH \rightarrow H_2O + CH_3CH_2CH_2CHOH$**	**$4.1\cdot10^9$**	**1000**	**Hesper and Herrmann, 2003**
147	**$NO_3 + CH_3CH_2CH_2CH_2OH \rightarrow CH_3CH_2CH_2CHOH + NO_3^- + H^+$**	**$1.9\cdot10^6$**		**(Shastri and Huie, 1990)**
148	$CH_3CH_2CH_2CHOH + O_2 \rightarrow CH_3CH_2CH_2CHO_2OH$	$2\cdot10^9$		Estimated after (von Sonntag, 1987)
149	$CH_3CH_2CH_2CHO_2OH \rightarrow CH_3CH_2CH_2CHO + HO_2$	1000		Estimated after (von Sonntag, 1987)
	Oxidation of Butyraldehyde			
150	**$CH_3CH_2CH_2CHO + OH \rightarrow CH_3CH_2CH_2CO + H_2O$**	**$3.9\cdot10^9$**	**900**	**Hesper and Herrmann, 2003**
151	**$NO_3 + CH_3CH_2CH_2CHO \rightarrow CH_3CH_2CH_2CO + NO_3^- + H^+$**	**$1.8\cdot10^8$**		**Calculated (Herrmann and Zellner, 1998) BDE's determined with Benson's incremental method(2)**
152	$CH_3CH_2CH_2CO + O_2 \rightarrow CH_3CH_2CH_2COO_2$	$2\cdot10^9$		Estimated after (von Sonntag, 1987)
153	$2\ CH_3CH_2CH_2COO_2 \rightarrow 2\ CH_3CH_2CH_2C(O)O\cdot + O_2$	$1.5\cdot10^8$		Estimated after the ACO_3 recombination, (Herrmann et al., 1999)

	Reaction	$k_{298\,K}$ [M^{-1} s^{-1}]	- E_A/R [K]	Comments
154	$CH_3CH_2CH_2C(O)O\cdot \rightarrow CH_3CH_2CH_2\cdot + CO_2$	$2\cdot10^9$		Estimated after $CH_3CH_2C(O)O\cdot$ (Hilborn and Pincock, 1991)
155	$CH_3CH_2CH_2\cdot + O_2 \rightarrow CH_3CH_2CH_2O_2\cdot$	$2\cdot10^9$		Estimated after (von Sonntag, 1987)
156	$2\ CH_3CH_2CH_2O_2\cdot \rightarrow 2\ CH_3CH_2CH_2O + O_2$	$1\cdot10^8$	750	Estimated after ETHP, (Herrmann et al., 1999)
157	$CH_3CH_2CH_2O + O_2 \rightarrow C_2H_5CH(O) + HO_2$	$6\cdot10^6$		Estimated
158	$2\ CH_3CH_2CH_2O_2 \rightarrow C_2H_5CH(O) + C_3H_7OH + O_2$	$6\cdot10^7$	750	Estimated after ETHP, (Herrmann et al., 1999)
	Oxidation of Butyraldehyde (hydrated form)			
159	$\mathbf{CH_3CH_2CH_2CH(OH)_2 + OH \rightarrow CH_3CH_2CH_2C\cdot(OH)_2}$	$\mathbf{3.9\cdot10^9}$	**900**	**Hesper and Herrmann, 2003**
160	$\mathbf{NO_3 + CH_3CH_2CH_2CH(OH)_2 \rightarrow CH_3CH_2CH_2C\cdot(OH)_2 + NO_3^- + H^+}$	$\mathbf{1.8\cdot10^8}$		**Calculated (Herrmann and Zellner, 1998) BDE's determined with Benson's incremental method(2)**
161	$CH_3CH_2CH_2C\cdot(OH)_2 + O_2 \rightarrow CH_3CH_2CH_2CO_2\cdot(OH)_2$	$2\cdot10^9$		Estimated after (von Sonntag, 1987)
162	$CH_3CH_2CH_2CO_2\cdot(OH)_2 \rightarrow CH_3CH_2CH_2COOH + HO_2$	1000		Estimated after (von Sonntag, 1987)
	Oxidation of Butyric acid			
163	$\mathbf{CH_3CH_2CH_2COOH + OH \rightarrow CH_3CH_2CHCOOH + H_2O}$	$\mathbf{2{,}2\cdot10^9}$		**(Scholes and Willson, 1967)**
164	$\mathbf{NO_3 + CH_3CH_2CH_2COOH \rightarrow CH_3CH_2CHCOOH + NO_3^- + H^+}$	$\mathbf{1.2\cdot10^7}$		**Calculated (Herrmann and Zellner, 1998) BDE's determined with Benson's incremental method(2)**
165	$CH_3CH_2CHCOOH + O_2 \rightarrow CH_3CH_2CHO_2COOH$	$2\cdot10^9$		Estimated after (von Sonntag, 1987)
166	$2\ CH_3CH_2CHO_2COOH \rightarrow 2\ CH_3CH_2C(O)COOH + H_2O_2$	$2\cdot10^7$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
167	$2\ CH_3CH_2CHO_2COOH \rightarrow CH_3CH_2C(O)COOH + CH_3CH_2CHOHCOOH + O_2$	$1.9\cdot10^7$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
168	$2\ CH_3CH_2CHO_2COOH \rightarrow 2\ CH_3CH_2CHO + 2\ CO_2 + H_2O_2$	$1.9\cdot10^7$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
169	$2\ CH_3CH_2CHO_2COOH + 2\ OH^- + O_2 \rightarrow 2\ CH_3CH_2C(O)COOH + 2\ O_2^- + 2\ H_2O$	$7.5\cdot10^6$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
	Oxidation of Butyrate			
170	$\mathbf{CH_3CH_2CH_2COO^- + OH \rightarrow CH_3CH_2CHCOO^- + H_2O}$	$\mathbf{2.0\cdot10^9}$		**(Anbar et al., 1966)**
171	$\mathbf{NO_3 + CH_3CH_2CH_2COO^- \rightarrow CH_3CH_2CHCOO^- + NO_3^- + H^+}$	$\mathbf{4.0\cdot10^9}$		**Calculated (Herrmann and Zellner, 1998) BDE's derived after correlation reported in (Gligorovski and Herrmann, 2004)(1)**

	Reaction	$k_{298\,K}$ [$M^{-1}\,s^{-1}$]	- E_A/R [K]	Comments
172	$CH_3CH_2CHCOO^- + O_2 \rightarrow CH_3CH_2CHO_2COO^-$	$2\cdot10^9$		Estimated after (von Sonntag, 1987)
173	$2\ CH_3CH_2CH(O_2)COO^- \rightarrow 2\ CH_3CH_2C(O)COO^- + H_2O_2$	$2\cdot10^7$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
174	$2\ CH_3CH_2CH(O_2)COO^- \rightarrow CH_3CH_2C(O)COO^- + CH_3CH_2CHOHCOO^- + O_2$	$1.9\cdot10^7$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
175	$2\ CH_3CH_2CH(O_2)COO^- + 2\ H_2O \rightarrow 2\ CH_3CH_2CHO + 2\ CO_2 + 2\ OH^- + H_2O_2$	$1.9\cdot10^7$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
176	$2\ CH_3CH_2CH(O_2)COO^- + 2\ OH^- + O_2 \rightarrow 2\ CH_3CH_2C(O)COO^- + 2\ O_2^- + 2\ H_2O$	$7.5\cdot10^6$		Estimated in analogy to $O_2CH_2COO^-$ recombination, (Schuchmann et al., 1985)
	Oxidation of 2-Butanol			
177	**$CH_3CH_2CHOHCH_3 + OH \rightarrow CH_3CH_2COHCH_3 + H_2O$**	**$3.5\cdot10^9$**	**910**	**Hesper and Herrmann, 2003**
178	**$NO_3 + CH_3CH_2CHOHCH_3 \rightarrow CH_3CH_2COHCH_3 + NO_3^- + H^+$**	**$2.4\cdot10^6$**		**Calculated (Herrmann and Zellner, 1998) BDE's determined with Benson's incremental method[(2)]**
179	$CH_3CH_2COHCH_3 + O_2 \rightarrow CH_3CH_2C(O_2)(OH)CH_3$	$2\cdot10^9$		Estimated after (von Sonntag, 1987)
180	$CH_3CH_2C(O_2)(OH)CH_3 \rightarrow HO_2 + CH_3C(O)CH_2CH_3$	1000		(vonSonntag et al., 1997)
	Oxidation of Methyl Ethyl Ketone			
181	**$CH_3C(O)CH_2CH_3 + OH \rightarrow CH_3C(O)CHCH_3 + H_2O$**	**$1.17\cdot10^9$**	**1451**	**Average of measurements within the MOST project**
182	**$CH_3C(O)CH_2CH_3 + OH \rightarrow CH_2C(O)CH_2CH_3 + H_2O$**	**$1.3\cdot10^8$**	**1451**	**Average of measurements within the MOST project**
183	**$NO_3 + CH_3C(O)CH_2CH_3 \rightarrow CH_3C(O)CHCH_3 + NO_3^- + H^+$**	**$7.38\cdot10^5$**		**Calculated (Herrmann and Zellner, 1998) BDE's determined with Benson's incremental method[(2)]**
184	**$NO_3 + CH_3C(O)CH_2CH_3 \rightarrow CH_2C(O)CH_2CH_3 + NO_3^- + H^+$**	**$8.2\cdot10^4$**		**Calculated (Herrmann and Zellner, 1998) BDE's determined with Benson's incremental method[(2)]**
185	$CH_3C(O)CHCH_3 + O_2 \rightarrow CH_3C(O)CH(OO)CH_3$	$3.1\cdot10^9$		(Glowa et al., 2000)
186	$2\ CH_3C(O)CH(OO)CH_3 \rightarrow O_2 + 2\ CH_3C(O)CHOCH_3$	$3.6\cdot10^8$		(Glowa et al., 2000) branching ratios after measurements within MOST by Poulain et al.,
187	$2\ CH_3C(O)CH(OO)CH_3 \rightarrow H_2O_2 + 2\ CH_3C(O)C(O)CH_3$	$4\cdot10^7$		(Glowa et al., 2000) branching ratios after measurements within MOST by Poulain et al.,

	Reaction	$k_{298\,K}$ [M^{-1} s^{-1}]	- E_A/R [K]	Comments
188	$CH_3C(O)CHOCH_3 \rightarrow CH_3CHO + CH_3CO$	1.3E+5	-6441	Estimated after gas phase rate const. (Baldwin et al., 1977)
	Oxidation of 2,3-Butanedione			
189	**$CH_3C(O)C(O)CH_3 + OH \rightarrow CH_3C(O)C(O)CH_2 + H_2O$**	**$1.4\cdot10^8$**	**2435**	**k(298) after Gligorovski and Herrmann, 2004 Branching ratio estimated based on the gas phase reaction (Christensen et al., 1998)**
190	**$CH_3C(O)C(O)CH_3 + OH \rightarrow CH_3COOH + CH_3CO\cdot$**	**$1.4\cdot10^8$**	**2435**	**k(298) after Gligorovski and Herrmann, 2004 Branching ratio estimated based on the gas phase reaction (Christensen et al., 1998)**
191	**$CH_3C(O)C(O)CH_3 + NO_3 \rightarrow CH_3C(O)C(O)CH_2 + NO_3^- + H^+$**	**$2.9\cdot10^3$**		**Calculated (Herrmann and Zellner, 1998) BDE's derived after correlation reported in (Gligorovski and Herrmann, 2004)[(1)]**
192	**$CH_3C(O)C(O)CH_3 + NO_3 \rightarrow CH_3C(O)NO_3 + CH_3CO\cdot$**	**$2.9\cdot10^3$**		**Calculated (Herrmann and Zellner, 1998) BDE's derived after correlation reported in (Gligorovski and Herrmann, 2004)[(1)]**
193	$CH_3C(O)C(O)CH_2 + O_2 \rightarrow CH_3C(O)C(O)CH_2OO\cdot$	$2\cdot10^9$		Estimated after (von Sonntag, 1987)
194	$2\ CH_3C(O)C(O)CH_2OO\cdot \rightarrow 2\ CH_3C(O)C(O)CH_2O\cdot + O_2$	$1.5\cdot10^8$		k(298) estimated after the $CH_3C(O)OO\cdot$ recombination
195	$CH_3C(O)C(O)CH_2OO\cdot + CH_3C(O)OO\cdot \rightarrow CH_3C(O)O\cdot + CH_3C(O)C(O)CH_2O\cdot + O_2$	$1.5\cdot10^8$		k(298) estimated after the $CH_3C(O)OO\cdot$ recombination
196	$CH_3C(O)C(O)CH_2O\cdot \rightarrow CH_3CO\cdot + HCHO + CO$	1.3E+5	-6441	k_{1st} estimated after reac. 188
197	$CH_2C(O)CH_2CH_3 + O_2 \rightarrow OOCH_2C(O)CH_2CH_3$	$3.1\cdot10^9$		By analogy with acetone
198	$2\ OOCH_2C(O)CH_2CH_3 \rightarrow O_2 + 2\ OCH_2C(O)CH_2CH_3$	$4\cdot10^8$		By analogy with acetone
199	$OCH_2C(O)CH_2CH_3 \rightarrow HCHO + C(O)CH_2CH_3$	1.3E+5	-6441	By analogy with reac. 188
200	$C(O)CH_2CH_3 + H_2O \rightarrow C(OH)_2CH_2CH_3$	360.4		By analogy with CH_3CO (Schuchmann and Vonsonntag, 1988)
201	$C(OH)_2CH_2CH_3 \rightarrow C(O)CH_2CH_3 + H_2O$	3E+4		By analogy with $CH_3C(OH)_2$ (Schuchmann and Vonsonntag, 1988)
202	$C(OH)_2CH_2CH_3 + O_2 \rightarrow OOC(OH)_2CH_2CH_3$	2E+9		Estimated after (von Sonntag, 1987)
203	$C(O)CH_2CH_3 + O_2 \rightarrow OOC(O)CH_2CH_3$	2E+9		Estimated after (von Sonntag, 1987)
204	$OOC(OH)_2CH_2CH_3 \rightarrow CH_3CH_2C(O)OH + HO_2$	1E+6		Estimated

