Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplement

Oxidation of substituted aromatic hydrocarbons in the tropospheric aqueous phase: Kinetic mechanism development and modelling

Erik H. Hoffmann, Andreas Tilgner, Ralf Wolke, Olaf Böge, Arno Walter, and Hartmut Herrmann

Corresponding author: herrmann@tropos.de

Table S1 Phase transfer data of CAPRAM-AM1.0.

Species	K	Ref.	α	Ref.	D_g / 10^6 m^2 s^{-1}	Ref.
Phenol	$6.47 \cdot 10^2 e^{(7684*(1/T-1/298))}$	Feigenbrugel et al. [1]	0.027	Heal et al. [2]	8.5	Fuller et al. [3]
Catechol	$8.31 \cdot 10^5$	Sander [4]	0.1	est.	8.2	Fuller et al. [3]
Cresol	$4.24 \cdot 10^2 e^{(8544*(1/T-1/298))}$	Feigenbrugel et al. [1]	0.027	Lahoutifard et al. [5]	7.7	Fuller et al. [3]
Methylcatechol	$5.45 \cdot 10^5$	est. ratio phenol/catechol	0.1	est.	7.5	Fuller et al. [3]
Benzyl alcohol	$3.11 \cdot 10^3$	Altschuh et al. [6]	0.1	est.	7.7	Fuller et al. [3]
Benzaldehyde	$3.31 \cdot 10^1 e^{(6258*(1/T-1/298))}$	Allou et al. [7]	0.1	est.	7.9	Fuller et al. [3]
Benzoic acid	$2.94 \cdot 10^4$	Li et al. [8]	0.1	est.	7.6	Fuller et al. [3]
2-Nitrophenol	$1.47 \cdot 10^2 e^{(5720*(1/T-1/298))}$	Guo and Brimblecombe [9]	0.0033	Leyssens et al. [10]	7.7	Fuller et al. [3]
4-Nitrophenol	$2.13 \cdot 10^4$	Guo and Brimblecombe [9]	0.1	est.	7.7	Fuller et al. [3]
6-Methyl-2-Nitrophenol	$2.98 \cdot 10^1$	Tremp et al. [11]	0.1	est.	7.1	Fuller et al. [3]
1,4-Benzoquinone	$5.27 \cdot 10^5$	est. same as MBQ	0.1	est.	7.7	Fuller et al. [3]
2-Methyl-1,4-benzoquinone	$5.27 \cdot 10^5$	Sander [4]	0.1	est.	7.1	Fuller et al. [3]
Dinitrophenol	$1.16 \cdot 10^4$	Tremp et al. [11]	0.1	est.	7.2	Fuller et al. [3]
Dinitrocresol	$4.41 \cdot 10^3$	Tremp et al. [11]	0.1	est.	6.7	Fuller et al. [3]
4-Nitrocatechol	$2.70 \cdot 10^7$	est. ratio phenol/4-nitrophenol	0.1	est.	7.5	Fuller et al. [3]
Nitromethylcatechol	$3.83 \cdot 10^4$	est. ratio cresol/2-nitrocresol	0.1	est.	6.9	Fuller et al. [3]
2-Chlorophenol	$3.64 \cdot 10^2 e^{(5700*(1/T-1/298))}$	Sander [4]	0.1	est.	7.7	Fuller et al. [3]
4-Chlorophenol	$1.42 \cdot 10^2 e^{(11000*(1/T-1/298))}$	Sander [4]	0.1	est.	7.7	Fuller et al. [3]
2,4-Dichlorophenol	$6.69 \cdot 10^2 e^{(6800*(1/T-1/298))}$	Sander [4]	0.1	est.	7.1	Fuller et al. [3]
2,6-Dichlorophenol	$3.75 \cdot 10^2$	Sander [4]	0.1	est.	7.1	Fuller et al. [3]
2,4,6-Trichlorophenol	$2.03 \cdot 10^2$	Sander [4]	0.1	est.	6.6	Fuller et al. [3]
2-Bromophenol	$4.56 \cdot 10^3$	Sander [4]	0.1	est.	8.1	Fuller et al. [3]
4-Bromophenol	$6.79 \cdot 10^3$	Sander [4]	0.1	est.	8.1	Fuller et al. [3]
2,4-Dibromophenol	$1.11 \cdot 10^4$	Sander [4]	0.1	est.	8.0	Fuller et al. [3]
2,6-Dibromophenol	$1.11 \cdot 10^4$	Sander [4]	0.1	est.	8.0	Fuller et al. [3]
2,4,6-Tribromophenol	$2.13 \cdot 10^4$	Sander [4]	0.1	est.	8.0	Fuller et al. [3]
4-Bromo-2-nitrophenol	$7.90 \cdot 10^1$	est. 4-Chloro-2-nitrophenol	0.1	est.	6.7	Fuller et al. [3]
2-Chlorobenzoic acid	$2.53 \cdot 10^4$	Sander [4]	0.1	est.	7.0	Fuller et al. [3]

Table S2 Aqueous-phase equilibriums of CAPRAM-AM1.0.

	Reaction	K	Ref.	$k_{f,298}$	$k_{b,298}$	Ref.
1	$C_6H_5OH \rightleftharpoons C_6H_5O^-$	$1.0 \cdot 10^{-10}$	Lahoutifard et al. [5]	$5.0 \cdot 10^{0}$	$5.0 \cdot 10^{10}$	est.
2	$C_6H_5OH^+ \rightleftharpoons C_6H_5O + H^+$	$1.0 \cdot 10^{+2}$	Dixon and Murphy [12]	$5.0 \cdot 10^{12}$	$5.0 \cdot 10^{10}$	est.
3	$C_6H_5OH^+ + H_2O \rightleftharpoons PHENHCHD + H^+$	$4.0 \cdot 10^{-2}$	lower limit Sehested and Holcman [13]	$2.0 \cdot 10^{7}$	$5.0 \cdot 10^{8}$	Sehested et al. [14]
4	$Fe^{3+} + C_6H_5OH \rightleftharpoons FeC_6H_5O^{2+} + H^+$	$1.67 \cdot 10^{-2}$	Milburn [15]	$1.00 \cdot 10^{0}$	$1.67 \cdot 10^{2}$	Nakamura et al. [16]
5	$FeOH^{2+} + 1,2\text{-}C_6H_4(OH)_2 \rightleftharpoons FeC_6H_4O_2^+ + H^+$	$4.35 \cdot 10^{-2}$	Mentasti and Pelizzetti [17]	$3.1 \cdot 10^{3}$	$7.13 \cdot 10^{4}$	
6	$C_7H_7OH \rightleftharpoons C_7H_7O^-$	$7.4 \cdot 10^{-11}$	Lahoutifard et al. [5]	$3.7 \cdot 10^{0}$	$5.0 \cdot 10^{10}$	est.
7	$C_7H_7OH^+ \rightleftharpoons C_7H_7O + H^+$	$6.31 \cdot 10^{+1}$	Dixon and Murphy [12]	$2.0 \cdot 10^{5}$	$3.17 \cdot 10^{3}$	Choure et al. [18]
8	$C_7H_7OH^+ + H_2O \rightleftharpoons CRESCHD + H^+$	$4.0 \cdot 10^{-2}$	lower limit Sehested and Holcman [13]	$2.0 \cdot 10^{7}$	$5.0 \cdot 10^{8}$	Sehested et al. [14]
9	$C_6H_5CH_2OH^+ + H_2O \rightleftharpoons ALKHCHD + H^+$	$2.40 \cdot 10^{-3}$	est. Steenken and Ramaraj [19]	$1.20 \cdot 10^{6}$	$5.0 \cdot 10^{8}$	Sehested et al. [14]
10	$C_6H_5CH(OH)_2^+ + H_2O \rightleftharpoons ALDHCHD + H^+$	$2.40 \cdot 10^{-3}$	est. Steenken and Ramaraj [19]	$1.20 \cdot 10^{6}$	$5.0 \cdot 10^{8}$	Sehested et al. [14]
11	$C_6H_5CHO + H_2O \rightleftharpoons C_6H_5CH(OH)_2$	$1.1 \cdot 10^{-2}$	Greenzaid [20]	$5.5 \cdot 10^{8}$	$5.0 \cdot 10^{10}$	est.
12	$HOC_6H_4CHO + H_2O \rightleftharpoons HOC_6H_4CH(OH)_2$	$1.1 \cdot 10^{-2}$	est.	$5.5 \cdot 10^{8}$	$5.0 \cdot 10^{10}$	est.
13	$(HO)_2C_6H_3CHO + H_2O \rightleftharpoons (HO)_2C_6H_3CH(OH)_2$	$1.1 \cdot 10^{-2}$	est.	$5.5 \cdot 10^{8}$	$5.0 \cdot 10^{10}$	est.
14	$C_6H_5CO_2H \rightleftharpoons C_6H_5CO_2^-$	$6.3 \cdot 10^{-5}$	Remucal and Manley [21]	$3.2 \cdot 10^{6}$	$5.0 \cdot 10^{10}$	est.
15	$HOC_6H_4CO_2H \rightleftharpoons HOC_6H_4CO_2^-$	$1.51 \cdot 10^{-3}$	Park [22]	$7.57 \cdot 10^{7}$	$5.0 \cdot 10^{10}$	est.
16	$HOC_6H_4CO_2^- + Fe^{3+} \rightleftharpoons FeHOC_6H_4CO_2^{2+}$	$2.51 \cdot 10^{4}$	Park [22]	$1.26 \cdot 10^{15}$	$5.0 \cdot 10^{10}$	est.
17	$(HO)_2C_6H_3CO_2H \rightleftharpoons (HO)_2C_6H_3CO_2^-$	$2.00 \cdot 10^{-3}$	est. 2,3-dihydroxybenzoic acid, Avdeef et al. [23]	$1.00 \cdot 10^{8}$	$5.0 \cdot 10^{10}$	est.
18	$(HO)_2C_6H_3CO_2H + Fe^{3+} \rightleftharpoons (O)Fe(CO_2)C_6H_3OH^+ + 2\ H^+$	$7.00 \cdot 10^{0}$	Xu and Jordan [24]	$3.50 \cdot 10^{11}$	$5.0 \cdot 10^{10}$	est.
19	$(HO)_2C_6H_3CO_2^- + Fe^{3+} + H^+ \rightleftharpoons (O)Fe(CO_2)C_6H_3OH^+ + 2\ H^+$	$3.50 \cdot 10^{3}$	Xu and Jordan [24]	$1.75 \cdot 10^{14}$	$5.0 \cdot 10^{10}$	est.
20	$(O)Fe(CO_2)C_6H_3OH^+ \rightleftharpoons Fe^+(O)_2C_6H_3CO_2^- + H^+$	$1.00 \cdot 10^{-6}$	Xu and Jordan [24]	$5.00 \cdot 10^{4}$	$5.0 \cdot 10^{10}$	est.
21	$(HO)_3C_6H_2CO_2H \rightleftharpoons (HO)_3C_6H_2CO_2^-$	$3.98 \cdot 10^{-5}$	est. gallic acid, Dwibedy et al. [25]	$1.99 \cdot 10^{6}$	$5.0 \cdot 10^{10}$	est.
22	$(HO)_3C_6H_2CO_2H + FeOH^{2+} \rightleftharpoons Fe(O)_2(HO)C_6H_2CO_2H^+ + H^+$	$1.42 \cdot 10^{2}$	Hynes and O Coinceanainn [26]	$2.83 \cdot 10^{3}$	$2.0 \cdot 10^{1}$	
23	$2\text{-}HOC_6H_4O + O_2 \rightleftharpoons 1,2\text{-}C_6H_4O_2 + HO_2$	$1.60 \cdot 10^{-2}$	Valgimigli et al. [27]	$1.6 \cdot 10^{6}$	$1.0 \cdot 10^{8}$	