	Reaction	$k_{298\,K}$ [M^{-1} s^{-1}]	- E_A/R [K]	Comments
	Oxidation of 1,4-Dioxo Butene			
205	**OH + OHCCH=CHCHO → OHCCH(OH)CH·CHO**	**$6\cdot10^9$**		**= k (Maleic acid), (Cabelli and Bielski, 1985)**
206	OHCCH(OH)CH·CHO + O_2 → OHCCH(OH)CHO$_2$CHO	$2\cdot10^9$		Estimated after (von Sonntag, 1987)
207	2 OHCCH(OH)CHO$_2$CHO → OHCCHOHC(O)CHO + OHCCHOHCHOHCHO + O_2	$1.6\cdot10^8$		Formation of keto and hydroxy species = k (2 ETHP)
	Oxidation of 2-Hydroxy, 3,4-Dioxo Butyraldehyde			
208	**OHCCH(OH)C(O)CHO + OH → OC·CH(OH)C(O)CHO + H_2O**	**$1.1\cdot10^9$**	**1516**	**Estimated after Glyoxal, (Buxton et al., 1997)**
209	**OHCCH(OH)C(O)CHO + NO_3 → OC·CH(OH)C(O)CHO + NO_3^- + H^+**	**$3\cdot10^6$**		**Calculated (Herrmann and Zellner, 1998) BDE's determined with Benson's incremental method(2)**
210	OC·CH(OH)C(O)CHO + O_2 → OCO$_2$CH(OH)C(O)CHO	$2\cdot10^9$		Estimated after (von Sonntag, 1987)
211	OCO$_2$CH(OH)C(O)CHO + H_2O → HOOCCH(OH)C(O)CHO + HO_2	1000		Estimated after (von Sonntag, 1987)
	Oxidation of 2-Hydroxy, 3,4-Dioxo Butyric acid			
212	**HOOCCH(OH)C(O)CHO + OH → HOOCCH(OH)C(O)C·O + H_2O**	**$3,6\cdot10^8$**	**1000**	**= k (Glyoxylic acid), (Ervens et al., 2003) k(298) is eventually overestimated, because k was set according to the fully hydrated form.**
213	**HOOCCH(OH)C(O)CHO + NO_3 → HOOCCH(OH)C(O)C·O + NO_3^- + H^+**	**$3.4\cdot10^6$**		**Calculated, (Herrmann and Zellner, 1998) BDE's determined with Benson's incremental method(2)**
214	HOOCCH(OH)C(O)C·O + O_2 → HOOCCH(OH)C(O)C(O)O_2	$2\cdot10^9$		Estimated after (von Sonntag, 1987)
215	HOOCCH(OH)C(O)C(O)O_2 + H_2O → HOOCCH(OH)C(O)COOH + HO_2	1000		Estimated after (von Sonntag, 1987)
216	HOOCCHOHC(O)COOH → CO_2 + CH$_2$OHC(O)COOH	$1\cdot10^{-5}$		Estimated after (Guthrie, 2002) and (Guthrie and Jordan, 1972)
	Oxidation of 2-Hydroxy, 3,4-Dioxo Butyrate			
217	**$^-$OOCCH(OH)C(O)CHO + OH → $^-$OOCCH(OH)C(O)C·O + H_2O**	**$2.6\cdot10^9$**	**4300**	**= k (Glyoxylate), (Ervens et al., 2003)**
218	**$^-$OOCCH(OH)C(O)CHO + NO_3 → $^-$OOCCH(OH)C(O)C·O + NO_3^- + H^+**	**$1.8\cdot10^5$**		**= k (Glyoxylate)**
219	$^-$OOCCH(OH)C(O)C·O + O_2 → $^-$OOCCH(OH)C(O)C(O)O_2	$2\cdot10^9$		Estimated after (von Sonntag, 1987)

	Reaction	$k_{298\,K}$ [$M^{-1}\,s^{-1}$]	- E_A/R [K]	Comments
220	$^{-}OOCCH(OH)C(O)C(O)O_2 + H_2O \rightarrow {}^{-}OOCCH(OH)C(O)COOH + HO_2$	1000		Estimated after (von Sonntag, 1987)
221	$^{-}OOCCHOHC(O)COOH \rightarrow CO_2 + CH_2OHC(O)COO^{-}$	$1\cdot10^{-5}$		Estimated after (Guthrie, 2002) and (Guthrie and Jordan, 1972)
	Oxidation of 2,3-Dihydroxy, 4-Oxo Butyraldehyde			
222	**$OHCCH(OH)CH(OH)CHO + OH \rightarrow OC\cdot CH(OH)CH(OH)CHO + H_2O$**	**$1.1\cdot10^{9}$**	**1516**	**Estimated after Glyoxal, (Buxton et al., 1997)**
223	**$OHCCH(OH)CH(OH)CHO + NO_3 \rightarrow OC\cdot CH(OH)CH(OH)CHO + NO_3^{-} + H^{+}$**	**$6\cdot10^{6}$**		**Calculated (Herrmann and Zellner, 1998) BDE's determined with Benson's incremental method(2)**
224	$OC\cdot CH(OH)CH(OH)CHO + O_2 \rightarrow OCO_2CH(OH)CH(OH)CHO$	$2\cdot10^{9}$		Estimated after (von Sonntag, 1987)
225	$OCO_2CH(OH)CH(OH)CHO + H_2O \rightarrow HOOCCH(OH)CH(OH)CHO + HO_2$	1000		Estimated after (von Sonntag, 1987)
	Oxidation of 2,3-Dihydroxy, 4-Oxo Butyric acid			
226	**$HOOCCH(OH)CH(OH)CHO + OH \rightarrow HOOCCH(OH)CH(OH)C\cdot O + H_2O$**	**$3.6\cdot10^{8}$**	**1700**	**Estimated after Malic acid (Gligorovski and Herrmann 2004)**
227	**$HOOCCH(OH)CH(OH)CHO + NO_3 \rightarrow HOOCCH(OH)CH(OH)C\cdot O + NO_3^{-} + H^{+}$**	**$6\cdot10^{6}$**		**Calculated (Herrmann and Zellner, 1998) BDE's determined with Benson's incremental method(2)**
228	$HOOCCH(OH)CH(OH)C\cdot O + O_2 \rightarrow HOOCCH(OH)CH(OH)C(O)O_2$	$2\cdot10^{9}$		Estimated after (von Sonntag, 1987)
229	$HOOCCH(OH)CH(OH)C(O)O_2 + H_2O \rightarrow HOOCCH(OH)CH(OH)COOH + HO_2$	1000		Estimated after (von Sonntag, 1987)
	Oxidation of 2,3-Dihydroxy, 4-Oxo Butyrate			
230	**$^{-}OOCCH(OH)CH(OH)CHO + OH \rightarrow {}^{-}OOCCH(OH)CH(OH)C\cdot O + H_2O$**	**$9.7\cdot10^{8}$**	**1575**	**Estimated after Malate (Gligorovski and Herrmann 2004)**
231	**$^{-}OOCCH(OH)CH(OH)CHO + NO_3 \rightarrow {}^{-}OOCCH(OH)CH(OH)C\cdot O + NO_3^{-} + H^{+}$**	**$1.2\cdot10^{9}$**		**= BDE (Malonate) Calculated (Herrmann and Zellner, 1998) BDE's derived after correlation reported in (Gligorovski and Herrmann, 2004)(1)**
232	$^{-}OOCCH(OH)CH(OH)C\cdot O + O_2 \rightarrow {}^{-}OOCCH(OH)CH(OH)C(O)O_2$	$2\cdot10^{9}$		Estimated after (von Sonntag, 1987)
233	$^{-}OOCCH(OH)CH(OH)C(O)O_2 + H_2O \rightarrow {}^{-}OOCCH(OH)CH(OH)COOH + HO_2$	1000		Estimated after (von Sonntag, 1987)
	Oxidation of Ethylene Glycol			

	Reaction	$k_{298\,K}$ [$M^{-1}\,s^{-1}$]	- E_A/R [K]	Comments
234	**$CH_2OHCH_2OH + OH \rightarrow C{\cdot}HOHCH_2OH + H_2O$**	**$1,4\cdot10^9$**		**Source for Hydroxyacetaldehyde (Adams et al., 1965)**
235	**$CH_2OHCH_2OH + NO_3 \rightarrow C{\cdot}HOHCH_2OH + NO_3^- + H^+$**	**$7.6\cdot10^5$**		**(Ito et al., 1989b)**
236	$C{\cdot}HOHCH_2OH + O_2 \rightarrow O_2CH(OH)CH_2OH$	$2\cdot10^9$		Estimated after (von Sonntag, 1987)
237	$O_2CH(OH)CH_2OH \rightarrow OHCCH_2OH + HO_2$	190		(von Sonntag, 1987)
	Oxidation of Glycolaldehyde			
238	**$OHCCH_2OH + OH \rightarrow CH_2OHC{\cdot}O + H_2O$**	**$3.6\cdot10^9$**		**= k (CH_3CHO) (Schuchmann and Vonsonntag, 1988)**
239	**$OHCCH_2OH + NO_3 \rightarrow CH_2OHC{\cdot}O + NO_3^- + H^+$**	**$1.1\cdot10^7$**		**Estimated**
240	$CH_2OHC{\cdot}O + O_2 \rightarrow CH_2OHCO_2O$	$2\cdot10^9$		Estimated after (von Sonntag, 1987)
241	$CH_2OHCO_2O + H_2O \rightarrow CH_2OHCOOH + HO_2$	190		Estimated after Ethylene Glycol (von Sonntag, 1987)
	Oxidation of Glycolaldehyde (hydrated form)			
242	**$(OH)_2CHCH_2OH + OH \rightarrow (OH)_2C{\cdot}CH_2OH$**	**$1.2\cdot10^9$**		**= k ($CH_3CH(OH)_2$) (Schuchmann and Vonsonntag, 1988)**
243	**$OHCCH_2OH + NO_3 \rightarrow CH_2OHC{\cdot}O + NO_3^- + H^+$**	**$1.1\cdot10^7$**		**Estimated**
244	$(OH)_2C{\cdot}CH_2OH + O_2 \rightarrow (OH)_2CO_2CH_2OH$	$2\cdot10^9$		Estimated after (von Sonntag, 1987)
245	$(OH)_2CO_2CH_2OH \rightarrow OC(OH)CH_2OH + HO_2$	190		Estimated after Ethylene Glycol (von Sonntag, 1987)
	Oxidation of 3-Hydroxy Pyruvic acid			
246	**$HOCH_2C(O)COOH + OH \rightarrow HOC{\cdot}HC(O)COOH + H_2O$**	**$5,4\cdot10^8$**		**=k (Glycolic acid), (Scholes and Willson, 1967)**
247	**$HOCH_2C(O)COOH + NO_3 \rightarrow HOC{\cdot}HC(O)COOH + NO_3^- + H^+$**	**$3.7\cdot10^6$**		**Calculated (Herrmann and Zellner, 1998) BDE's determined with Benson's incremental method(2)**
248	$HOC{\cdot}HC(O)COOH + O_2 \rightarrow HOCO_2HC(O)COOH$	$2\cdot10^9$		Estimated after (von Sonntag, 1987)
249	$HOCO_2HC(O)COOH \rightarrow OHCC(O)COOH + HO_2$	665		Estimated after Isopropanol, (von Sonntag, 1987)
250	$OHCC(O)COOH + H_2O \rightarrow CH_3CH(O) + CO_2 + O_2$	$1\cdot10^{-5}$		Estimated after (Guthrie, 2002) and (Guthrie and Jordan, 1972)
	Oxidation of 3-Hydroxy Pyruvate			
251	**$HOCH_2C(O)COO^- + OH \rightarrow HOC{\cdot}HC(O)COO^- + H_2O$**	**$1.2\cdot10^9$**		**=k (Glycolate), (Logan, 1989)**

	Reaction	$k_{298\,K}$ [M^{-1} s^{-1}]	- E_A/R [K]	Comments
252	**$HOCH_2C(O)COO^- + NO_3 \rightarrow HOC{\cdot}HC(O)COO^- + NO_3^- + H^+$**	**$1.8{\cdot}10^9$**		**= BDE (Glycolate) Calculated (Herrmann and Zellner, 1998) BDE's derived after correlation reported in (Gligorovski and Herrmann, 2004)(1)**
253	$HOC{\cdot}HC(O)COO^- + O_2 \rightarrow HOCO_2HC(O)COO^-$	$2{\cdot}10^9$		Estimated after (von Sonntag, 1987)
254	$HOCO_2HC(O)COO^- \rightarrow OHCC(O)COO^- + HO_2$	665		Estimated after Isopropanol, (von Sonntag, 1987)
255	$OHCC(O)COO^- + H_2O \rightarrow CH(O)CH(O) + CO_2 + OH^-$	$1{\cdot}10^{-6}$		Estimated after (Guthrie, 2002) and (Guthrie and Jordan, 1972)
	Oxidation of 3-Oxo, Pyruvic acid			
256	**$OHCC(O)COOH + OH \rightarrow OC{\cdot}C(O)COOH + H_2O$**	**$3,6{\cdot}10^8$**	**1000**	**= k (Glyoxylic acid) (Ervens et al., 2003) Additional source of mesoxalic acid**
257	**$OHCC(O)COOH + NO_3 \rightarrow OC{\cdot}C(O)COOH + NO_3^- + H^+$**	**$3.4{\cdot}10^6$**		**Calculated (Herrmann and Zellner, 1998) BDE's determined with Benson's incremental method(2)**
258	$OC{\cdot}C(O)COOH + O_2 \rightarrow OCO_2C(O)COOH$	2.10^9		Estimated after (von Sonntag, 1987)
259	$OCO_2C(O)COOH + H_2O \rightarrow HOOCC(O)COOH + HO_2$	665		Estimated after Isopropanol, Von Sonntag, 1987
	Oxidation of 3-Oxo, Pyruvate			
260	**$OHCC(O)COO^- + OH \rightarrow OC{\cdot}C(O)COO^- + H_2O$**	**$2.6{\cdot}10^9$**	**4300**	**= k (Glyoxylate) (Ervens et al., 2003) Additional source of mesoxalate**
261	**$OHCC(O)COO^- + NO_3 \rightarrow OC{\cdot}C(O)COO^- + NO_3^- + H^+$**	**$9.3{\cdot}10^9$**		**= BDE (Glyoxylate) Calculated (Herrmann and Zellner, 1998) BDE's derived after correlation reported in (Gligorovski and Herrmann, 2004)(1)**
262	$OC{\cdot}C(O)COO^- + O_2 \rightarrow OCO_2C(O)COO^-$	2.10^9		Estimated after (von Sonntag, 1987)
263	$OCO_2C(O)COO^- + H_2O \rightarrow HOOCC(O)COO^- + HO_2$	665		Estimated after Isopropanol, Von Sonntag, 1987
	Oxidation of Malic acid			
264	**$HOOCCH(OH)CH_2COOH + OH \rightarrow HOOCC{\cdot}(OH)CH_2COOH + H_2O$**	**$3.6{\cdot}10^8$**	**1575**	**Gligorovski and Herrmann, 2004**
265	**$HOOCCH(OH)CH_2COOH + NO_3 \rightarrow HOOCC{\cdot}(OH)CH_2COOH + NO_3^- + H^+$**	**$2.4{\cdot}10^6$**		**Calculated, Herrmann and Zellner 1998 BDE's determined with Benson's incremental method(2)**
266	$HOOCC{\cdot}(OH)CH_2COOH + O_2 \rightarrow HOOCCO_2(OH)CH_2COOH$	$2{\cdot}10^9$		Estimated after (von Sonntag, 1987)

	Reaction	$k_{298\,K}$ [M^{-1} s^{-1}]	- E_A/R [K]	Comments
267	$HOOCCO_2(OH)CH_2COOH \rightarrow HOOCC(O)CH_2COOH + HO_2$	1000		Estimated after (von Sonntag, 1987)
	Oxidation of Malate			
268	**$HOOCCH(OH)CH_2COO^- + OH \rightarrow HOOCC\cdot(OH)CH_2COO^- + H_2O$**	**$9.7\cdot10^8$**	**1700**	**Gligorovski and Herrmann, 2004**
269	**$HOOCCH(OH)CH_2COO^- + NO_3 \rightarrow HOOCC\cdot(OH)CH_2COO^- + NO_3^- + H^+$**	**$1.3\cdot10^9$**		**Calculated (Herrmann and Zellner, 1998) BDE's derived after correlation reported in (Gligorovski and Herrmann, 2004)(1)**
270	$HOOCC\cdot(OH)CH_2COO^- + O_2 \rightarrow HOOCCO_2(OH)CH_2COO^-$	$2\cdot10^9$		Estimated after (von Sonntag, 1987)
271	$HOOCCO_2(OH)CH_2COO^- \rightarrow HOOCC(O)CH_2COO^- + HO_2$	1000		Estimated after (von Sonntag, 1987)
	Oxidation of Oxalacetic acid			
272	**$HOOCC(O)CH_2COOH + OH \rightarrow HOOCC(O)CH\cdot COOH + H_2O$**	**$1.1\cdot10^8$**	**1300**	**= k ($C_2H_4(COOH)_2$) (Ervens et al., 2003)**
273	**$HOOCC(O)CH_2COOH + NO_3 \rightarrow HOOCC(O)CH\cdot COOH + NO_3^- + H^+$**	**$2.2\cdot10^5$**		**Calculated (Herrmann and Zellner, 1998) BDE's determined with Benson's incremental method(2)**
274	$HOOCC(O)CH\cdot COOH + O_2 \rightarrow HOOCC(O)CH(O_2)COOH$	$2\cdot10^9$		Estimated after (von Sonntag, 1987)
275	$2\ HOOCC(O)CH(O_2)COOH \rightarrow HOOCC(O)CH(OH)COOH + HOOCC(O)C(O)COOH + O_2$	$1{,}6\cdot10^8$		Formation from Keto- und Hydroxyacids = k (2 ETHP)
276	$HOOCC(O)C(O)COOH \rightarrow CO_2 + OHCC(O)COOH$	$1\cdot10^{-5}$		Estimated after (Guthrie, 2002) and (Guthrie and Jordan, 1972)
277	$HOOCC(O)CH(OH)COOH \rightarrow CO_2 + OHCCH(OH)COOH$	$1\cdot10^{-5}$		Estimated after (Guthrie, 2002) and (Guthrie and Jordan, 1972)
278	**$OH + OHCCH(OH)COOH \rightarrow OHCC(OH)COOH$**	**$4.3\cdot10^8$**		**Estimated after Lactic acid**
279	**$NO_3 + OHCCH(OH)COOH \rightarrow OHCC(OH)COOH + NO_3^- + H^+$**	**$3\cdot10^6$**		**Estimated after Lactic acid**
280	$OHCC(OH)COOH + O_2 \rightarrow OHCC(OH)O_2COOH$	$2\cdot10^9$		Estimated after (von Sonntag, 1987)
281	$OHCC(OH)O_2COOH \rightarrow OHCC(O)COOH + HO_2$	1000		Estimated after (von Sonntag, 1987)
	Oxidation of Oxalacetate			
282	**$HOOCC(O)CH_2COO^- + OH \rightarrow HOOCC(O)CH\cdot COO^- + H_2O$**	**$5\cdot10^8$**	**1300**	**= k ($C_2H_4(COO^-)_2$) (Ervens et al., 2003)**
283	**$HOOCC(O)CH_2COO^- + NO_3 \rightarrow HOOCC(O)CH\cdot COO^- + NO_3^- + H^+$**	**$5.5\cdot10^7$**		**= k ($HOOCCH_2CH_2COO^-$)**
284	$HOOCC(O)CH\cdot COO^- + O_2 \rightarrow HOOCC(O)CH(O_2)COO^-$	$2\cdot10^9$		Estimated after (von Sonntag, 1987)

	Reaction	$k_{298\,K}$ [M^{-1} s^{-1}]	- E_A/R [K]	Comments
285	2 $HOOCC(O)CH(O_2)COO^-$ → $HOOCC(O)CH(OH)COO^-$ + $HOOCC(O)C(O)COO^-$ + O_2	$1,6 \cdot 10^8$		Formation from Keto- und Hydroxyacids = k (2 ETHP)
286	$HOOCC(O)C(O)COO^-$ → CO_2 + $OHCC(O)COO^-$	$1 \cdot 10^{-6}$		Estimated after (Guthrie, 2002) and (Guthrie and Jordan, 1972)
287	$HOOCC(O)CH(OH)COO^-$ → CO_2 + $OHCCH(OH)COO^-$	$1 \cdot 10^{-6}$		Estimated after (Guthrie, 2002) and (Guthrie and Jordan, 1972)
288	**OH + $OHCCH(OH)COO^-$ → $OHCC(OH)COO^-$ + H_2O**	**$1.2 \cdot 10^9$**		**Estimated after Lactate**
289	**NO_3 + $OHCCH(OH)COO^-$ → $OHCC(OH)COO^-$ + NO_3^- + H^+**	**$5.4 \cdot 10^9$**		**Estimated after Lactate**
290	$OHCC(OH)COO^-$ + O_2 → $OHCC(OH)O_2COO^-$	$2 \cdot 10^9$		Estimated after (von Sonntag, 1987)
291	$OHCC(OH)O_2COO^-$ → $OHCC(O)COO^-$ + HO_2	1000		Estimated after (von Sonntag, 1987)
	Oxidation of Tartronic acid			
292	**HOOCCH(OH)COOH + OH → HOOCC·(OH)COOH + H_2O**	**$1.7 \cdot 10^8$**		**(Schuchmann et al., 1995)**
293	**HOOCCH(OH)COOH + NO_3 → HOOCC·(OH)COOH + NO_3^- + H^+**	**$3 \cdot 10^6$**		**Calculated (Herrmann and Zellner, 1998) BDE's determined with Benson's incremental method(2)**
294	HOOCC·(OH)COOH + O_2 → $HOOCCO_2(OH)COOH$	$2 \cdot 10^9$		Estimated after (von Sonntag, 1987)
295	$HOOCCO_2(OH)COOH$ → HOOCC(O)COOH + HO_2	665		Estimated after Isopropanal (von Sonntag, 1987)
296	HOOCC(O)COOH + H_2O → CO_2 + $CH(OH)_2COOH$	$1 \cdot 10^{-5}$		Estimated after (Guthrie, 2002) and (Guthrie and Jordan, 1972)
	Oxidation of Tartronate			
297	**$HOOCCH(OH)COO^-$ + OH → $HOOCC·(OH)COO^-$ + H_2O**	**$3.6 \cdot 10^8$**		**(Schuchmann et al., 1995)**
298	**$HOOCCH(OH)COO^-$ + NO_3 → $HOOCC·(OH)COO^-$ + NO_3^- + H^+**	**$1.1 \cdot 10^6$**		**= k ($HOOCCH_2COO^-$)**
299	$HOOCC·(OH)COO^-$ + O_2 → $HOOCCO_2(OH)COO^-$	$2 \cdot 10^9$		Estimated after (von Sonntag, 1987)
300	$HOOCCO_2(OH)COO^-$ → $HOOCC(O)COO^-$ + HO_2	665		Estimated after Isopropanal (von Sonntag, 1987)
301	$HOOCC(O)COO^-$ + H_2O → CO_2 + $CH(OH)_2COO^-$	$1 \cdot 10^{-6}$		Estimated after (Guthrie, 2002) and (Guthrie and Jordan, 1972)
	Oxidation of Methyl Isobutyl Ketone			
302	**$CH_3C(O)CH_2CH(CH_3)_2$ + OH → $CH_3C(O)CHCH(CH_3)_2$ + H_2O**	**$2.38 \cdot 10^9$**	**1360**	**Average of measurements within the MOST project**
303	**$CH_3C(O)CH_2CH(CH_3)_2$ + OH → $CH_3C(O)CH_2C(CH_3)_2$ + H_2O**	**$1.02 \cdot 10^9$**	**1360**	**Average of measurements within the MOST project**

	Reaction	$k_{298\,K}$ [$M^{-1}\,s^{-1}$]	- E_A/R [K]	Comments
304	**$NO_3 + CH_3C(O)CH_2CH(CH_3)_2 \rightarrow CH_3C(O)CHCH(CH_3)_2 + NO_3^- + H^+$**	**$1.05\cdot10^5$**		**Calculated (Herrmann and Zellner, 1998) BDE's derived after correlation reported in (Gligorovski and Herrmann, 2004)[(1)]**
305	**$NO_3 + CH_3C(O)CH_2CH(CH_3)_2 \rightarrow CH_3C(O)CH_2C(CH_3)_2 + NO_3^- + H^+$**	**$4.5\cdot10^4$**		**Calculated (Herrmann and Zellner, 1998) BDE's derived after correlation reported in (Gligorovski and Herrmann, 2004)[(1)]**
306	$CH_3C(O)CHCH(CH_3)_2 + O_2 \rightarrow CH_3C(O)CH(OO)CH(CH_3)_2$	$2\cdot10^9$		Estimated after (von Sonntag, 1987)
307	$2\ CH_3C(O)CH(OO)CH(CH_3)_2 \rightarrow O_2 + 2\ CH_3C(O)CHOCH(CH_3)_2$	$1.6\cdot10^8$		Estimated after $CH_3C(O)CH_2OO$; branching ratios after measurements within MOST by Poulain et al.,
308	$2\ CH_3C(O)CH(OO)CH(CH_3)_2 \rightarrow H_2O_2 + 2\ CH_3C(O)C(O)CH(CH_3)_2$	$1.2\cdot10^8$		Estimated after $CH_3C(O)CH_2OO$; branching ratios after measurements within MOST by Poulain et al.,
309	$2\ CH_3C(O)CH(OO)CH(CH_3)_2 \rightarrow O_2 + CH_3C(O)C(O)CH(CH_3)_2 + CH_3C(O)CH(OH)CH(CH_3)_2$	$1.2\cdot10^8$		Estimated after $CH_3C(O)CH_2OO$; branching ratios after measurements within MOST by Poulain et al.,
310	$CH_3C(O)CHOCH(CH_3)_2 \rightarrow CH_3CO + H(O)CCH(CH_3)_2$	$1.6\cdot10^6$		By analogy with acetone and with the gas phase (Mellouki et al.,)
311	$CH_3C(O)CH_2C(CH_3)_2 + O_2 \rightarrow CH_3C(O)CH_2C(OO)(CH_3)_2$	$2\cdot10^9$		Estimated after (von Sonntag, 1987)
312	$2\ CH_3C(O)CH_2C(OO)(CH_3)_2 \rightarrow O_2 + 2\ CH_3C(O)CH_2CO(CH_3)_2$	$4\cdot10^8$		Estimated
313	$CH_3C(O)CH_2CO(CH_3)_2 \rightarrow CH_3C(O)CH_3 + CH_3COCH_2$	$1.28\cdot10^6$		By analogy with the gas phase, (Mellouki et al.,) By analogy with t-butanol
314	$CH_3C(O)CH_2CO(CH_3)_2 \rightarrow CH_2C(O)CH_2C(OH)(CH_3)_2$	$3.2\cdot10^5$		By analogy with the gas phase, (Mellouki et al.,)
315	$CH_2C(O)CH_2C(OH)(CH_3)_2 + O_2 \rightarrow OOCH_2C(O)CH_2C(OH)(CH_3)_2$	$3.1\cdot10^9$		By analogy with acetone
316	$2\ OOCH_2C(O)CH_2C(OH)(CH_3)_2 \rightarrow H_2O_2 + 2\ H(O)CC(O)CH_2C(OH)(CH_3)_2$	$1.2\cdot10^8$		By analogy with acetone
317	$2\ OOCH_2C(O)CH_2C(OH)(CH_3)_2 \rightarrow O_2 + H(O)CC(O)CH_2C(OH)(CH_3)_2 + CH_2(OH)C(O)CH_2C(OH)(CH_3)_2$	$6\cdot10^7$		By analogy with acetone
318	$2\ OOCH_2C(O)CH_2C(OH)(CH_3)_2 \rightarrow O_2 + 2\ OCH_2C(O)CH_2C(OH)(CH_3)_2$	$1.96\cdot10^8$		By analogy with acetone
319	$2\ OCH_2C(O)CH_2C(OH)(CH_3)_2 \rightarrow H(O)CC(O)CH_2C(OH)(CH_3)_2 + CH_2(OH)C(O)CH_2C(OH)(CH_3)_2$	$1\cdot10^6$		By analogy with acetone