	Reaction	K	Ref.	$k_{f,298}$	$k_{b,298}$	Ref.
24	$4\text{-}HOC_6H_4O + O_2 \rightleftharpoons 1,4\text{-}C_6H_4O_2 + HO_2$	$1.60 \cdot 10^{-2}$	Valgimigli et al. [27]	$1.6 \cdot 10^{6}$	$1.0 \cdot 10^{8}$	
25	$2,4\text{-}C_6H_4N_2O_5 \rightleftharpoons 2,4\text{-}C_6H_3N_2O_5^- + H^+$	$8.13 \cdot 10^{-5}$	cal.	$4.06 \cdot 10^{6}$	$5.0 \cdot 10^{10}$	est.
26	$2,4\text{-}C_7H_6N_2O_5 \rightleftharpoons 2,4\text{-}C_6H_5N_2O_5^- + H^+$	$3.55 \cdot 10^{-5}$	cal.	$1.77 \cdot 10^{6}$	$5.0 \cdot 10^{10}$	est.
27	$4\text{-}C_6H_5NO_4 \rightleftharpoons 4\text{-}C_6H_4NO_4^- + H^+$	$1.35 \cdot 10^{-7}$	cal.	$6.74 \cdot 10^{3}$	$5.0 \cdot 10^{10}$	est.
28	$4\text{-}C_7H_7NO_4 \rightleftharpoons 4\text{-}C_7H_6NO_4^- + H^+$	$1.38 \cdot 10^{-7}$	cal.	$6.90 \cdot 10^{3}$	$5.0 \cdot 10^{10}$	est.
29	$2\text{-}C_6H_4ClOH \rightleftharpoons 2\text{-}C_6H_4ClO^-$	$2.75 \cdot 10^{-9}$	Deborde and von Gunten [28]	$1.38 \cdot 10^{2}$	$5.0 \cdot 10^{10}$	est.
30	$4\text{-}C_6H_4ClOH \rightleftharpoons 4\text{-}C_6H_4ClO^-$	$3.72 \cdot 10^{-10}$	Deborde and von Gunten [28]	$1.86 \cdot 10^{1}$	$5.0 \cdot 10^{10}$	est.
31	$2,4\text{-}C_6H_3Cl_2OH \rightleftharpoons 2,4\text{-}C_6H_3Cl_2O^-$	$1.41 \cdot 10^{-8}$	Deborde and von Gunten [28]	$7.05 \cdot 10^{2}$	$5.0 \cdot 10^{10}$	est.
32	$2,6\text{-}C_6H_3Cl_2OH \rightleftharpoons 2,6\text{-}C_6H_3Cl_2O^-$	$1.07 \cdot 10^{-7}$	Deborde and von Gunten [28]	$5.35 \cdot 10^{3}$	$5.0 \cdot 10^{10}$	est.
33	$2,4,6\text{-}C_6H_2Cl_3OH \rightleftharpoons 2,4,6\text{-}C_6H_2Cl_3O^-$	$7.10 \cdot 10^{-7}$	Deborde and von Gunten [28]	$3.55 \cdot 10^{4}$	$5.0 \cdot 10^{10}$	est.
34	$2\text{-}C_6H_4BrOH \rightleftharpoons 2\text{-}C_6H_4BrO^-$	$3.55 \cdot 10^{-9}$	Deborde and von Gunten [28]	$1.78 \cdot 10^{2}$	$5.0 \cdot 10^{10}$	est.
35	$4\text{-}C_6H_4BrOH \rightleftharpoons 4\text{-}C_6H_4BrO^-$	$6.76 \cdot 10^{-10}$	Deborde and von Gunten [28]	$3.38 \cdot 10^{1}$	$5.0 \cdot 10^{10}$	est.
36	$2,4\text{-}C_6H_3Br_2OH \rightleftharpoons 2,4\text{-}C_6H_3Br_2O^-$	$1.41 \cdot 10^{-8}$	Deborde and von Gunten [28]	$7.05 \cdot 10^{2}$	$5.0 \cdot 10^{10}$	est.
37	$2,6\text{-}C_6H_3Br_2OH \rightleftharpoons 2,6\text{-}C_6H_3Br_2O^-$	$1.07 \cdot 10^{-7}$	Deborde and von Gunten [28]	$5.35 \cdot 10^{3}$	$5.0 \cdot 10^{10}$	est.
38	$2,4,6\text{-}C_6H_2Br_3OH \rightleftharpoons 2,4,6\text{-}C_6H_2Br_3O^-$	$7.10 \cdot 10^{-7}$	Deborde and von Gunten [28]	$3.55 \cdot 10^{4}$	$5.0 \cdot 10^{10}$	est.
39	$2\text{-}ClC_6H_4CO_2H \rightleftharpoons 2\text{-}ClC_6H_5CO_2^-$	$1.29 \cdot 10^{-3}$	cal.	$6.44 \cdot 10^{7}$	$5.0 \cdot 10^{10}$	est.
40	$HOC_6H_3BrCO_2H \rightleftharpoons HOC_6H_3BrCO_2^-$	$2.24 \cdot 10^{-3}$	cal.	$1.12 \cdot 10^{8}$	$5.0 \cdot 10^{10}$	est.

Table S3 Aqueous-phase reactions of CAPRAM-AM1.0.