	Reaction	$k_{298\,K}$ [$M^{-1}\,s^{-1}$]	- E_A/R [K]	Comments
320	$OCH_2C(O)CH_2C(OH)(CH_3)_2 \rightarrow HCHO + C(O)CH_2C(OH)(CH_3)_2$	$1.6 \cdot 10^6$		By analogy with acetone By analogy with the gas phase (Mellouki et al.)
321	$C(O)CH_2C(OH)(CH_3)_2 \rightarrow OHCCH_2C(OH)CH_3CH_2$	$3.2 \cdot 10^5$		By analogy with $CH_3C(O)CH_2CO(CH_3)_2$
322	$OHCCH_2C(OH)CH_3CH_2 + O_2 \rightarrow OHCCH_2C(OH)CH_3CH_2O_2$	$2 \cdot 10^9$		Estimated after (von Sonntag, 1987)
323	$2\ OHCCH_2C(OH)CH_3CH_2O_2 \rightarrow OHCCH_2C(OH)CH_3CH_2OH + OHCCH_2C(OH)CH_3CHO + O_2$	$6 \cdot 10^7$		Estimated after $OOCH_2C(O)CH_2C(OH)(CH_3)_2$
324	$C_2H_5OCHO + H_2O \rightarrow C_2H_5OH + HCOOH$	$4.7 \cdot 10^{-6}$	$1.1 \cdot 10^4$	(Mata-Segreda, 2000)
325	$C_2H_5OCHO + H_3O^+ \rightarrow C_2H_5OH + HCOOH + H^+$	$2.6 \cdot 10^{-3}$	$7.22 \cdot 10^3$	(Mata-Segreda, 2000)
	Oxidation of Ethyl Formate			
326	**$C_2H_5OCHO + {}^\bullet OH \rightarrow C_2H_5OC^\bullet(O) + H_2O$**	**$3.34 \cdot 10^8$**	**2106**	**Average of measurements within the MOST project**
327	**$C_2H_5OCHO + {}^\bullet OH \rightarrow CH_3{}^\bullet CHOCHO + H_2O$**	**$4.56 \cdot 10^7$**	**2106**	**Average of measurements within the MOST project**
328	**$NO_3 + C_2H_5OCHO \rightarrow C_2H_5OC^\bullet(O) + NO_3^- + H^+$**	**$8.4 \cdot 10^4$**		**Calculated (Herrmann and Zellner, 1998) BDE's determined with Benson's incremental method(2)**
329	**$NO_3 + C_2H_5OCHO \rightarrow CH_3{}^\bullet CHOCHO + NO_3^- + H^+$**	**$1.1 \cdot 10^4$**		**Calculated (Herrmann and Zellner, 1998) BDE's determined with Benson's incremental method(2)**
330	$C_2H_5OC^\bullet(O) + O_2 \rightarrow C_2H_5OC(O)OO^\bullet$	$2 \cdot 10^9$		Estimated after (von Sonntag, 1987)
331	$C_2H_5OC(O)OO^\bullet + H_2O \rightarrow C_2H_5OH + CO_2 + HO_2^\bullet$	$4.7 \cdot 10^{-6}$	$1.1 \cdot 10^4$	Estimated after reaction 332
332	$C_2H_5OC(O)OO^\bullet + H_3O^+ \rightarrow C_2H_5OH + CO_2 + HO_2^\bullet + H^+$	$2.6 \cdot 10^{-3}$	$7.22 \cdot 10^3$	Estimated after reaction 333
333	$C_2H_5OC(O)OO^\bullet \rightarrow C_2H_5OC(O)O^\bullet + \frac{1}{2} O_2$	$6.51 \cdot 10^{-3}$		Estimated based on product studies carried out within MOST by Poulain et al.,
334	$CH_3CH_2OC(O)O^\bullet \rightarrow C_2H_5O^\bullet + CO_2$	$1 \cdot 10^9$		Wang 2001
335	$CH_3CH_2OC(O)O^\bullet \rightarrow {}^\bullet CH_2CH_2OC(O)OH$	$3 \cdot 10^{-3}$		Estimated
336	$2\ CH_3CH(OO^\bullet)OH \rightarrow H_2O_2 + 2\ CH_3C(O)OH$	$3.5 \cdot 10^8$		(Neta et al., 1990)
337	${}^\bullet CH_2CH_2OC(O)OH + O_2 \rightarrow {}^\bullet OOCH_2CH_2OC(O)OH$	$2 \cdot 10^9$		Estimated
338	$2\ {}^\bullet OOCH_2CH_2OC(O)OH \rightarrow 2\ {}^\bullet OCH_2CH_2OC(O)OH + O_2$	$5 \cdot 10^8$		Estimated
339	${}^\bullet OCH_2CH_2OC(O)OH \rightarrow HCHO + {}^\bullet CH_2OC(O)OH$	$1.6 \cdot 10^6$		Estimated in analogy with $CH_3C(O)CH_2O\cdot$
340	${}^\bullet CH_2OC(O)OH \rightarrow HCHO + {}^\bullet COOH$	$1.6 \cdot 10^6$		Estimated in analogy with $CH_3C(O)CH_2O\cdot$
341	$CH_3C^\bullet HOCHO + O_2 \rightarrow CH_3CH(OO^\bullet)OCHO$	$2 \cdot 10^9$		Estimated after (von Sonntag, 1987)

	Reaction	$k_{298\,K}$ [M^{-1} s^{-1}]	- E_A/R [K]	Comments
342	$CH_3CH(OO^{\bullet})OCHO + H_2O \rightarrow CH_3CH(OO^{\bullet})OH + HCOOH$	$4.7 \cdot 10^{-6}$	$1.1 \cdot 10^{4}$	In analogy with Ethyl Formate, (Mata-Segreda, 2000)
343	$CH_3CH(OO^{\bullet})OCHO + H_3O^{+} \rightarrow CH_3CH(OO^{\bullet})OH + HCOOH + H^{+}$	$2.6 \cdot 10^{-3}$	$7.22 \cdot 10^{3}$	In analogy with Ethyl Formate, (Mata-Segreda, 2000)
	Oxidation of N Methyl Pyrrolidinone			
344	**$CH_2CH_2CH_2C(O)NCH_3 + OH \rightarrow CH_2CH_2C(O)NCH_3CH\bullet + H_2O$**	**$6.21 \cdot 10^{9}$**		**Average of measurements within the MOST project**
345	**$CH_2CH_2CH_2C(O)NCH_3 + OH \rightarrow CH_2CH_2CH_2C(O)NC\bullet H_2 + H_2O$**	**$6.9 \cdot 10^{8}$**		**Average of measurements within the MOST project**
346	**$NO_3 + CH_2CH_2CH_2C(O)NCH_3 \rightarrow CH_2CH_2C(O)NCH_3CH\bullet + NO_3^{-} + H^{+}$**	**$7.4 \cdot 10^{5}$**		**Calculated (Herrmann and Zellner, 1998) BDE's derived after correlation reported in (Gligorovski and Herrmann, 2004)[(1)]**
347	**$NO_3 + CH_2CH_2CH_2C(O)NCH_3 \rightarrow CH_2CH_2CH_2C(O)NC\bullet H_2 + NO_3^{-} + H^{+}$**	**$8.2 \cdot 10^{4}$**		**Calculated (Herrmann and Zellner, 1998) BDE's derived after correlation reported in (Gligorovski and Herrmann, 2004)[(1)]**
348	$CH_2CH_2C(O)NCH_3CH\bullet + O_2 \rightarrow CH_2CH_2C(O)NCH_3CHO_2\bullet$	$2 \cdot 10^{9}$		Estimated after (von Sonntag, 1987)
349	$2\ CH_2CH_2C(O)NCH_3CHO_2\bullet \rightarrow 2\ CH_2CH_2C(O)NCH_3CHO\bullet + O_2$	$1 \cdot 10^{8}$		k(298) estimated after the ethyl peroxy radical (Herrmann et al., 1999)
350	$CH_2CH_2C(O)NCH_3CHO\bullet + O_2 \rightarrow CH_2CH_2C(O)NCH_3C(O) + HO_2$	$6 \cdot 10^{6}$		k(298) estimated after the reaction CH3CH2O + O2 (214 in CAPRAM 2.4)
351	**$CH_2CH_2C(O)NCH_3C(O) + OH \rightarrow CH_2CH_2C(O)NC\bullet H_2C(O) + H_2O$**	**$6.9 \cdot 10^{9}$**		**Estimated after NMP**
352	**$NO_3 + CH_2CH_2C(O)NCH_3C(O) \rightarrow CH_2CH_2C(O)NC\bullet H_2C(O) + NO_3^{-} + H^{+}$**	**$2.6 \cdot 10^{7}$**		**Calculated (Herrmann and Zellner, 1998) BDE's derived after correlation reported in (Gligorovski and Herrmann, 2004)[(3)]**
353	$CH_2CH_2C(O)NC\bullet H_2C(O) + O_2 \rightarrow CH_2CH_2C(O)NCH_2OO\bullet C(O)$	$2 \cdot 10^{9}$		Estimated after (von Sonntag, 1987)
354	$2\ CH_2CH_2C(O)NCH_2OO\bullet C(O) + O_2 \rightarrow 2\ CH_2CH_2C(O)NHC(O) + 2\ CO_2 + H_2O_2$	$1 \cdot 10^{8}$		k(298) estimated after the ethyl peroxy radical (Herrmann et al., 1999)
355	$CH_2CH_2CH_2C(O)NC\bullet H_2 + O_2 \rightarrow CH_2CH_2CH_2C(O)NCH_2O_2\bullet$	$2 \cdot 10^{9}$		Estimated after (von Sonntag, 1987)
356	$2\ CH_2CH_2CH_2C(O)NCH_2O_2\bullet + O_2 \rightarrow 2\ CH_2CH_2C(O)NHCH_2 + 2\ CO_2 + H_2O_2$	$1 \cdot 10^{8}$		k(298) estimated after the ethyl peroxy radical (Herrmann et al., 1999)
357	**$CH_2CH_2C(O)NHCH_2 + OH \rightarrow CH_2CH_2C(O)NHC\bullet H + H_2O$**	**$6.9 \cdot 10^{9}$**		**Estimated after NMP**
358	**$NO_3 + CH_2CH_2C(O)NHCH_2 \rightarrow CH_2CH_2C(O)NHC\bullet H + NO_3^{-} + H^{+}$**	**$8.2 \cdot 10^{5}$**		**Estimated after NMP**
359	$CH_2CH_2C(O)NHC\bullet H + O_2 \rightarrow CH_2CH_2C(O)NHCHO_2$	$2 \cdot 10^{9}$		Estimated after (von Sonntag, 1987)

	Reaction	$k_{298\,K}$ [M^{-1} s^{-1}]	- E_A/R [K]	Comments
360	2 $CH_2CH_2C(O)NHCHO_2\bullet \rightarrow$ 2 $CH_2CH_2C(O)NHCHO\bullet + O_2$	$1\cdot10^{8}$		k(298) estimated after the ethyl peroxy radical (Herrmann et al., 1999)
361	$CH_2CH_2C(O)NHCHO\bullet + O_2 \rightarrow CH_2CH_2C(O)NHC(O) + HO_2$	$6\cdot10^{6}$		k(298) estimated after the reaction CH3CH2O + O2 (214 in CAPRAM 2.4)
	HO_2 elimination from $CH_3C(OH)_2O_2$			
362	$CH_3C(OH)_2O_2 \rightarrow CH_3COOH + HO_2$	1000		Estimated after (von Sonntag, 1987)

Remarks:

(1): Contribution of H-abs back calculated using correlation for the reaction of NO_3 with aliphatic compounds in aqueous solution (Herrmann and Zellner, 1998) where the BDEs were derived from the correlation reported in (Gligorovski and Herrmann, 2004) for the reaction of OH with organic compounds.

(2): Calculated using the correlation for the reaction of NO3 with aliphatic compounds in aqueous solution (Herrmann and Zellner, 1998). The BDEs determined with Benson´s incremental method.

(3): Contribution of H-abs back calculated using correlation for the reaction of NO_3 with aliphatic compounds in aqueous solution (Herrmann and Zellner, 1998) where the BDEs were derived from the correlation (gas-phase) reported in (Gligorovski and Herrmann, 2004) for the reaction of OH with organic compounds.

Equilibrium reactions:

	Equilibrium	K	Ea/R	k_{for}	k_{back}	Comments
E1	$HOOCCH_2COO^- \rightleftharpoons H^+ + CH_2(COO^-)_2$	$2{,}04\cdot10^{-6}$	-117	$1{,}02\cdot10^{5}$	$5\cdot10^{10}$	Lit.: Handb. Of Org. Comp. T-dependency between 0 and 30°C
E2	$CH_3C(O)COOH \rightleftharpoons H^+ + CH_3C(O)COO^-$	$3{,}55\cdot10^{-3}$		$1{,}8\cdot10^{8}$	$5\cdot10^{10}$	Lit.: Handb. Of Org. Comp.
E3	$CH_3CH_2COOH \rightleftharpoons H^+ + CH_3CH_2COO^-$	$1{,}349\cdot10^{-5}$	60	$6{,}75\cdot10^{5}$	$5\cdot10^{10}$	T-dependency between 5 and 20°C
E4	$CH_3C(O)CHO + H_2O \rightleftharpoons CH_3C(O)CH(OH)_2$	48.6		21,5	0.543	(Betterton and Hoffmann, 1988) k_{hin} as for Glyoxal
E5	$C_2H_4(COOH)_2 \rightleftharpoons H^{+-} + OOCC_2H_4COOH$	$6{,}46\cdot10^{-5}$		$3{,}2\cdot10^{6}$	$5\cdot10^{10}$	
E6	$^-OOCC_2H_4COOH \rightleftharpoons H^{+-} + C_2H_4(COO^-)_2$	$2{,}29\cdot10^{-6}$		$1{,}15\cdot10^{5}$	$5\cdot10^{10}$	
E7	$CH_3CHOHCOOH \rightleftharpoons CH_3CHOHCOO^- + H^+$	$1{,}35\cdot10^{-5}$		$6{,}75\cdot10^{5}$	$5\cdot10^{10}$	α-Hydroxy-Propionate is formed by the recombination of the propionate peroxy radical. No sinks implemented until now for α-Hydroxy-Propionate = K, k (Propanoic acid)
E8	$CH_2OHCOOH \rightleftharpoons CH_2OHCOO^- + H^+$	$1{,}48\cdot10^{-4}$		$7{,}4\cdot10^{6}$	$5\cdot10^{10}$	(Lide, 1995)
E9	$CH_3CH_2CH_2COOH \rightleftharpoons CH_3CH_2CH_2COO^- +$	$1{,}54\cdot10^{-5}$	-500	$7{,}7\cdot10^{5}$	$5\cdot10^{10}$	(Lide, 1995)

	Equilibrium	K	Ea/R	k_{for}	k_{back}	Comments
	H^+					
E10	$ACO_3 + H_2O \rightleftharpoons CH_3C(OH)_2O_2$	367		$1.1\cdot10^{7}$	$3\cdot10^{4}$	Estimated in analogy with the acetyl radical
E11	$HO_2CH_2COOH \rightleftharpoons HO_2CH_2COO^- + H^+$	$1.74\cdot10^{-5}$		$8.7\cdot10^{5}$	$5\cdot10^{10}$	Estimated after acetic acid (Lide, 1995)
E12	$HOOCCH(OH)C(O)CHO \rightleftharpoons {}^-OOCCH(OH)C(O)CHO + H^+$	$4.57\cdot10^{-5}$		$2.29\cdot10^{6}$	$5\cdot10^{10}$	Estimated after the second step dissociation constant of tartaric acid (Lide, 1995)
E13	$HOOCCHOHC(O)COOH \rightleftharpoons {}^-OOCCHOHC(O)COOH + H^+$	$6.03\cdot10^{-3}$		$3.01\cdot10^{8}$	$5\cdot10^{10}$	Estimated after oxalacetic acid (Lide, 1995)
E14	$CH_2OHC(O)COOH \rightleftharpoons CH_2OHC(O)COO^- + H^+$	$3.55\cdot10^{-3}$		$1.8\cdot10^{8}$	$5\cdot10^{10}$	Estimated after pyruvic acid (Lide, 1995)
E15	$HOOCCH(OH)CH(OH)CHO \rightleftharpoons {}^-OOCCH(OH)CH(OH)CHO + H^+$	$4.57\cdot10^{-5}$		$2.29\cdot10^{6}$	$5\cdot10^{10}$	Estimated after the second step dissociation constant of tartaric acid (Lide, 1995)
E16	$HOOCCH(OH)CH(OH)COOH \rightleftharpoons {}^-OOCCH(OH)CH(OH)COOH + H^+$	$1.05\cdot10^{-3}$		$5.25\cdot10^{7}$	$5\cdot10^{10}$	(Lide, 1995)
E17	$OHCC(O)COOH \rightleftharpoons OHCC(O)COO^- + H^+$	$3.55\cdot10^{-3}$		$1.8\cdot10^{8}$	$5\cdot10^{10}$	Estimated after pyruvic acid (Lide, 1995)
E18	$HOOCC(O)COOH \rightleftharpoons HOOCC(O)COO^- + H^+$	$3.16\cdot10^{-3}$		$1.58\cdot10^{8}$	$5\cdot10^{10}$	(Albalat et al., 1989)
E19	$HOOCCH(OH)CH_2COOH \rightleftharpoons HOOCCH(OH)CH_2COO^- + H^+$	$1.48\cdot10^{-3}$		$7.4\cdot10^{7}$	$5\cdot10^{10}$	(Lide, 1995)
E20	$HOOCCH(OH)CH_2COO^- \rightleftharpoons {}^-OOCCH(OH)CH_2COO^- + H^+$	$8.0\cdot10^{-6}$			$5\cdot10^{10}$	(Lide, 1995)
E21	$HOOCC(O)CH_2COOH \rightleftharpoons HOOCC(O)CH_2COO^- + H^+$	$6.03\cdot10^{-3}$		$3.02\cdot10^{8}$	$5\cdot10^{10}$	(Lide, 1995)
E22	$HOOCC(O)CH_2COO^- \rightleftharpoons {}^-OOCC(O)CH_2COO^-$	$4.3\cdot10^{-5}$			$5\cdot10^{10}$	(Lide, 1995)
E23	$HOOCC(O)C(O)COOH \rightleftharpoons HOOCC(O)CH_2COO^- + H^+$	$3.16\cdot10^{-3}$		$1.58\cdot10^{8}$	$5\cdot10^{10}$	Estimated after mesoxalic acid (Albalat et al., 1989)
E24	$HOOCCH(OH)COOH \rightleftharpoons HOOCCH(OH)COO^- + H^+$	$9.55\cdot10^{-3}$		$4.77\cdot10^{8}$	$5\cdot10^{10}$	(Campi, 1963)
E25	$HOOCCH(OH)COO^- \rightleftharpoons {}^-OOCCH(OH)COO^- + H^+$	$5.75\cdot10^{-5}$			$5\cdot10^{10}$	(Campi, 1963)
E26	$HOOCCH_2COOH \rightleftharpoons HOOCCH_2COO^- + H^+$	$1.4\cdot10^{-3}$		$7.1\cdot10^{7}$	$5\cdot10^{10}$	Smith and Marthell, 1989
E27	$CH_3CH_2C(O)COOH \rightleftharpoons CH_3CH_2C(O)COO^- + H^+$	$3.16\cdot10^{-3}$			$5\cdot10^{10}$	Ojelund and Wadso, 1967
E28	$OHCCH(OH)COOH \rightleftharpoons OHCCH(OH)COO^- + H^+$	$1.35\cdot10^{-5}$			$5\cdot10^{10}$	Estimated after Propanoic acid
E29	$OHCCH_2COOH \rightleftharpoons OHCCH_2COO^- + H^+$	$1.35\cdot10^{-5}$			$5\cdot10^{10}$	Estimated after Propanoic acid
E30	$C_2H_5CH(O) + H_2O \rightleftharpoons C_2H_5CH(OH)_2$	$1.84\cdot10^{-2}$		$1.05\cdot10^{-4}$	$5.69\cdot10^{-3}$	Xu et al., 1992 k_{back} estimated after acetaldehyde
E31	$CH_3CH_2CH_2CHO + H_2O \rightleftharpoons CH_3CH_2CH_2CH(OH)_2$	$9.01\cdot10^{-3}$		$5.13\cdot10^{-5}$	$5.69\cdot10^{-3}$	Xu et al., 1992 k_{back} estimated after acetaldehyde

	Equilibrium	K	Ea/R	k_{for}	k_{back}	Comments
E32	$OHCCH_2OH + H_2O \rightleftharpoons (OH)_2CHCH_2OH$	$1.80 \cdot 10^{-1}$		$1.02 \cdot 10^{-3}$	$5.69 \cdot 10^{-3}$	Betterton and Hoffmann 1988 k_{back} estimated after acetaldehyde
E33	$OHCCH_2COOH + H_2O \rightleftharpoons CH(OH)_2CH_2COOH$	$1.84 \cdot 10^{-2}$			$5.69 \cdot 10^{-3}$	Estimated after acetaldehyde
E34	$OHCCH_2COO^- + H_2O \rightleftharpoons CH(OH)_2CH_2COO^-$	$1.84 \cdot 10^{-2}$			$5.69 \cdot 10^{-3}$	Estimated after acetaldehyde

Photolysis rates:

	Reaction	j_{max}	Reference
P1	$HO_2CH_2COOH \rightarrow OH + OCH_2COOH$	$7{,}64 \cdot 10^{-6}$	Photochemical rate constant estimated equal to $J(H_2O_2)$

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Table II: Classification of the diurnal behaviors of the organics compounds considered in CAPRAM 3.0 for the three different scenarios (remote, urban and marine)

Compound	Remote	Urban	Marine
1,2-dioxo 4-hydroxy isohexane	A(1)	A	A
1,4-dihydroxy 2-oxo isohexane	A	A	A
2-buten-1,4-dial	B1(2)	B1	B1
1-butanol	B2(3)	A	A
1-propanol	B2	A	B1
2,3-butanedione	A	A	A
2,3-dihydroxy 4-oxo butyraldehyde	B1	A	B1
2,3-dihydroxy 4-oxo butyric acid	B1	A	B1
2,3-dioxo isohexane	A	A	A
2-butanol	B2	A	A
2-hydroxy 3,4-dioxo butyraldehyde	B1	A	B1
2-hydroxy 3,4-dioxo butyric acid	B1	A	B1
2-hydroxy 3-oxo propanoic acid	B1	A	B2
2-hydroxy 3-oxo succinic acid	B1	B1	B2
2-oxo 3-hydroxy isohexane	A	A	A
2-propanol	B2	A	A
2-pyrrolidinone	C(4)	C	C
3-hydroxy pyruvic acid	B1	A	B2
3-oxo propanoic acid	C	A	C
3-oxo pyruvic acid	B1	A	C
Acetic acid hydroperoxide	B1	B1	A
Acetone	A	A	A
Butyraldehyde	B(5)	A	D(6)
Butyric acid	A	A	D
Dioxo succinic acid	D	D	A
Ethyl formate	D	D	D
Ethylene glycol	B1	B1	D
Glycolaldehyde	B1	A	D
Hydroxy acetone	C	A	A
Hydroxy butyric acid	A	A	A
Lactic acid	A	A	D
Malic acid	C	B	C

Compound	Remote	Urban	Marine
Malonic acid	D	D	D
Methyl ethyl ketone	A	A	A
Mesoxalic acid	A	A	A
Methylglyoxal	C	B	C
Methyl isobutyl ketone	A	A	A
N-methylsuccinimide	C	C	C
N-methylpyrrolidinone	C	C	C
Oxalacetic acid	C	A	C
Oxo butyric acid	A	A	A
Oxo isobutane	A	A	A
Propanoic acid	A	A	D
Propionaldehyde	B	A	D
Pyruvic acid	C	A	C
Succinic acid	D	D	D
Succinimide	D	A	D
Tartaric acid	A	A	A
Tartronic acid	C	A	D

Comments to the table:
(1): A: Increasing concentration throughout the simulation time
(2): B1: Concentration having a strong diurnal variation with an increasing daily peak concentration
(3): B2: Concentration having a strong diurnal variation with a decreasing daily peak concentration
(4): C: Decreasing concentration profile after a reached maximum concentration
(5): B: Concentration having a strong diurnal variation without a clear increase or decrease in time
(6): D: Diurnal concentration profiles which could not be included in either of the above described cases

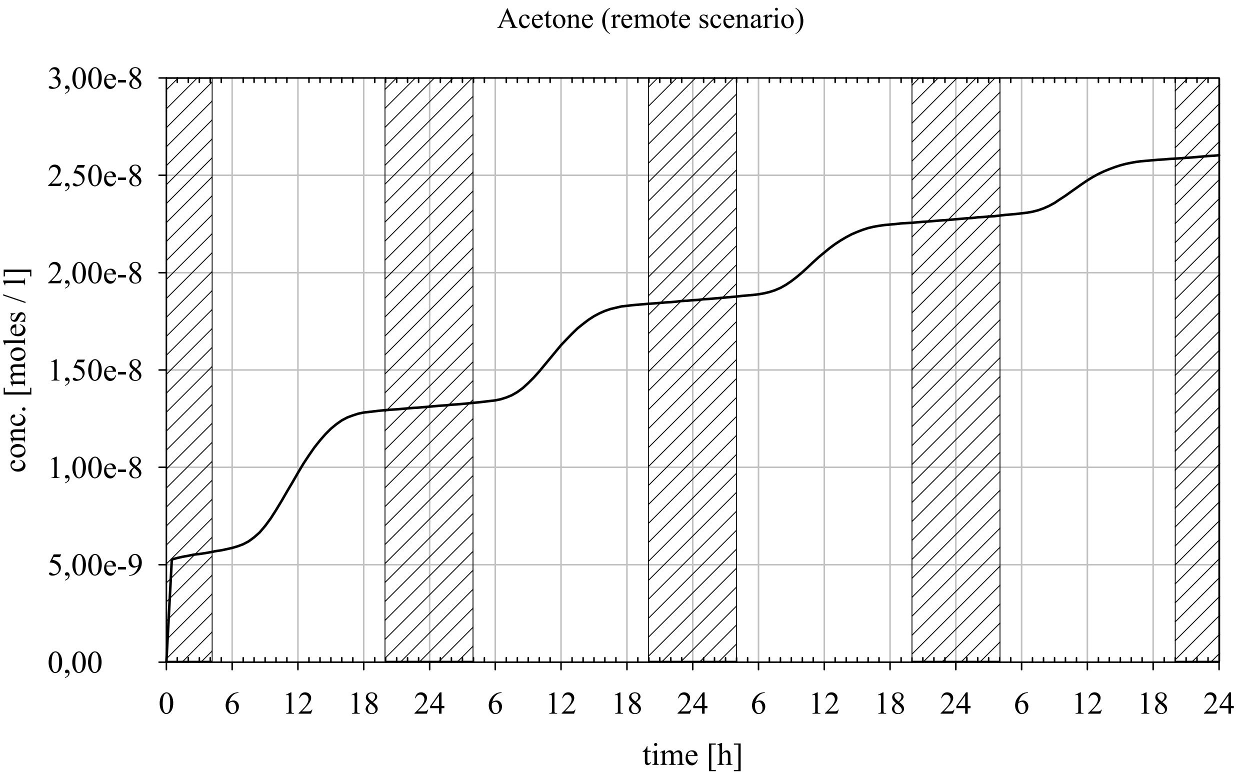


Figure I: Aqueous phase concentration of acetone for the standard scenario (remote).