	Reaction	k_{298}	$-E_A/R$	Comment	Reference
A1	$C_6H_5OH + OH \rightarrow 0.92\ PHENHCHD + 0.08\ C_6H_5O$	$8.41 \cdot 10^9$		Raghavan and Steenken [29]	Bonin et al. [30]
A2	$C_6H_5OH + NO_3 \rightarrow C_6H_5OH^+ + NO_3^-$	$1.90 \cdot 10^9$	-2100	ETR	Umschlag et al. [31]
A3	$C_6H_5OH + SO_4^- \rightarrow C_6H_5OH^+ + SO_4^{2-}$	$8.80 \cdot 10^9$		ETR	Ziajka and Pasiuk-Bronikowska [32]
A4	$C_6H_5OH + Cl \rightarrow C_6H_5OH^+ + Cl^-$	$2.50 \cdot 10^{10}$		ETR	Alfassi et al. [33]
A5	$C_6H_5OH + Cl_2^- \rightarrow C_6H_5OH^+ + 2\ Cl^-$	$3.20 \cdot 10^8$	-878	ETR after Vione et al. [34]	Alfassi et al. [35]
A6	$C_6H_5OH + Br_2^- \rightarrow C_6H_5OH^+ + 2\ Br^-$	$6.10 \cdot 10^6$	-2080	ETR	Alfassi et al. [35]
A7	$C_6H_5OH + CO_3^- \rightarrow C_6H_5OH^+ + CO_3^{2-}$	$2.20 \cdot 10^7$		ETR	Chen and Hoffman [36]
A8	$C_6H_5OH + NO_2 \rightarrow C_6H_5OH^+ + NO_2^-$	$7.90 \cdot 10^2$		ETR	Vione et al. [37]
A9	$C_6H_5O^- + NO_2 \rightarrow C_6H_5O + NO_2^-$	$1.50 \cdot 10^7$	-4126	ETR	Alfassi et al. [35]
A10	$C_6H_5OH + NO_2^+ \rightarrow$ $0.6\ 2\text{-}C_6H_5NO_3 + 0.4\ 4\text{-}C_6H_5NO_3 + H^+$	$1.00 \cdot 10^{10}$		diffusion limited	Heal et al. [38]
A11	$C_6H_5OH + O_3 \rightarrow$ $0.46\ 1,4\text{-}C_6H_4O_2 + 0.08\ 1,4\text{-}C_6H_4(OH)_2 + 0.23\ 1,2\text{-}C_6H_4(OH)_2 + 0.23\ C_6H_6O_4 + 0.46\ H_2O_2 - 0.54\ H^+$	$1.30 \cdot 10^3$		yields pH = 2 Mvula and von Sonntag [39]	Hoigne and Bader [40]
A12	$C_6H_5O^- + O_3 \rightarrow$ $0.57\ 1,4\text{-}C_6H_4O_2 + 0.04\ C_6H_5O + 0.01\ 1,4\text{-}C_6H_4(OH)_2 + 0.04\ O_3^- + 0.36\ 1,2\text{-}C_6H_4(OH)_2 + 0.02\ C_6H_5O_4^- + 0.57\ H_2O_2 - 0.94\ H^+$	$1.40 \cdot 10^9$		yields pH = 10 Mvula and von Sonntag [39]	Hoigne and Bader [40]
A13	$HOCl + C_6H_5OH \rightarrow$ $0.8\ 2\text{-}C_6H_4ClOH + 0.2\ 4\text{-}C_6H_4ClOH + H_2O$	$3.60 \cdot 10^{-1}$			Gallard and Von Gunten [41]
A14	$HOCl + C_6H_5OH + H^+ \rightarrow$ $0.8\ 2\text{-}C_6H_4ClOH + 0.2\ 4\text{-}C_6H_4ClOH + H_2O + H^+$	$3.52 \cdot 10^4$			Gallard and Von Gunten [41]
A15	$HOCl + C_6H_5O^- \rightarrow$ $0.8\ 2\text{-}C_6H_4ClO^- + 0.2\ 4\text{-}C_6H_4ClO^- + H_2O$	$2.19 \cdot 10^4$			Gallard and Von Gunten [41]
A16	$HOBr + C_6H_5OH \rightarrow$ $0.67\ 2\text{-}C_6H_4BrOH + 0.33\ 4\text{-}C_6H_4BrOH + H_2O$	$5.00 \cdot 10^2$			Gallard et al. [42]
A17	$HOBr + C_6H_5O^- \rightarrow$	$1.80 \cdot 10^8$			Gallard et al. [42]

	Reaction	k_{298}	$-E_A/R$	Comment	Reference
	0.67 2-$C_6H_4BrO^-$ + 0.33 4-$C_6H_4BrO^-$ + H_2O				
A18	$C_6H_5OH + HONO \rightarrow$ 4-$C_6H_5NO_2 + H_2O$	$9.20 \cdot 10^{-3}$			Vione et al. [37]
A19	4-$C_6H_5NO_2 \rightarrow$ 4-$C_6H_5NO_3$	$3.00 \cdot 10^{-5}$			Vione et al. [37]
A20	$C_6H_5OH^+ + Fe^{2+} \rightarrow C_6H_5OH + Fe^{3+}$	$6.00 \cdot 10^{8}$		est. same as for Anisole	Walling et al. [43]
A21	$C_6H_5O + HO_2 \rightarrow C_6H_5OH + O_2$	$2.00 \cdot 10^{9}$			Vione et al. [34]
A22	$C_6H_5O + O_2^- \rightarrow$ 1,4-$C_6H_4O_2 - H^+$ - H_2O	$1.00 \cdot 10^{9}$			Mvula and von Sonntag [39]
A23	$C_6H_5O + Cl_2^- \rightarrow$ 0.8 2-C_6H_4ClOH + 0.2 4-C_6H_4ClOH + Cl^-	$3.00 \cdot 10^{3}$		yields est. like for HOCl	Martire et al. [44]
A24	$C_6H_5O + Br_2^- \rightarrow$ 0.67 2-C_6H_4BrOH + 0.33 4-C_6H_4BrOH + Br^-	$1.80 \cdot 10^{5}$		60 times higher formation rate of bromophenols	Calza et al. [45]
A25	$C_6H_5O + NO_2 \rightarrow$ 0.67 2-$C_6H_5NO_3$ + 0.33 4-$C_6H_5NO_3$	$3.00 \cdot 10^{9}$			Vione et al. [46]
A26	$C_6H_5O + C_6H_5O \rightarrow C_{12}H_{10}O_2$	$2.45 \cdot 10^{9}$			Mvula and von Sonntag [39]
A27	2-$C_6H_5NO_3 + h\nu \rightarrow$ $C_6H_4(OH)_2$ + HONO – H_2O	$1.896 \cdot 10^{-06}$	$\cos(\chi)^{0.670}\exp(-0.081/\cos(\chi))$		Alif et al. [47]
A28	PHENHCHD + $O_2 \rightarrow$ 0.5 1,2-$C_6H_4(OH)_2$ + 0.5 1,4-$C_6H_4(OH)_2$ + HO_2	$1.20 \cdot 10^{9}$		yields Barzaghi and Herrmann [48]	Mvula et al. [49]
A29	PHENHCHD + $Fe^{3+} \rightarrow$ 0.5 1,2-$C_6H_4(OH)_2$ + 0.5 1,4-$C_6H_4(OH)_2$ + Fe^{2+} + H^+	$7.00 \cdot 10^{3}$			Metelitsa [50]
A30	2 PHENHCHD $\rightarrow$ 0.5 1,2-$C_6H_4(OH)_2$ + 0.5 1,4-$C_6H_4(OH)_2$ + C_6H_5OH	$1.00 \cdot 10^{8}$		as HCHD, Mantaka et al. [51]	Mvula et al. [49]
A31	PHENHCHD + $NO_2 \rightarrow$ 0.5 2-$C_6H_5NO_3$ + 0.5 4-$C_6H_5NO_3$	$8.20 \cdot 10^{9}$			Barzaghi and Herrmann [48]
A32	1,2-$C_6H_4(OH)_2$ + OH $\rightarrow$ 1,2-$C_6H_4O_2$ + HO_2 - O_2 + H_2O	$4.70 \cdot 10^{9}$		Scheck and Frimmel [52]	mean from Smith et al. [53]
A33	1,2-$C_6H_4(OH)_2$ + $NO_3 \rightarrow$ 2-HOC_6H_4O + NO_3^- + H^+	$5.20 \cdot 10^{8}$	-4691	H-abstraction	Barzaghi and Herrmann [54]
A34	1,2-$C_6H_4(OH)_2$ + $SO_4^- \rightarrow$ 2-HOC_6H_4O + SO_4^{2-} + H^+	$5.20 \cdot 10^{8}$	-4691	H-abstraction	est. after Herrmann et al. [55]
A35	1,2-$C_6H_4(OH)_2$ + $HO_2 \rightarrow$ 2-HOC_6H_4O + H_2O_2	$4.70 \cdot 10^{4}$		H-abstraction	Bielski et al. [56]
A36	1,2-$C_6H_4(OH)_2$ + $O_2^- \rightarrow$ 2-HOC_6H_4O + $H_2O_2 - H^+$	$2.70 \cdot 10^{5}$		H-abstraction	Bielski et al. [56]
A37	1,2-$C_6H_4(OH)_2$ + $O_3 \rightarrow$ $C_6H_6O_4$ + H_2O_2 - H_2O	$5.20 \cdot 10^{5}$		est.	Mvula and von Sonntag [39]
A38	1,2-$C_6H_4(OH)_2$ + 2 HONO $\rightarrow$ 1,2-$C_6H_4O_2$ + 2 NO + 2 H_2O	$4.51 \cdot 10^{0}$			Khalafi and Rafiee [57]
A39	$FeC_6H_5O^{2+} + h\nu \rightarrow Fe^{2+} + C_6H_5O$	$4.764 \cdot 10^{-02}$	$\cos(\chi)^{0.829}\exp(-0.291/\cos(\chi))$		est. $Fe(OH)_2^{2+}$ Arakaki et al. [58]