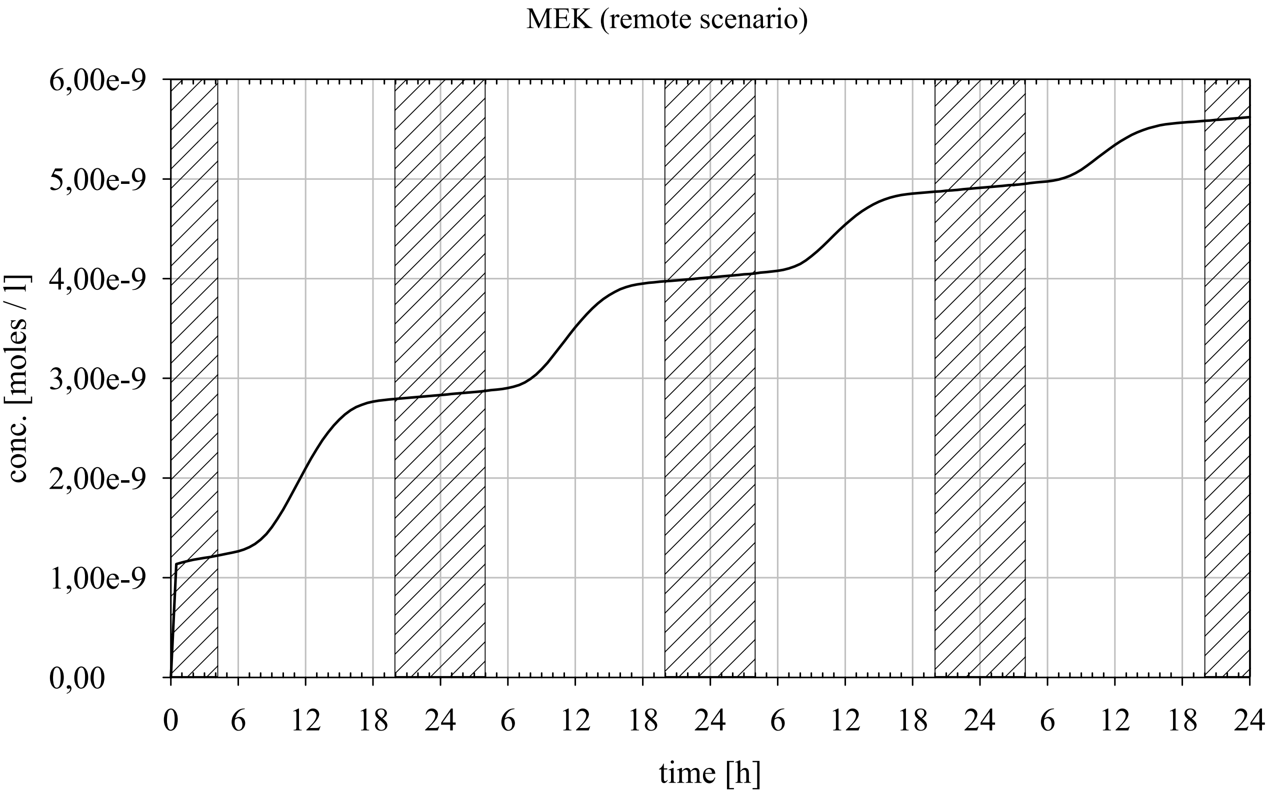


Figure II: Aqueous phase concentration of MEK for the standard scenario (remote).

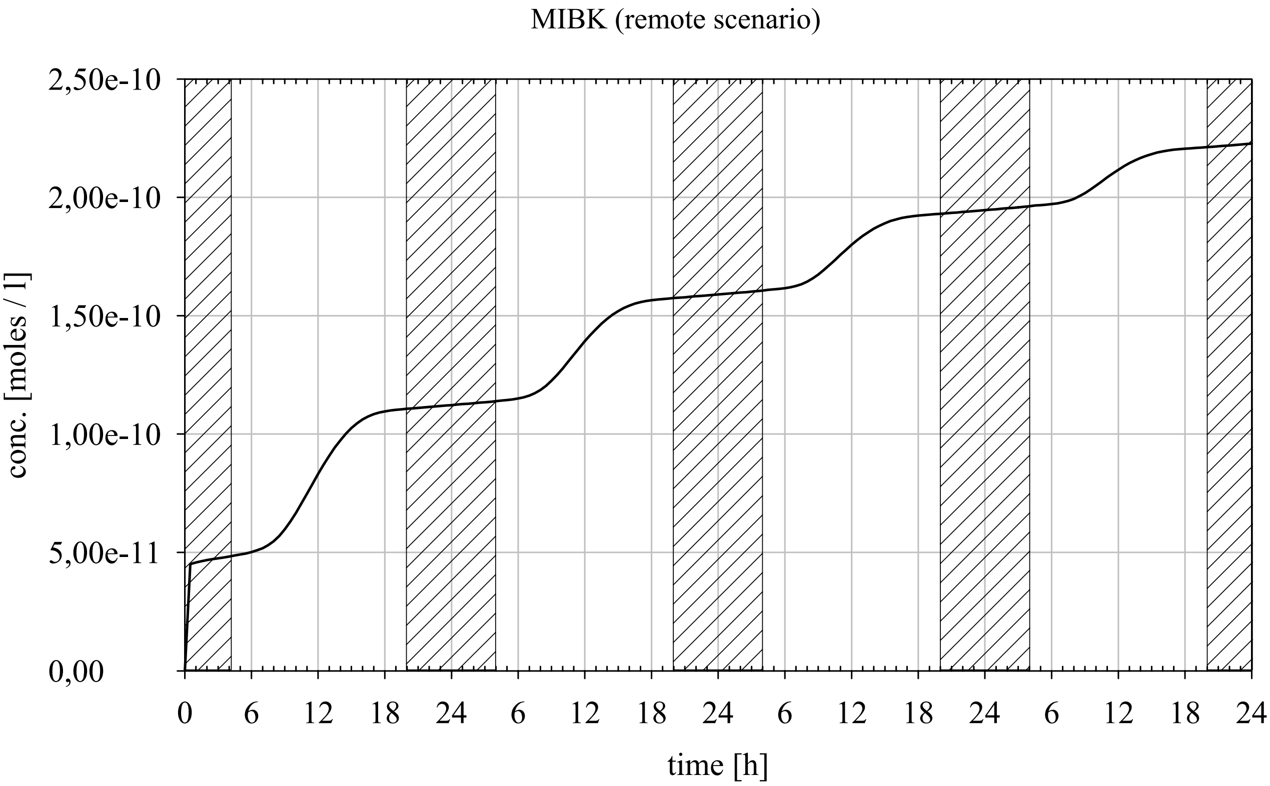


Figure III: Aqueous phase concentration of MIBK for the standard scenario (remote).

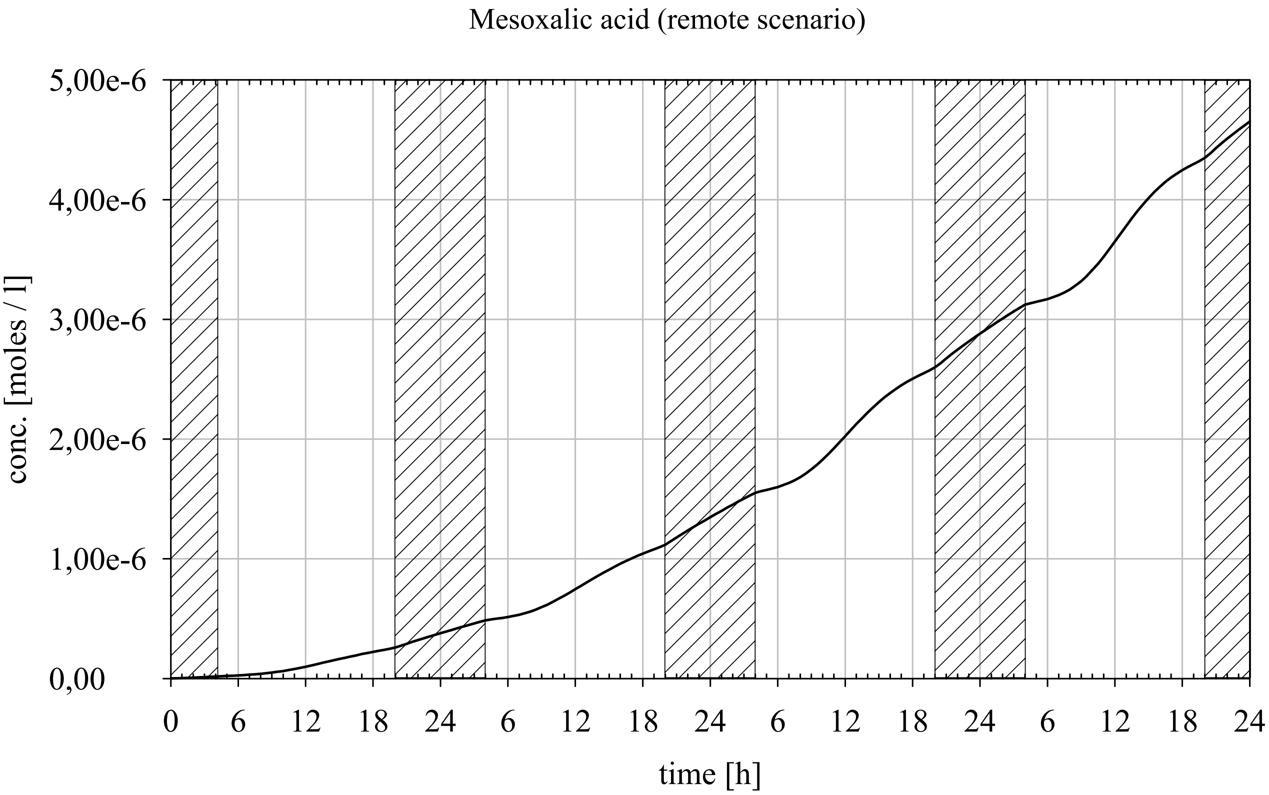


Figure IV: Aqueous phase concentration of mesoxalic acid for the standard scenario (remote).

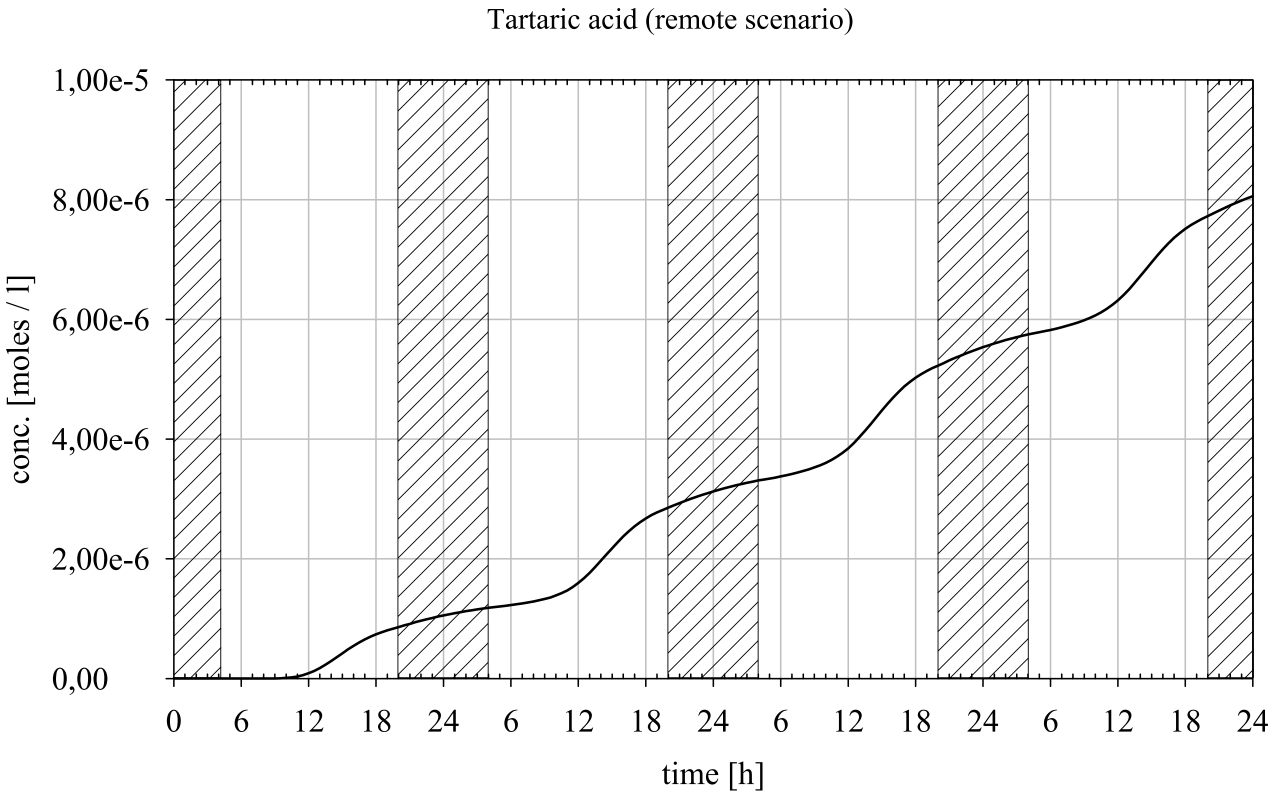


Figure V: Aqueous phase concentration of tartaric acid for the standard scenario (remote).

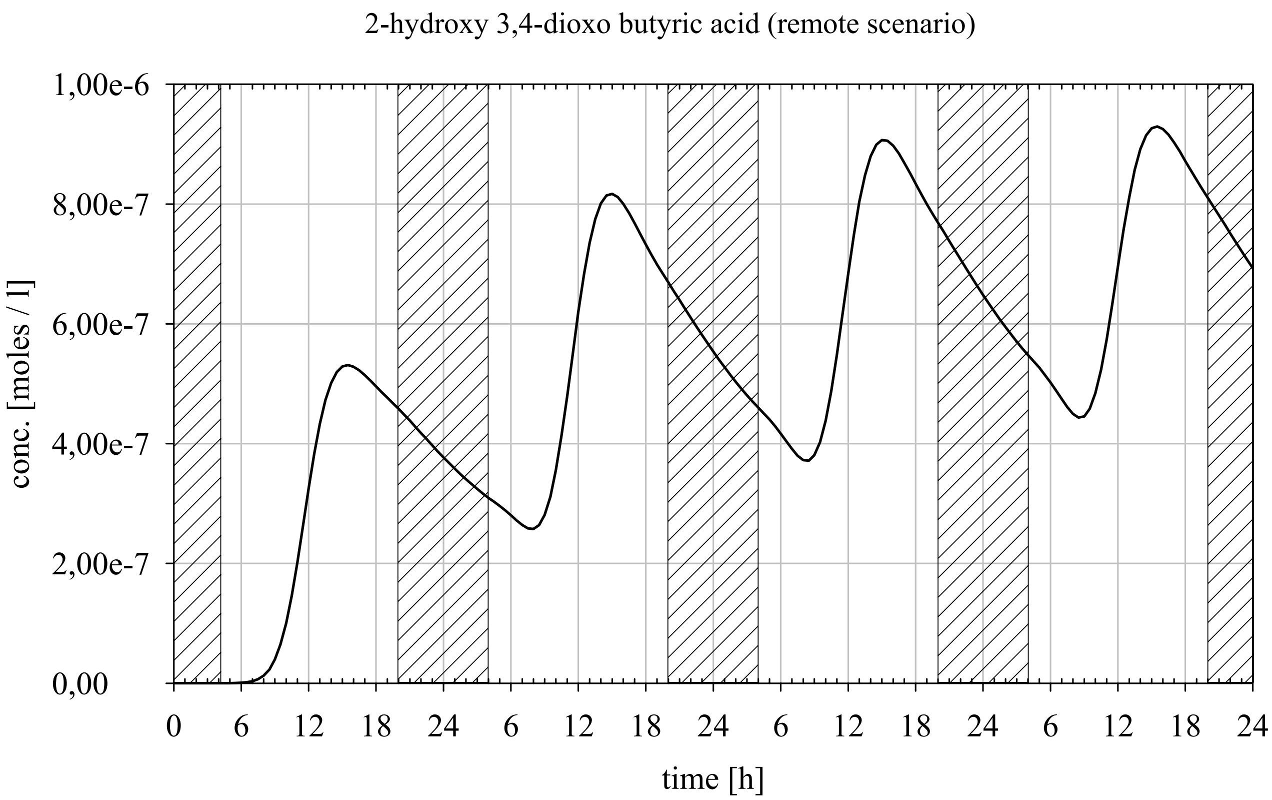


Figure VI: Aqueous phase concentration of 2-hydroxy-3,4-butyric acid for the standard scenario (remote).