	Reaction	k_{298}	$-E_A/R$	Comment	Reference
A40	$FeC_6H_4O_2^+ + h\nu \rightarrow Fe^{2+} + 2\text{-}HOC_6H_4O - H^+$	$1.343 \cdot 10^{-02} \cos(\chi)^{0.855} \exp(-0.300/\cos(\chi))$			est. $Fe(OH)_2^+$ Arakaki et al. [58]
A41	$1,4\text{-}C_6H_4(OH)_2 + OH \rightarrow 1,4\text{-}C_6H_4O_2 + HO_2 - O_2 + H_2O$	$1.60 \cdot 10^{10}$		products after Scheck and Frimmel [52]	Oturan et al. [59]
A42	$1,4\text{-}C_6H_4(OH)_2 + NO_3 \rightarrow 4\text{-}HOC_6H_4O + NO_3^- + H^+$	$8.80 \cdot 10^{8}$		H-abstraction	Barzaghi and Herrmann [54]
A43	$1,4\text{-}C_6H_4(OH)_2 + SO_4^- \rightarrow 4\text{-}HOC_6H_4O + SO_4^{2-} + H^+$	$8.80 \cdot 10^{8}$		H-abstraction	est. after Herrmann et al. [55]
A44	$1,4\text{-}C_6H_4(OH)_2 + HO_2 \rightarrow 4\text{-}HOC_6H_4O + H_2O_2$	$8.50 \cdot 10^{3}$		H-abstraction	Nadezhdin and Dunford [60]
A45	$1,4\text{-}C_6H_4(OH)_2 + O_2^- \rightarrow 4\text{-}HOC_6H_4O + H_2O_2 - H^+$	$1.70 \cdot 10^{7}$		H-abstraction	Rao and Hayon [61]
A46	$1,4\text{-}C_6H_4(OH)_2 + O_3 \rightarrow 1,4\text{-}C_6H_4O_2 + HO_2 + OH$	$1.80 \cdot 10^{6}$		product est.	Mvula and von Sonntag [39]
A47	$1,2\text{-}C_6H_4O_2 + OH \rightarrow C_6H_6O_4 + HO_2 - O_2$	$6.60 \cdot 10^{9}$		products after Scheck and Frimmel [52]	Schuchmann et al. [62]
A48	$1,2\text{-}C_6H_4O_2 + NO_2^- \rightarrow NO_2C_6H_3(OH)_2 + OH^- - H_2O$	$1.16 \cdot 10^{1}$			Khalafi and Rafiee [57]
A49	$1,4\text{-}C_6H_4O_2 + OH \rightarrow C_4H_4O_4 + C_2H_2O_2 + HO_2 - 2\ O_2$	$6.60 \cdot 10^{9}$		products after Scheck and Frimmel [52]	Schuchmann et al. [62]
A50	$1,4\text{-}C_6H_4O_2 + NO_3 \rightarrow C_4H_4O_4 + C_2H_2O_2 + HO_2 + NO_3^- + H^+ - 2\ O_2$	$1.00 \cdot 10^{8}$			est. after Herrmann et al. [55]
A51	$1,4\text{-}C_6H_4O_2 + SO_4^- \rightarrow C_4H_4O_4 + C_2H_2O_2 + HO_2 + SO_4^{2-} + H^+ - 2\ O_2$	$1.00 \cdot 10^{8}$			Criquet and Leitner [63]
A52	$2\text{-}HOC_6H_4O + Fe^{2+} + H^+ \rightarrow 1,2\text{-}C_6H_4(OH)_2 + Fe^{3+}$	$1.50 \cdot 10^{5}$		est same $4\text{-}HOC_6H_4O$	Neta and Grodkowski [64]
A53	$2\text{-}HOC_6H_4O + Fe^{3+} \rightarrow 1,2\text{-}C_6H_4O_2 + Fe^{2+} + H^+$	$7.00 \cdot 10^{5}$		est same $4\text{-}HOC_6H_4O$	Neta and Grodkowski [64]
A54	$2\ 2\text{-}HOC_6H_4O \rightarrow 1,2\text{-}C_6H_4(OH)_2 + 1,2\text{-}C_6H_4O_2$	$1.09 \cdot 10^{9}$			Adams and Michael [65]
A55	$4\text{-}HOC_6H_4O + Fe^{2+} + H^+ \rightarrow 1,4\text{-}C_6H_4(OH)_2 + Fe^{3+}$	$1.50 \cdot 10^{5}$			Neta and Grodkowski [64]
A56	$4\text{-}HOC_6H_4O + Fe^{3+} \rightarrow 1,4\text{-}C_6H_4O_2 + Fe^{2+} + H^+$	$7.00 \cdot 10^{5}$			Neta and Grodkowski [64]
A57	$2\ 4\text{-}HOC_6H_4O \rightarrow 1,4\text{-}C_6H_4(OH)_2 + 1,4\text{-}C_6H_4O_2$	$1.09 \cdot 10^{9}$			Adams and Michael [65]
A58	$HOCl + 2\text{-}C_6H_4ClO^- \rightarrow 0.7\ 2,6\text{-}C_6H_3Cl_2O^- + 0.3\ 2,4\text{-}C_6H_3Cl_2O^- + H_2O$	$2.42 \cdot 10^{3}$			Gallard and von Gunten [66]
A59	$HOCl + 4\text{-}C_6H_4ClOH \rightarrow 2,4\text{-}C_6H_3Cl_2OH + H_2O$	$2.00 \cdot 10^{-2}$			Gallard and von Gunten [66]
A60	$HOCl + 4\text{-}C_6H_4ClO^- \rightarrow 2,4\text{-}C_6H_3Cl_2O^- + H_2O$	$2.67 \cdot 10^{3}$			Gallard and von Gunten [66]
A61	$HOCl + 2,6\text{-}C_6H_3Cl_2O^- \rightarrow 2,4,6\text{-}C_6H_2Cl_3O^- + H_2O$	$1.94 \cdot 10^{2}$			Gallard and von Gunten [66]

	Reaction	k_{298}	$-E_A/R$	Comment	Reference
A62	$HOCl + 2,4\text{-}C_6H_3Cl_2O^- \rightarrow 2,4,6\text{-}C_6H_2Cl_3O^- + H_2O$	$3.03 \cdot 10^2$			Gallard and von Gunten [66]
A63	$HOBr + 2\text{-}C_6H_4BrO^- \rightarrow$ $0.7\ 2,6\text{-}C_6H_3Br_2O^- + 0.3\ 2,4\text{-}C_6H_3Br_2O^- + H_2O$	$6.40 \cdot 10^6$			Echigo and Minear [67]
A64	$HOBr + 4\text{-}C_6H_4BrO^- \rightarrow 2,4\text{-}C_6H_3Br_2O^- + H_2O$	$4.80 \cdot 10^6$			Echigo and Minear [67]
A65	$HOBr + 2,6\text{-}C_6H_3Br_2OH \rightarrow 2,4,6\text{-}C_6H_2Br_3OH + H_2O$	$1.70 \cdot 10^4$			Acero et al. [68]
A66	$HOBr + 2,6\text{-}C_6H_3Br_2O^- \rightarrow 2,4,6\text{-}C_6H_2Br_3O^- + H_2O$	$4.80 \cdot 10^5$			Acero et al. [68]
A67	$HOBr + 2,4\text{-}C_6H_3Br_2OH \rightarrow 2,4,6\text{-}C_6H_2Br_3OH + H_2O$	$1.20 \cdot 10^4$			Acero et al. [68]
A68	$HOBr + 2,4\text{-}C_6H_3Br_2O^- \rightarrow 2,4,6\text{-}C_6H_2Br_3O^- + H_2O$	$8.90 \cdot 10^5$			Acero et al. [68]
A69	$C_7H_7OH + OH \rightarrow C_7H_6(OH)_2$	$1.10 \cdot 10^{10}$		product Zhang et al. [69]	Buxton et al. [70]
A70	$C_7H_7OH + NO_3 \rightarrow C_7H_7OH^+ + NO_3^-$	$1.10 \cdot 10^9$			Umschlag et al. [31]
A71	$C_7H_7OH + SO_4^- \rightarrow C_7H_7OH^+ + SO_4^{2-}$	$3.40 \cdot 10^9$			Choure et al. [18]
A72	$C_7H_7OH + Cl_2^- \rightarrow C_7H_7OH^+ + 2\ Cl^-$	$4.30 \cdot 10^7$			Herrmann [71]
A73	$C_7H_7OH + Br_2^- \rightarrow C_7H_7OH^+ + 2\ Br^-$	$4.30 \cdot 10^6$			est. one order of magnitude lower as Cl_2^-
A74	$C_7H_7O^- + NO_2 \rightarrow C_7H_7O + NO_2^-$	$3.40 \cdot 10^7$			Alfassi et al. [72]
A75	$C_7H_7OH + NO_2^+ \rightarrow 2\text{-}C_7H_7NO_3 + H^+$	$4.07 \cdot 10^5$		est. same as for guaiacol	Kroflic et al. [73]
A76	$C_7H_7OH + O_3 \rightarrow C_7H_6(OH)_2 + O_2$	$5.48 \cdot 10^4$	-5300		Zheng and Kuo [74]
A77	$C_7H_7OH + HONO \rightarrow 2\text{-}C_7H_7NO_2$	$9.20 \cdot 10^{-3}$		est. same as for phenol	Vione et al. [37]
A78	$2\text{-}C_7H_7NO_2 \rightarrow 2\text{-}C_7H_7NO_3$	$3.00 \cdot 10^{-5}$		est. same as for nitrosophenol	Vione et al. [37]
A79	$C_7H_7OH^+ + Fe^{2+} \rightarrow C_7H_7OH + Fe^{3+}$	$6.00 \cdot 10^8$		est. same as for Anisole	Walling et al. [43]
A80	CRESCHD + $O_2 \rightarrow$ $0.4\ C_7H_6(OH)_2 + 0.4\ HO_2 + 0.6$ CRESO2	$2.00 \cdot 10^6$		yields from calculations in Merga et al. [75]	PSSA Fang et al. [76]
A81	CRESCHD + $Fe^{3+} \rightarrow C_7H_6(OH)_2 + Fe^{2+} + H^+$	$7.00 \cdot 10^3$		est. like PHENHCHD	Metelitsa [50]
A82	CRESCHD + $NO_2 \rightarrow 2\text{-}C_7H_7NO_3$	$8.20 \cdot 10^9$		est. same as for PHENHCHD	Barzaghi and Herrmann [48]
A83	2 CRESCHD $\rightarrow C_7H_6(OH)_2 + C_7H_7OH$	$1.00 \cdot 10^8$		as HCHD, Mantaka et al. [51]	Mvula et al. [49]
A84	2 CRESO2 $\rightarrow$ $1.36\ C_5H_6O_3 + 1.36\ C_2H_2O_2 + 0.64\ C_7H_6O_2 + 2\ HO_2$	$1.00 \cdot 10^6$		yields after recombination in MCM	Tilgner and Herrmann [77]