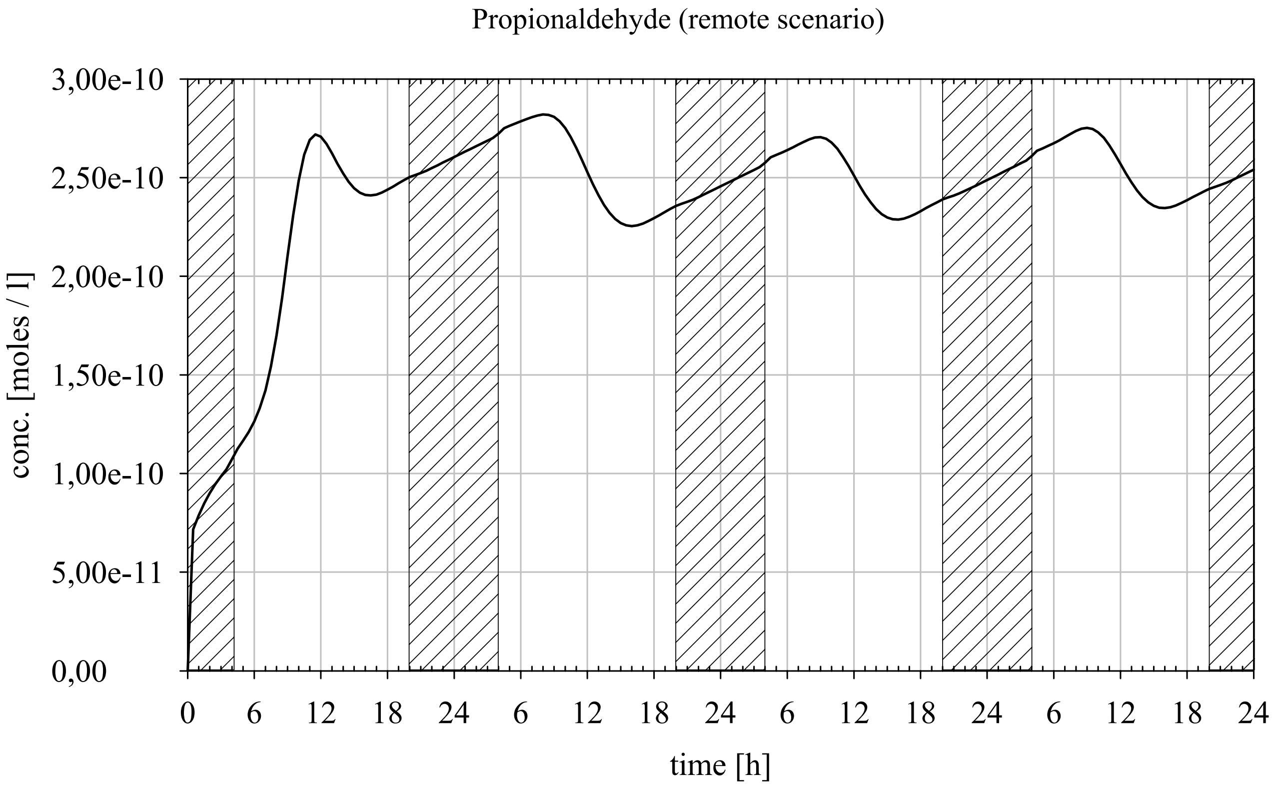


Figure VII: Aqueous phase concentration of propionaldehyde for the standard scenario (remote).

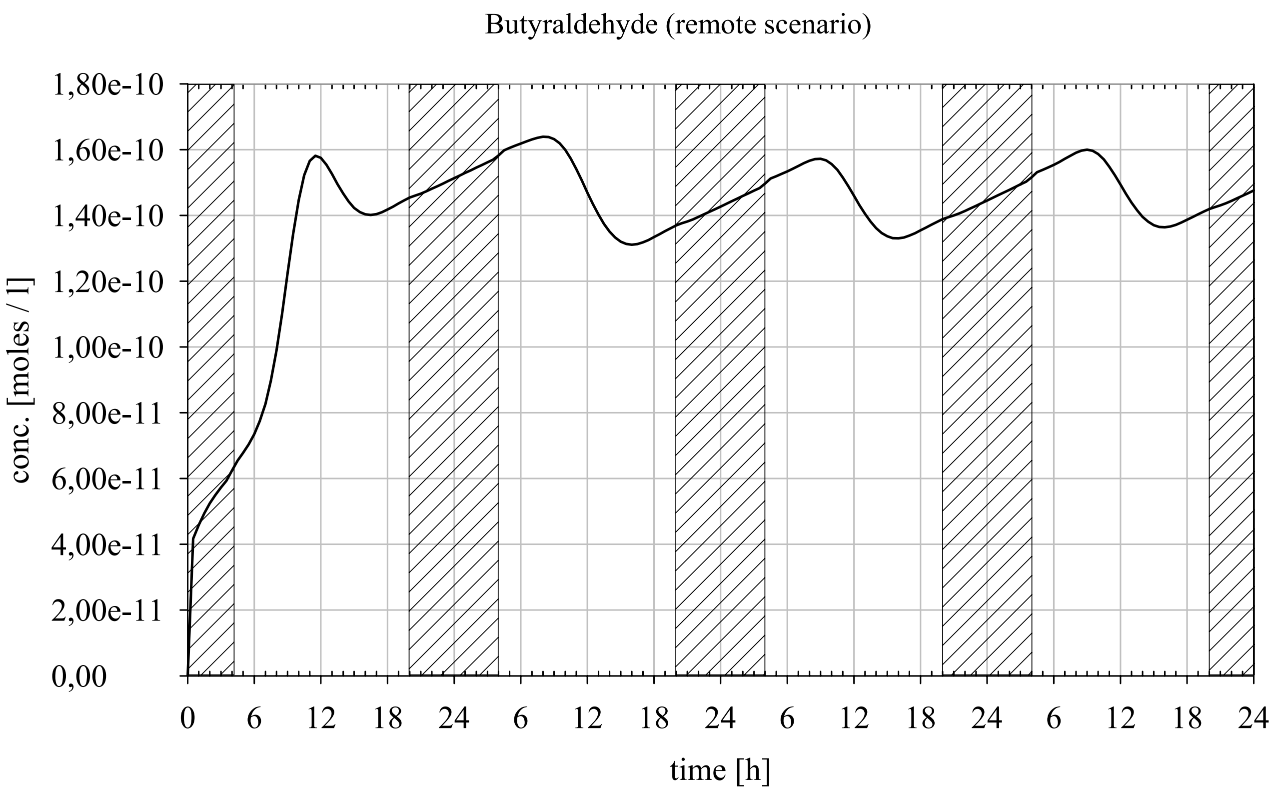


Figure VIII: Aqueous phase concentration of butyraldehyde for the standard scenario (remote).

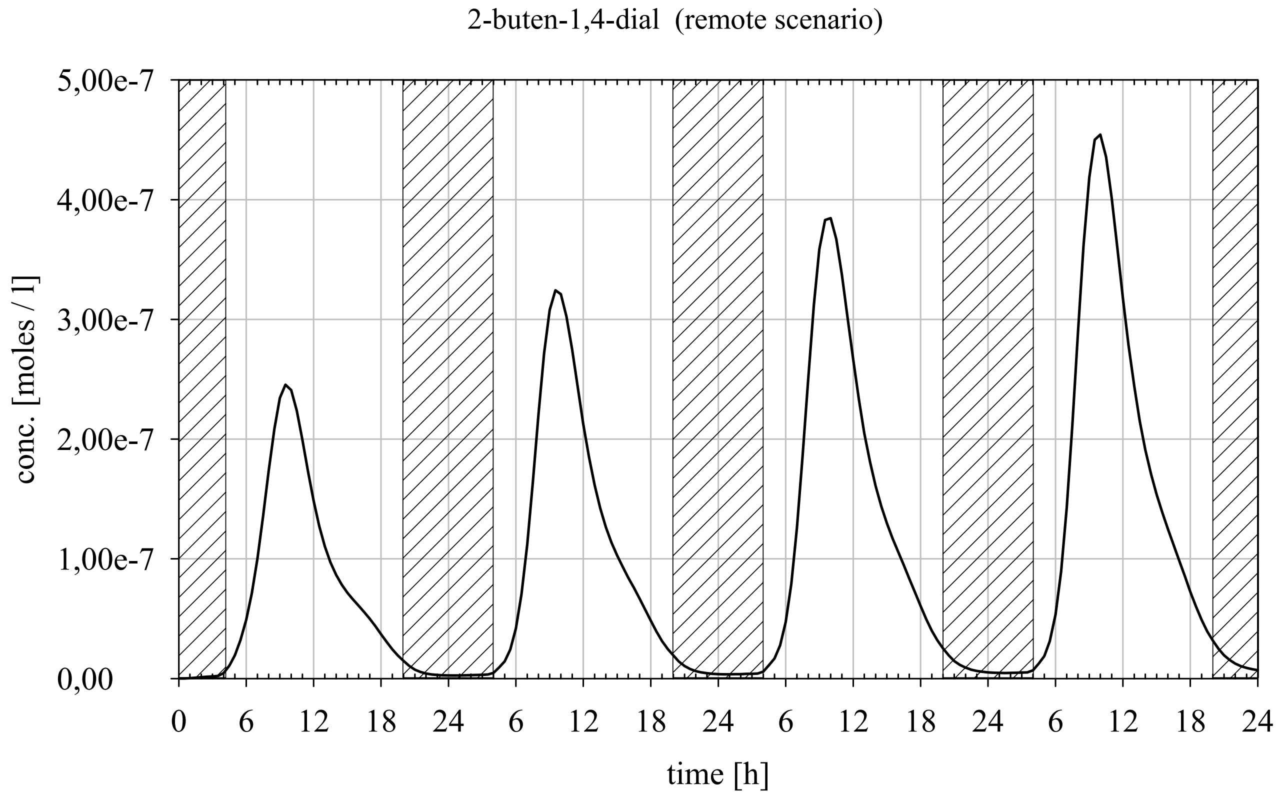


Figure XIX: Aqueous phase concentration of 2-buten-1,4-dial for the standard scenario (remote).

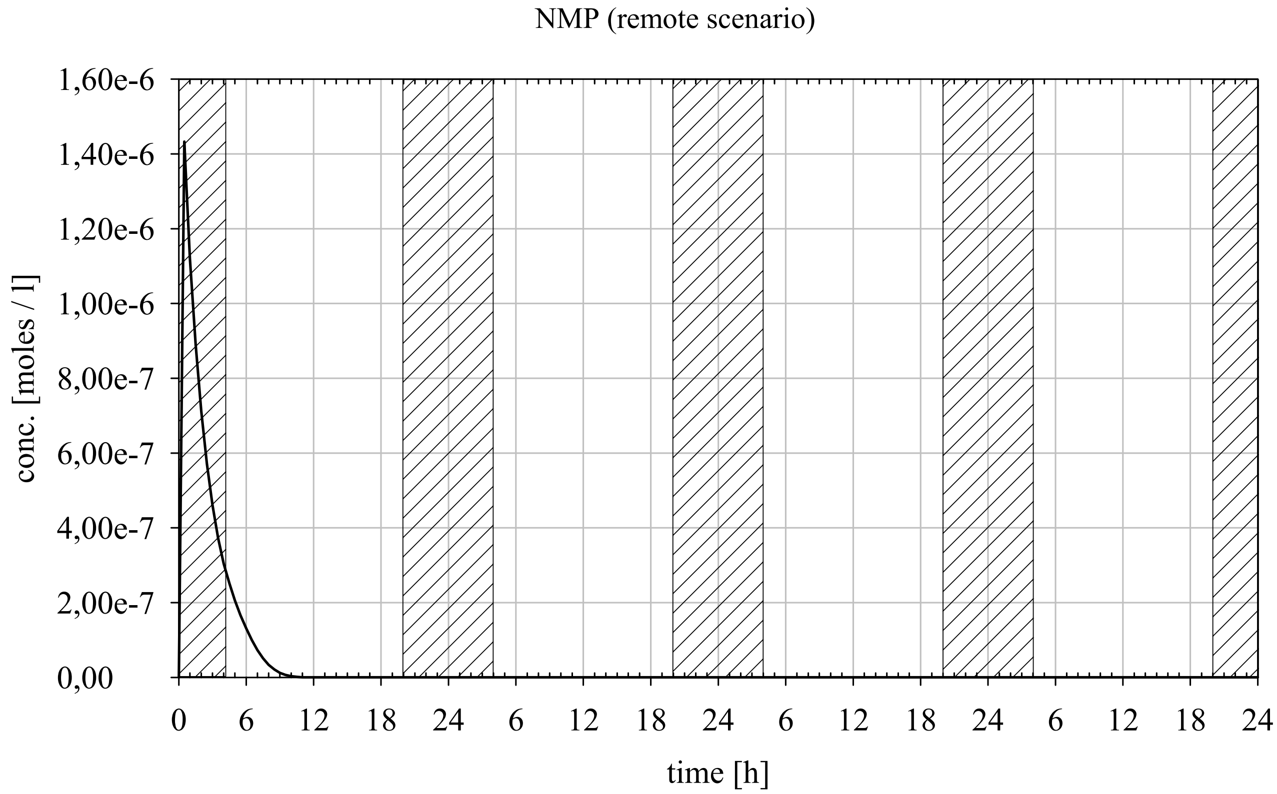


Figure X: Aqueous phase concentration of NMP for the standard scenario (remote).