	Reaction	k_{298}	$-E_A/R$	Comment	Reference
A85	CRESO2 → 0.4 $C_5H_7O_2$ + 0.2 $C_5H_6O_3$ + 0.6 $C_2H_2O_2$ + 0.4 $C_3H_4O_2$ + 0.2 $C_4H_4O_2$ + 0.2 $C_4H_4O_3$ + 2 HO_2	$2.00 \cdot 10^{2}$		HO_2 elimination	Bräuer [78]
A86	$C_7H_7O + HO_2 \rightarrow C_7H_7OH$	$2.0 \cdot 10^{9}$			Vione et al. [34]
A87	$C_7H_7O + O_2^- \rightarrow C_7H_6O_2 - H^+ - H_2O$	$1.00 \cdot 10^{9}$			Mvula and von Sonntag [39]
A88	$C_7H_7O + NO_2 \rightarrow 2\text{-}C_7H_7NO_3$	$3.00 \cdot 10^{9}$		est. same as for C_6H_5O	Vione et al. [46]
A89	$C_7H_7O + C_7H_7O \rightarrow C_{14}H_{12}O_2$	$2.45 \cdot 10^{9}$			Mvula and von Sonntag [39]
A90	$C_7H_6(OH)_2 + OH \rightarrow C_7H_6O_2 + HO_2 - O_2 + H_2O$	$1.60 \cdot 10^{10}$		products Zhang et al. [69]	Gohn and Getoff [79]
A91	$C_7H_6O_2 + OH \rightarrow C_7H_8O_4 + HO_2 - O_2 - H_2O$	$2.00 \cdot 10^{10}$			Zhang et al. [69]
A92	$4\text{-}C_6H_5NO_3 + OH \rightarrow 0.7$ HONO + 0.7 $4\text{-}HOC_6H_4O$ + 0.3 NIPHENHCHD	$3.80 \cdot 10^{9}$		products Eiben et al. [80]	Cercek and Ebert [81]
A93	$4\text{-}C_6H_5NO_3 + NO_3 \rightarrow$ NIPHENHCHD + $NO_3^- + H^+$	$7.70 \cdot 10^{8}$			Hoffmann [82]
A94	$4\text{-}C_6H_5NO_3 + SO_4^- \rightarrow$ NIPHENHCHD + $SO_4^{2-} + H^+$	$7.70 \cdot 10^{8}$			est. after Herrmann et al. [55]
A95	$4\text{-}C_6H_5NO_3 + HOBr \rightarrow C_6H_4NO_3Br + H_2O$	$9.20 \cdot 10^{3}$			Heeb et al. [83]
A96	$2\text{-}C_6H_5NO_3 + OH \rightarrow$ 0.16 $C_6H_4(OH)_2$ + 0.16 NO_2 + 0.84 NIPHENHCHD	$5.90 \cdot 10^{9}$		products Tanaka et al. [84]	Vione et al. [85]
A97	$2\text{-}C_6H_5NO_3 + NO_3 \rightarrow$ NIPHENHCHD + $H^+ + NO_3^-$	$8.30 \cdot 10^{8}$			Weller et al. [86]
A98	$2\text{-}C_6H_5NO_3 + SO_4^- \rightarrow$ NIPHENHCHD + $SO_4^{2-} + H^+$	$8.30 \cdot 10^{8}$			est. after Herrmann et al. [55]
A99	$4\text{-}C_6H_5NO_4 + OH \rightarrow$ NICATHCHD	$1.00 \cdot 10^{10}$			Oturan et al. [59]
A100	$2,4\text{-}C_6H_4N_2O_5 + OH \rightarrow 4\text{-}C_6H_5NO_4 + NO_2$	$1.76 \cdot 10^{9}$		products Tanaka et al. [84]	Albinet et al. [87]
A101	$2,4\text{-}C_6H_4N_2O_5 + h\nu \rightarrow 4\text{-}C_6H_5NO_4$ + HONO	$1.675 \cdot 10^{-06}\cos(\chi)^{0.846}\exp(-0.096/\cos(\chi))$			Albinet et al. [87]
A102	$2,4\text{-}C_6H_3N_2O_5^- + OH \rightarrow 4\text{-}C_6H_4NO_4^- + NO_2$	$2.33 \cdot 10^{9}$		products Tanaka et al. [84]	Albinet et al. [87]
A103	$2,4\text{-}C_6H_3N_2O_5^- + h\nu \rightarrow 4\text{-}C_6H_4NO_4^-$ + HONO	$1.0 \cdot 10^{-05}\cos(\chi)^{0.546}\exp(-0.117/\cos(\chi))$			Albinet et al. [87]
A104	$2\text{-}C_7H_7NO_3 + OH \rightarrow$ 0.16 $C_7H_6(OH)_2$ + 0.16 NO_2 + 0.84 NICRESHCHD	$1.05 \cdot 10^{10}$		est. as 2-nitro-pcresol	Rindone et al. [88]
A105	$2\text{-}C_7H_7NO_3 + NO_3 \rightarrow$ NICRESHCHD + $H^+ + NO_3^-$	$1.00 \cdot 10^{8}$		est. as 2-nitro-pcresol	Umschlag et al. [31]
A106	$2\text{-}C_7H_7NO_3 + SO_4^- \rightarrow$ NICRESHCHD + $SO_4^{2-} + H^+$	$1.00 \cdot 10^{8}$		est. as 2-nitro-pcresol	est. after Herrmann et al. [55]

	Reaction	k_{298}	$-E_A/R$	Comment	Reference
A107	2-$C_7H_7NO_3$ + Cl_2^- → NICRESHCHD + H^+ + 2 Cl^-	$1.50 \cdot 10^8$			Walter [89]
A108	2-$C_7H_7NO_3$ + hν → $C_7H_6(OH)_2$ + HONO – H_2O	$1.896 \cdot 10^{-06} \cos(\chi)^{0.670} \exp(-0.081/\cos(\chi))$			est. 2-nitrophenol
A109	NIPHENHCHD + O_2 → 4-$C_6H_5NO_4$ + HO_2	$2.00 \cdot 10^6$		products vonSonntag et al. [90]	PSSA Fang et al. [76]
A110	NIPHENHCHD + Fe^{3+} → 4-$C_6H_5NO_4$ + Fe^{2+} + H^+	$7.00 \cdot 10^3$			Metelitsa [50]
A111	NIPHENHCHD + NO_2 → 2,4-$C_6H_4N_2O_5$	$1.00 \cdot 10^7$			est. according to Vione et al. [85]
A112	2 NIPHENHCHD → 4-$C_6H_5NO_4$ + 4-$C_6H_5NO_3$	$5.00 \cdot 10^8$		as HCHD, Mantaka et al. [51]	Metelitsa [50]
A113	NICATHCHD + O_2 → NICATO2	$2.00 \cdot 10^6$			PSSA Fang et al. [76]
A114	2 NICATO2 → 2 $C_4H_4O_4$ + 2 NO_2 + 2 $C_2H_2O_3$ + 2 HO_2 – 2 H_2O	$1.00 \cdot 10^6$		yields recombination MCM	Bräuer [78]
A115	NICATO2 → $C_4H_4O_4$ + NO_2 + $C_2H_2O_2$ + 2 HO_2 – H_2O	$2.00 \cdot 10^2$		yields est.	Bräuer [78]
A116	NICRESHCHD + O_2 → 0.6 NICRESO2 + 0.4 2-$C_7H_7NO_4$ + 0.4 HO_2	$2.00 \cdot 10^6$			PSSA Fang et al. [76]
A117	NICRESHCHD + Fe^{3+} → 2-$C_7H_7NO_4$ + Fe^{2+} + H^+	$7.00 \cdot 10^3$			Metelitsa [50]
A118	NICRESHCHD + NO_2 → 2,4-$C_7H_6N_2O_5$	$1.00 \cdot 10^7$		as for NIPHENHCHD	est.
A119	2 NICRESHCHD → 2-$C_7H_7NO_4$ + 2-$C_7H_7NO_3$	$1.00 \cdot 10^8$		as HCHD, Mantaka et al. [51]	Mvula et al. [49]
A120	2,4-$C_7H_6N_2O_5$ + hν → 2-$C_7H_7NO_4$ + HONO	$1.675 \cdot 10^{-06} \cos(\chi)^{0.846} \exp(-0.096/\cos(\chi))$			est.
A121	2,4-$C_7H_5N_2O_5^-$ + hν → 2-$C_7H_6NO_4^-$ + HONO	$1.0 \cdot 10^{-05} \cos(\chi)^{0.546} \exp(-0.117/\cos(\chi))$			est.
A122	2 NICRESO2 → 2 $C_5H_6O_3$ + 2 $C_2H_2O_2$ + 2 HO_2 + 2 NO_2	$1.00 \cdot 10^6$		yields est.	Bräuer [78]
A123	NICRESO2 → 0.4 $C_5H_7O_2$ + 0.2 $C_5H_6O_3$ + 0.6 $C_2H_2O_2$ + 0.4 $C_3H_4O_2$ + 0.2 $C_4H_4O_2$ + 0.2 $C_4H_4O_3$ + 2 HO_2	$2.00 \cdot 10^2$		yields est.	Bräuer [78]
A124	$C_6H_5CH_2OH$ + OH → 0.04 C_6H_5OH + 0.04 HCHO + 0.81 ALKHCHD + 0.15 C_6H_5CHOH + 0.19 H_2O	$6.40 \cdot 10^9$			Steenken and Ramaraj [19]
A125	$C_6H_5CH_2OH$ + NO_3 → C_6H_5CHOH + NO_3^- + H^+	$4.50 \cdot 10^8$			Ito et al. [91]
A126	$C_6H_5CH_2OH$ + SO_4^-→ $C_6H_5CH_2OH^+$ + SO_4^{2-}	$3.20 \cdot 10^9$			Steenken and Ramaraj [19]
A127	ALKHCHD + O_2 → 0.4 $HOC_6H_4CH_2OH$ + 0.4 HO_2 + 0.6 ALKHCHDOX	$2.00 \cdot 10^6$		Steenken and Ramaraj [19], Mantaka et al. [51]	PSSA Fang et al. [76]
A128	ALKHCHD + Fe^{3+} → $HOC_6H_5CH_2OH$ + Fe^{2+} + H^+	$7.00 \cdot 10^3$		Steenken and Ramaraj [19]	Metelitsa [50]

	Reaction	k_{298}	$-E_A/R$	Comment	Reference
A129	2 ALKHCHD → $C_6H_5CH_2OH$ + $HOC_6H_4CH_2OH$	$1.00 \cdot 10^8$		as HCHD, Mantaka et al. [51]	Mvula et al. [49]
A130	2 ALKHCHDOX → 1.2 $C_2H_2O_2$ + 0.8 $C_5H_6O_3$ + 0.4 $C_5H_8O_4$ + 0.8 $C_3H_4O_3$ + 0.4 $C_4H_4O_2$ + 0.4 $C_4H_4O_3$ + 2 HO_2	$7.30 \cdot 10^8$		yields analogy recombination TLBIPERO2 in MCM	Bräuer [78]
A131	$C_6H_5CH_2OH^+ \rightarrow C_6H_5CHOH + H^+$	$5.00 \cdot 10^7$		lower limit	Steenken and Ramaraj [19]
A132	$C_6H_5CHOH + O_2 \rightarrow C_6H_5CHO + HO_2$	$2.00 \cdot 10^9$		CAPRAM Standard	Bräuer [78]
A133	$HOC_6H_4CH_2OH + OH \rightarrow$ 0.14 HOC_6H_4CHOH + 0.14 H_2O + 0.86 ALKOHHCHD	$5.27 \cdot 10^9$			Dhiman and Naik [92]
A134	$HOC_6H_4CH_2OH + Cl_2^- \rightarrow$ ALKOHHCHD + 2 Cl^- + H^+	$2.80 \cdot 10^8$		products est.	Dhiman and Naik [92]
A135	$HOC_6H_4CHOH + O_2 \rightarrow HOC_6H_4CHO + HO_2$	$2.00 \cdot 10^9$		CAPRAM Standard	Bräuer [78]
A136	ALKOHHCHD + O_2 → 0.4 $(HO)_2C_6H_3CH_2OH$ + 0.4 HO_2 + 0.6 ALKOHHCHDOX	$2.00 \cdot 10^6$		Steenken and Ramaraj [19], Mantaka et al. [51]	PSSA Fang et al. [76]
A137	ALKOHHCHD + Fe^{3+} → 0.4 $(HO)_2C_6H_4CH_2OH$ + Fe^{2+} + H^+	$7.00 \cdot 10^3$		Steenken and Ramaraj [19]	Metelitsa [50]
A138	2 ALKOHHCHD → $C_6H_5CH_2OH$ + $(HO)_2C_6H_4CH_2OH$	$1.00 \cdot 10^8$		as HCHD, Mantaka et al. [51]	Mvula et al. [49]
A139	2 ALKOHHCHDOX → 1.36 $C_5H_6O_4$ + 1.36 $C_2H_2O_2$ + 0.64 1,4-$C_7H_6O_3$ + 2 HO_2	$1.00 \cdot 10^6$		yields analogy recombination CRESO2 in MCM	Tilgner and Herrmann [77]
A140	ALKOHHCHDOX → 0.6 $C_2H_2O_2$ + 0.4 $C_5H_6O_3$ + 0.2 $C_5H_8O_4$ + 0.4 $C_3H_4O_3$ + 0.2 $C_4H_4O_2$ + 0.2 $C_4H_4O_3$ + 2 HO_2	$2.00 \cdot 10^2$		HO_2 elimination	Bräuer [78]
A141	$(HO)_2C_6H_3CH_2OH + OH \rightarrow (HO)_2C_6H_3CHOH + H_2O$	$5.00 \cdot 10^9$		est.	est.
A142	$(HO)_2C_6H_3CHOH + O_2 \rightarrow (HO)_2C_6H_3CHO + HO_2$	$2.00 \cdot 10^9$		CAPRAM Standard	Bräuer [78]
A143	$C_6H_5CHO + OH$ → 0.75 ALDHCHD + 0.25 $C_6H_5O_2$ + 0.25 H_2O + 0.25 CO	$2.60 \cdot 10^9$		yields Sharma et al. [93]	Buxton et al. [70]
A144	$C_6H_5CH(OH)_2 + OH \rightarrow C_6H_5C(OH)_2 + H_2O$	$2.60 \cdot 10^9$		yields Sharma et al. [93]	Buxton et al. [70]
A145	$C_6H_5CH(OH)_2 + NO_3 \rightarrow$ 0.8 $C_6H_5C(OH)_2$ + 0.8 H^+ + 0.2 $C_6H_5CH(OH)_2^+$ + NO_3^-	$7.10 \cdot 10^8$		yields Sharma et al. [93]	est. after Herrmann et al. [55]
A146	$C_6H_5CH(OH)_2 + SO_4^- \rightarrow$ 0.8 $C_6H_5C(OH)_2$ + 0.8 H^+ + 0.2 $C_6H_5CH(OH)_2^+$ + SO_4^{2-}	$7.10 \cdot 10^8$		yields Sharma et al. [93]	Sharma et al. [93]
A147	ALDHCHD + O_2 →	$2.00 \cdot 10^6$		yields Sharma et al. [93]	PSSA Fang et al. [76]

	Reaction	k_{298}	$-E_A/R$	Comment	Reference
	0.4 HOC_6H_4CHO + 0.4 HO_2 + 0.6 ALDHCHDOX				
A148	ALDHCHD + Fe^{3+} → HOC_6H_4CHO + Fe^{2+} + H^+	$7.00 \cdot 10^3$		yields Sharma et al. [93]	Metelitsa [50]
A149	2 ALDHCHD → C_6H_5CHO + HOC_6H_4CHO	$1.00 \cdot 10^8$		Mantaka et al. [51]	Mvula et al. [49]
A150	2 ALDHCHDOX → 1.2 $C_2H_2O_2$ + 0.8 $C_5H_4O_3$ + 0.4 $C_5H_6O_4$ + 0.8 $C_3H_4O_3$ + 0.4 $C_4H_4O_2$ + 0.4 $C_4H_4O_3$ + 2 HO_2	$7.30 \cdot 10^8$		yields analogy recombination TLBIPERO2 in MCM	Bräuer [78]
A151	$C_6H_5CH(OH)_2^+$ → $C_6H_5CH(OH)_2$ + H^+	$5.00 \cdot 10^7$		est. $C_6H_5CH_2OH^+$	Steenken and Ramaraj [19]
A152	$C_6H_5C(OH)_2$ + O_2 → $C_6H_5CO_2H$ + HO_2	$2.00 \cdot 10^9$		CAPRAM Standard	Bräuer [78]
A153	HOC_6H_4CHO + OH → 0.33 $HOC_6H_4O_2$ + 0.33 CO + 0.33 H_2O + 0.67 ALDOHHCHD	$1.21 \cdot 10^{10}$		est. p-hydroxybenzaldehyde	Geeta et al. [94]
A154	$HOC_6H_4CH(OH)_2$ + OH → $HOC_6H_4CH(OH)_2$	$1.21 \cdot 10^{10}$		est. p-hydroxybenzaldehyde	Geeta et al. [94]
A155	HOC_6H_4CHO + NO_3 → $HOC_6H_4CHO^+$ + NO_3^-	$5.90 \cdot 10^9$		est. p-hydroxybenzaldehyde	est. after Herrmann et al. [55]
A156	$HOC_6H_4CH(OH)_2$ + NO_3 → $HOC_6H_4CH(OH)_2^+$ + NO_3^-	$5.90 \cdot 10^9$		est. p-hydroxybenzaldehyde	est. after Herrmann et al. [55]
A157	HOC_6H_4CHO + SO_4^- → $HOC_6H_4CHO^+$ + SO_4^{2-}	$5.90 \cdot 10^9$		est. p-hydroxybenzaldehyde	Geeta et al. [94]
A158	$HOC_6H_4CH(OH)_2$ + SO_4^- → $HOC_6H_4CH(OH)_2^+$ + SO_4^{2-}	$5.90 \cdot 10^9$		est. p-hydroxybenzaldehyde	Geeta et al. [94]
A159	$HOC_6H_4CHO^+$ → $HOC_6H_4O_2$ + CO + H^+	$5.00 \cdot 10^7$		est. $C_6H_5CH_2OH^+$	Steenken and Ramaraj [19]
A160	$HOC_6H_4CH(OH)_2^+$ → $HOC_6H_4CH(OH)_2$ + H^+	$5.00 \cdot 10^7$		est. $C_6H_5CH_2OH^+$	Steenken and Ramaraj [19]
A161	$HOC_6H_4CH(OH)_2$ + O_2 → $HOC_6H_4CO_2H$ + HO_2	$2.00 \cdot 10^9$		CAPRAM Standard	Bräuer [78]
A162	ALDOHHCHD + O_2 → 0.4 $(HO)_2C_6H_3CHO$ + 0.4 HO_2 + 0.6 ALDOHHCHDOX	$2.00 \cdot 10^6$		Geeta et al. [94]	PSSA Fang et al. [76]
A163	ALDOHHCHD + Fe^{3+} → $(HO)_2C_6H_4CHO$ + Fe^{2+} + H^+	$7.00 \cdot 10^3$		Sharma et al. [93]	Metelitsa [50]
A164	2 ALDOHHCHD → HOC_6H_5CHO + $(HO)_2C_6H_4CHO$	$1.00 \cdot 10^8$		Mantaka et al. [51]	Mvula et al. [49]
A165	2 ALDOHHCHDOX → 1.36 $C_5H_4O_4$ + 1.36 $C_2H_2O_2$ + 0.64 1,4-$C_7H_4O_3$ + 2 HO_2	$1.00 \cdot 10^6$		yields analogy recombination CRESO2 in MCM	Tilgner and Herrmann [77]
A166	ALDOHHCHDOX → 0.6 $C_2H_2O_2$ + 0.4 $C_5H_4O_3$ + 0.2 $C_5H_6O_4$ + 0.4 $C_3H_4O_3$ + 0.2 $C_4H_4O_2$ + 0.2 $C_4H_6O_3$ + 2 HO_2	$2.00 \cdot 10^2$		HO_2 elimination	Bräuer [78]
A167	$(HO)_2C_6H_3CH(OH)_2$ + OH → $(HO)_2C_6H_4CH(OH)_2$	$1.00 \cdot 10^{10}$		est.	est.
A168	$(HO)_2C_6H_4CH(OH)_2$ + O_2 → $(HO)_2C_6H_4CO_2H$ + HO_2	$2.00 \cdot 10^9$		CAPRAM Standard	Bräuer [78]
A169	$C_6H_5CO_2H$ + OH → ACIDHCHD	$1.80 \cdot 10^9$			Remucal and Manley [21]