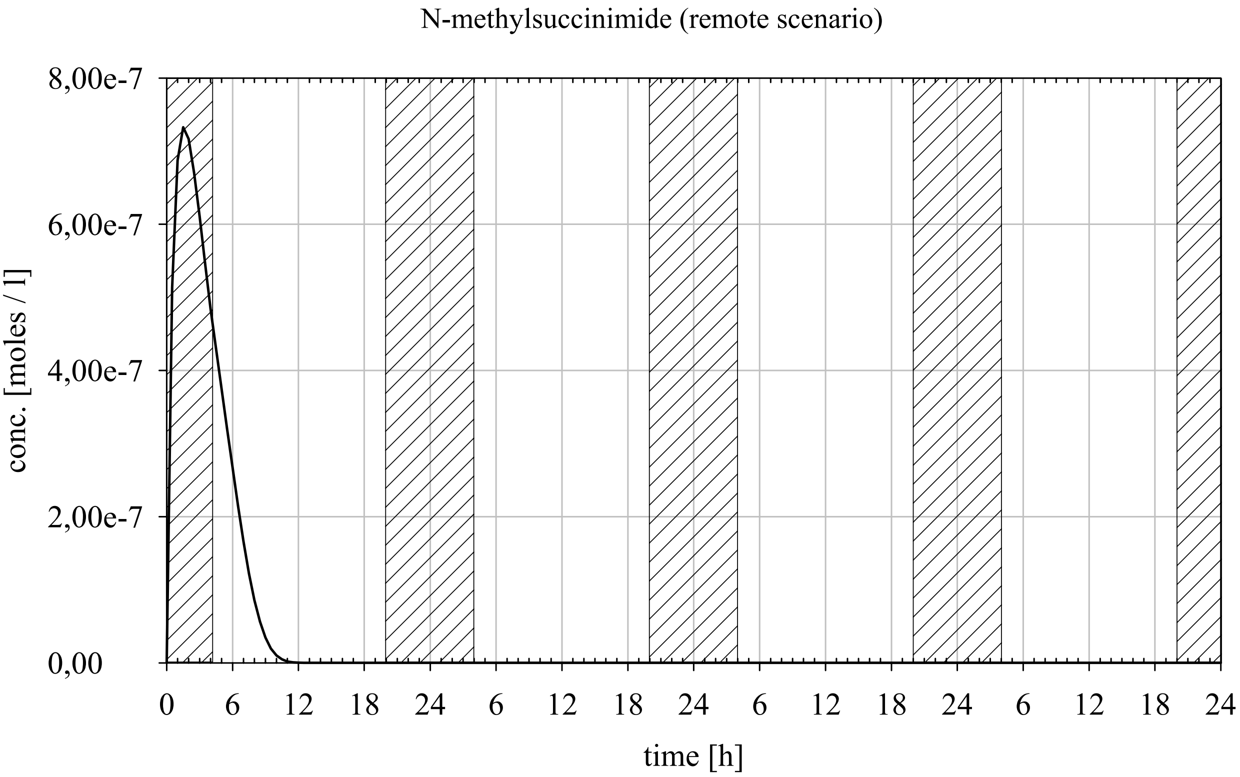


Figure XI: Aqueous phase concentration of N-methylsuccinimide for the standard scenario (remote).

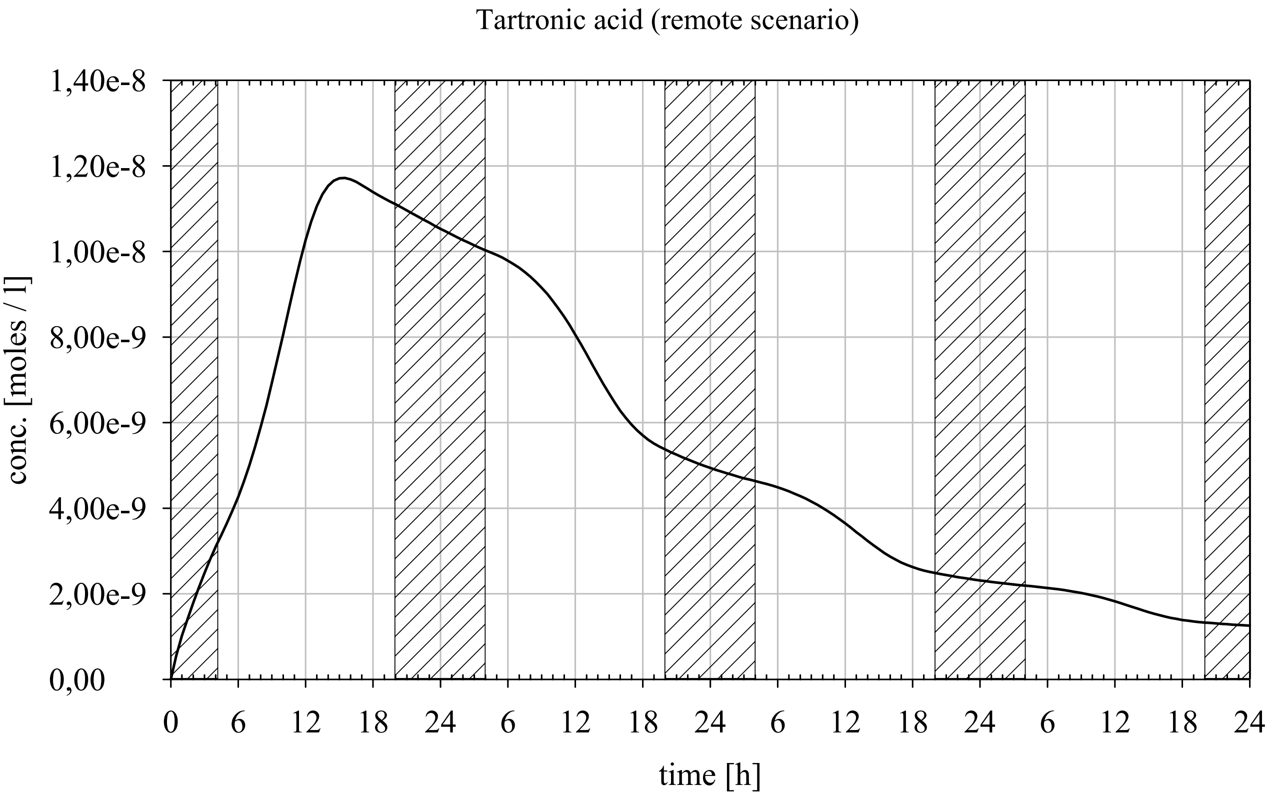


Figure XII: Aqueous phase concentration of tartronic acid for the standard scenario (remote).

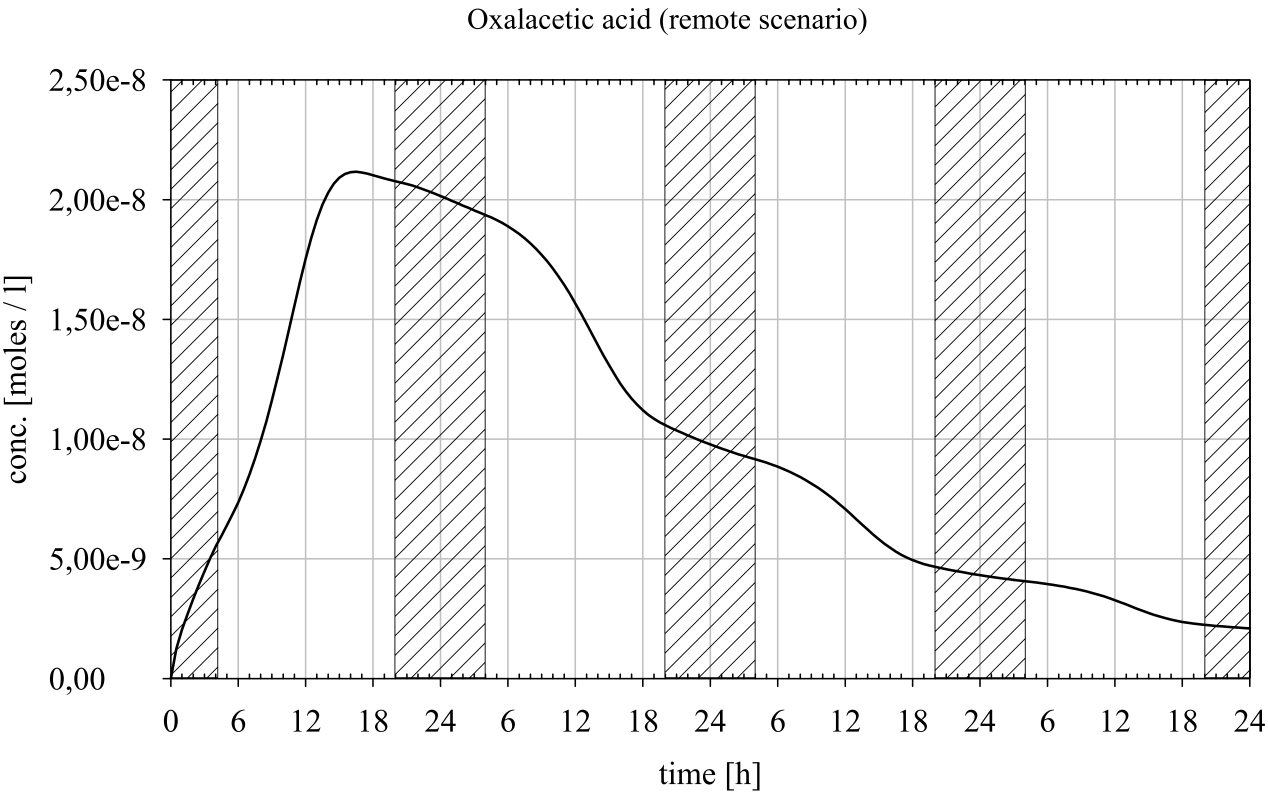
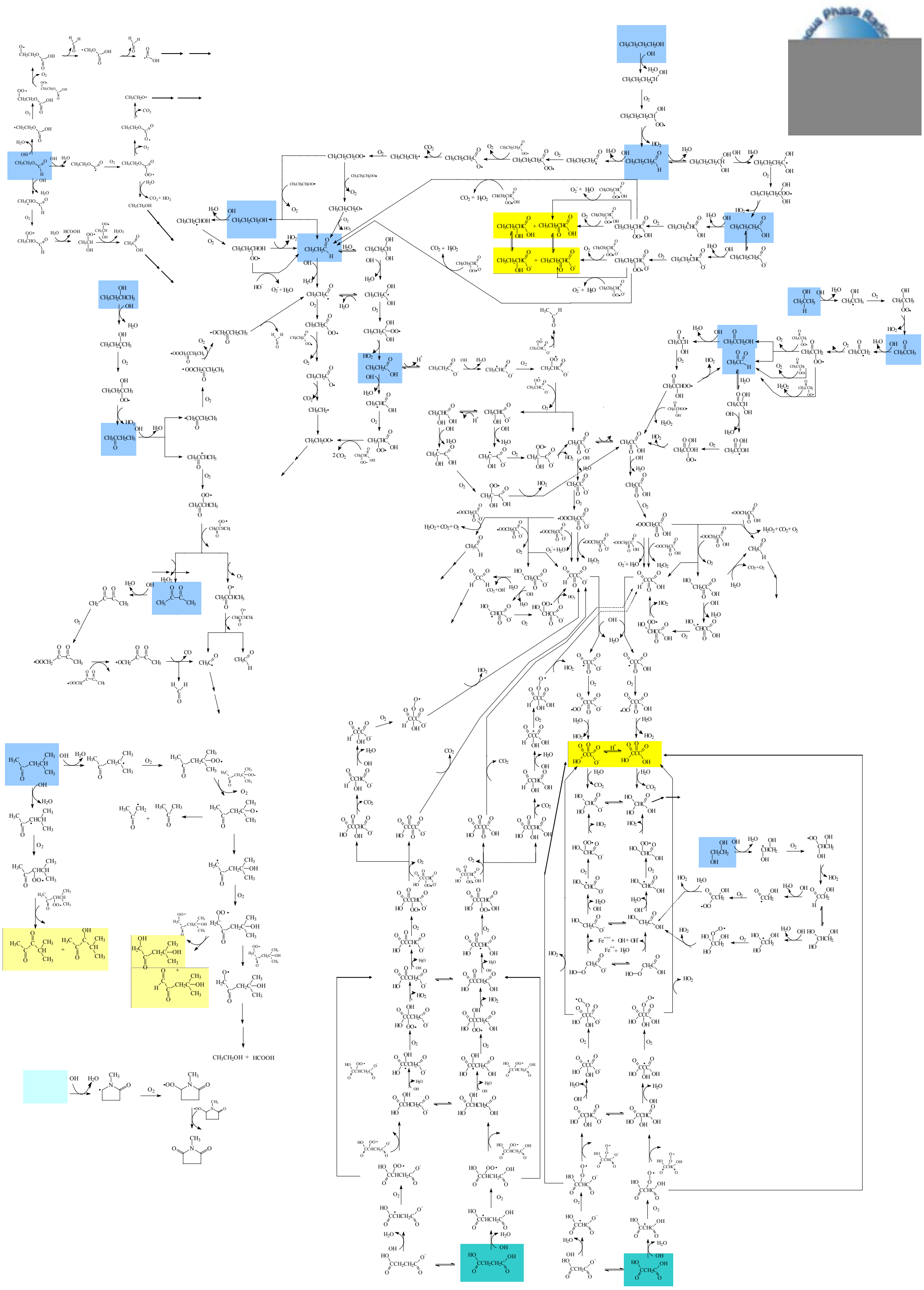


Figure XIII: Aqueous phase concentration of oxalacetic acid for the standard scenario (remote).



Scheme I: Oxidation pathways implemented in CAPRAM 3.0