	Reaction	k_{298}	$-E_A/R$	Comment	Reference
A170	$C_6H_5CO_2H + NO_3 \rightarrow$ ACIDHCHD + $H^+ + NO_3^- - H_2O$	$6.50 \cdot 10^7$	-1300		Umschlag et al. [31]
A171	$C_6H_5CO_2H + SO_4^- \rightarrow$ ACIDHCHD + $H^+ + SO_4^{2-} - H_2O$	$6.50 \cdot 10^7$	-1300		est. after Herrmann et al. [55]
A172	$C_6H_5CO_2H + Cl \rightarrow$ ACIDCLCHD	$1.80 \cdot 10^{10}$			Martire et al. [44]
A173	$C_6H_5CO_2H + Cl_2^- \rightarrow$ ACIDCLCHD + Cl^-	$2.00 \cdot 10^5$			Martire et al. [44]
A174	$C_6H_5CO_2^- + OH \rightarrow 0.93$ ACIDHCHD$^-$ + 0.07 $C_6H_5O_2$ + 0.07 CO_2 + 0.07 OH^-	$5.90 \cdot 10^9$		Deng et al. [95]	Buxton et al. [70]
A175	$C_6H_5CO_2^- + NO_3 \rightarrow C_6H_5O_2 + NO_3^-$	$1.20 \cdot 10^9$		ETR assumed	est. after Herrmann et al. [55]
A176	$C_6H_5CO_2^- + SO_4^- \rightarrow C_6H_5O_2 + SO_4^{2-}$	$1.20 \cdot 10^9$		ETR assumed	Neta et al. [96]
A177	$C_6H_5CO_2^- + Cl_2^- \rightarrow C_6H_5O_2 + 2\ Cl^-$	$2.00 \cdot 10^6$		ETR assumed	Hasegawa and Neta [97]
A178	ACIDHCHD + $O_2 \rightarrow HOC_6H_4CO_2H + HO_2$	$2.00 \cdot 10^6$		Klein et al. [98], Merga et al. [75]	PSSA Fang et al. [76]
A179	ACIDHCHD + $Fe^{3+} \rightarrow$ 0.93 $HOC_6H_4CO_2H$ + 0.07 C_6H_5OH + 0.07 CO_2 + 0.07 H_2O + $Fe^{2+} + H^+$	$7.00 \cdot 10^3$		Klein et al. [98]	Metelitsa [50]
A180	2 ACIDHCHD $\rightarrow C_6H_5CO_2H + HOC_6H_4CO_2H + H_2O$	$3.95 \cdot 10^8$		Klein et al. [98]	Metelitsa [50]
A181	ACIDHCHD$^-$ + $O_2 \rightarrow HOC_6H_4CO_2^- + HO_2$	$2.00 \cdot 10^6$		Klein et al. [98], Merga et al. [75]	PSSA Fang et al. [76]
A182	ACIDHCHD$^-$ + $Fe^{3+} \rightarrow$ 0.93 $HOC_6H_4CO_2^-$ + 0.07 $C_6H_5O^-$ + 0.07 CO_2 + 0.07 H_2O + $Fe^{2+} + H^+$	$7.00 \cdot 10^3$		Klein et al. [98]	Metelitsa [50]
A183	2 ACIDHCHD$^- \rightarrow C_6H_5CO_2^- + HOC_6H_4CO_2^- + H_2O$	$3.95 \cdot 10^8$		Klein et al. [98]	Metelitsa [50]
A184	ACIDCLCHD + $O_2 \rightarrow$ 2-$ClC_6H_4CO_2H + HO_2$	$2.00 \cdot 10^6$			PSSA Fang et al. [76]
A185	ACIDCLCHD + $Fe^{3+} \rightarrow$ 2-$ClC_6H_4CO_2H + Fe^{2+} + H^+$	$7.00 \cdot 10^3$			Metelitsa [50]
A186	2 ACIDCLCHD $\rightarrow C_6H_5CO_2H$ + 2-$ClC_6H_4CO_2H$ + HCl	$1.00 \cdot 10^8$		as HCHD, Mantaka et al. [51]	Mvula et al. [49]
A187	2 $C_6H_5O_2 \rightarrow 2\ C_6H_5O + O_2$	$1.00 \cdot 10^6$			Tilgner and Herrmann [77]
A188	$HOC_6H_4CO_2H + OH \rightarrow$ SAHCHD	$2.20 \cdot 10^{10}$		est. Salicylic acid Huang et al. [99]	Buxton et al. [70]
A189	$HOC_6H_4CO_2H + NO_3 \rightarrow$ SAHCHD + $H^+ + NO_3^- - H_2O$	$1.50 \cdot 10^9$			Weller et al. [86]
A190	$HOC_6H_4CO_2H + SO_4^- \rightarrow$ SAHCHD + $H^+ + SO_4^{2-} - H_2O$	$1.50 \cdot 10^9$			est. after Herrmann et al. [55]
A191	$HOC_6H_4CO_2H + Cl_2^- \rightarrow HOC_6H_4O_2 + 2\ Cl^- + CO_2 + H^+$	$1.10 \cdot 10^8$		est. Salicylic acid	Hasegawa and Neta [97]

	Reaction	k_{298}	$-E_A/R$	Comment	Reference
A192	$HOC_6H_4CO_2H + Br_2 \rightarrow HOC_6H_3BrCO_2H + Br^- + H^+$	$4.42 \cdot 10^9$	-4030	est. Salicylic acid	Patil et al. [100]
A193	$HOC_6H_4CO_2H + O_3 \rightarrow (HO)_2C_6H_3CO_2H + O_2$	$2.00 \cdot 10^2$		est.	Benitez et al. [101]
A194	$HOC_6H_4CO_2^- + OH \rightarrow 0.93\ SAHCHD^- + 0.07\ COO^- + 0.07\ 1,4\text{-}C_6H_4(OH)_2$	$1.60 \cdot 10^{10}$		Santos et al. [102]	Buxton et al. [70]
A195	$HOC_6H_4CO_2^- + NO_3 \rightarrow HOC_6H_4O_2 + NO_3^- + CO_2 + H^+$	$1.60 \cdot 10^9$		est. Salicylic acid	est. after Herrmann et al. [55]
A196	$HOC_6H_4CO_2^- + SO_4^- \rightarrow HOC_6H_4O_2 + SO_4^{2-} + CO_2 + H^+$	$1.60 \cdot 10^9$		est. Salicylic acid	Kishore and Mukherjee [103]
A197	$HOC_6H_4CO_2^- + O_3 \rightarrow (HO)_2C_6H_3CO_2^- + O_2$	$1.78 \cdot 10^5$		est.	Benitez et al. [101]
A198	$FeHOC_6H_4CO_2^{2+} + h\nu \rightarrow Fe^{2+} + HOC_6H_4O_2 + CO_2 - O_2$	$4.764 \cdot 10^{-02}\cos(\chi)^{0.829}\exp(-0.291/\cos(\chi))$			est. $Fe(OH)^{2+}$ Arakaki et al. [58]
A199	$SAHCHD + O_2 \rightarrow 0.75\ HOC_6H_4O_2 + 0.75\ CO_2 + 0.25\ (HO)_2C_6H_3CO_2H + HO_2$	$2.00 \cdot 10^6$		products after Scheck and Frimmel [52]	PSSA Fang et al. [76]
A200	$SAHCHD + Fe^{3+} \rightarrow 0.75\ HOC_6H_4O_2 + 0.75\ CO_2 + 0.25\ (HO)_2C_6H_3CO_2H + Fe^{2+} + H^+$	$7.00 \cdot 10^3$		products after Scheck and Frimmel [52]	Metelitsa [50]
A201	$2\ SAHCHD \rightarrow HOC_6H_4CO_2H + 0.75\ HOC_6H_4O_2 + 0.75\ CO_2 + 0.25\ (HO)_2C_6H_3CO_2H$	$1.00 \cdot 10^8$		Mantaka et al. [51]	Mvula et al. [49]
A202	$SAHCHD^- + O_2 \rightarrow 0.75\ HOC_6H_4O_2 + 0.75\ CO_2 + 0.25\ (HO)_2C_6H_3CO_2^- + HO_2 - 0.75\ H^+$	$2.00 \cdot 10^6$		products after Scheck and Frimmel [52]	PSSA Fang et al. [76]
A203	$SAHCHD^- + Fe^{3+} \rightarrow 0.75\ HOC_6H_4O_2 + 0.75\ CO_2 + 0.25\ (HO)_2C_6H_3CO_2^- + Fe^{2+} + H^+$	$7.00 \cdot 10^3$		products after Scheck and Frimmel [52]	Metelitsa [50]
A204	$2\ SAHCHD^- \rightarrow HOC_6H_4CO_2^- + 0.75\ HOC_6H_4O_2 + 0.75\ CO_2 + 0.25\ (HO)_2C_6H_3CO_2^-$	$1.00 \cdot 10^8$		Mantaka et al. [51]	Mvula et al. [49]
A205	$2\ HOC_6H_4O_2 \rightarrow 2\text{-}HOC_6H_4O + 2\text{-}HOC_6H_4O + O_2$	$1.00 \cdot 10^6$			Bräuer [78]
A206	$(HO)_2C_6H_3CO_2H + OH \rightarrow TRIACIDHCHD$	$8.00 \cdot 10^9$			Duesteberg and Waite [104]
A207	$(HO)_2C_6H_3CO_2H + HO_2 \rightarrow TRIACIDHCHD + H_2O_2 - H^+$	$3.90 \cdot 10^4$		est.	Bielski et al. [56]

	Reaction	k_{298}	$-E_A/R$	Comment	Reference
A208	TRIACIDHCHD + O_2 → 0.4 $(HO)_3C_6H_2CO_2H$ + 0.4 HO_2 + 0.6 TRIACIDHCHDOX	$2.00 \cdot 10^6$		products est. Duesteberg and Waite [104]	PSSA Fang et al. [76]
A209	TRIACIDHCHD + Fe^{3+} → $(HO)_3C_6H_4CO_2H$ + Fe^{2+} + H^+	$7.00 \cdot 10^3$		products est. Duesteberg and Waite [104]	Metelitsa [50]
A210	2 TRIACIDHCHD → $(HO)_2C_6H_4CO_2H$ + $(HO)_3C_6H_4CO_2H$	$1.00 \cdot 10^8$		Mantaka et al. [51]	Mvula et al. [49]
A211	$(HO)_3C_6H_2CO_2H$ + OH → $(HO)_3C_6H_2O_2$	$6.40 \cdot 10^9$		est. Santos et al. [102]	Dwibedy et al. [25]
A212	$(HO)_3C_6H_2CO_2H$ + NO_3 → $(HO)_3C_6H_2O_2$ + NO_3^- + CO_2 + H^+	$6.30 \cdot 10^8$		ETR assumed	est. after Herrmann et al. [55]
A213	$(HO)_3C_6H_2CO_2H$ + SO_4^- → $(HO)_3C_6H_2O_2$ + SO_4^{2-} + CO_2 + H^+	$6.30 \cdot 10^8$		ETR assumed	Caregnato et al. [105]
A214	$(HO)_3C_6H_2CO_2H$ + Cl_2^- → $(HO)_3C_6H_2O_2$ + 2 Cl^- + CO_2 + H^+	$1.90 \cdot 10^9$		ETR assumed	Dwibedy et al. [25]
A215	$(HO)_3C_6H_2CO_2H$ + O_3 → $C_7H_6O_7$ + H_2O_2 – H_2O	$9.70 \cdot 10^4$		products est. Beltrán et al. [106]	Beltrán et al. [106]
A216	$(HO)_3C_6H_2CO_2^-$ + OH → $(HO)_3C_6H_2O_2$ + CO_2 + OH^-	$1.10 \cdot 10^{10}$		ETR assumed	Dwibedy et al. [25]
A217	$(HO)_3C_6H_2CO_2^-$ + NO_3 → $(HO)_3C_6H_2O_2$ + NO_3^- + CO_2 + H^+	$2.90 \cdot 10^9$		ETR assumed	est. after Herrmann et al. [55]
A218	$(HO)_3C_6H_2CO_2^-$ + SO_4^- → $(HO)_3C_6H_2O_2$ + SO_4^{2-} + CO_2 + H^+	$2.90 \cdot 10^9$		ETR assumed	Caregnato et al. [105]
A219	$(HO)_3C_6H_2CO_2^-$ + Br_2^- → $(HO)_3C_6H_2O_2$ + 2 Br^- + CO_2 + H^+	$3.30 \cdot 10^9$		ETR assumed	Dwibedy et al. [25]
A220	$(HO)_3C_6H_2CO_2^-$ + O_3 → $C_7H_5O_7^-$ + H_2O_2 – H_2O	$4.70 \cdot 10^5$		products est. Beltrán et al. [106]	Beltran et al. [107]
A221	2 $(HO)_3C_6H_2O_2$ → $(HO)_3C_6H_2O$	$1.00 \cdot 10^6$			Bräuer [78]
A222	2 $(HO)_3C_6H_2O$ → $(HO)_2C_6H_2(O)_2$ + $C_6H_2(OH)_4$	$1.09 \cdot 10^9$			Adams and Michael [65]
A223	$C_6H_2(OH)_4$ + OH → $(HO)_2C_6H_2(O)_2$ + HO_2 – 1.5 O_2	$1.00 \cdot 10^{10}$		est. analogy 1,4-$C_6H_4(OH)_2$	est. analogy 1,4-$C_6H_4(OH)_2$
A224	$(HO)_2C_6H_2(O)_2$ + OH → HOOCCOCHCHCOCOOH + HO_2 – 1.5 O_2	$2.00 \cdot 10^8$		est. Mousset et al. [108]	Mousset et al. [108]

Table S4 Namelist of compounds.

Name	Molecular formular
Phenol	C_6H_5OH
Catechol	$1,2\text{-}C_6H_4(OH)_2$
Hydroquinone	$1,4\text{-}C_6H_4(OH)_2$
1,2-Benzoquinone	$1,2\text{-}C_6H_4O_2$
1,4-Benzoquinone	$1,4\text{-}C_6H_4O_2$
Biphenol	$C_{12}H_{10}O_2$
Cresol	C_7H_7OH
Methylcatechol	$C_7H_6(OH)_2$
Methylbenzoquinone	$C_7H_6O_2$
Bicresol	$C_{14}H_{12}O_2$
Benzylalcohol	$C_6H_5CH_2OH$
Hydroxy benzylalcohol	$HOC_6H_4CH_2OH$
Dihydroxy benzylalcohol	$(HO)_2C_6H_3CH_2OH$
Benzaldehyde	C_6H_5CHO
Hydrated benzaldehyde	$C_6H_5CH(OH)_2$
Hydroxy benzaldehyde	HOC_6H_4CHO
Hydrated hydroxy benzaldehyde	$HOC_6H_4CH(OH)_2$
Dihydroxy benzaldehyde	$(HO)_2C_6H_5CHO$
Hydrated dihydroxy benzaldehyde	$(HO)_2C_6H_5CH(OH)_2$
Benzoic acid	$C_6H_5CO_2H$
Hydroxy benzoic acid	$HOC_6H_4CO_2H$
Dihydroxy benzoic acid	$(HO)_2C_6H_4CO_2H$
Trihydroxy benzoic acid	$(HO)_3C_6H_4CO_2H$
2-chloro benzoic acid	$2\text{-}ClC_6H_4CO_2H$
Hydroxy bromo benzoic acid	$HOC_6H_3BrCO_2H$
4-Nitrosophenol	$4\text{-}C_6H_5NO_2$
2-Nitrophenol	$2\text{-}C_6H_5NO_3$

Name	Molecular formular
4-Nitrophenol	4-$C_6H_5NO_3$
2-bromo-4-nitrophenol	$C_6H_4NO_3Br$
Nitrocatechol	$NO_2C_6H_3(OH)_2$
2-Nitrosocresol	2-$C_7H_7NO_2$
2-Methyl-6-Nitrophenol	2-$C_7H_7NO_3$
4-Nitrocatechol	4-$C_6H_5NO_4$
Nitromethylcatechol	2-$C_7H_7NO_4$
2-Chlorophenol	2-C_6H_4ClOH
4-Chlorophenol	4-C_6H_4ClOH
2,4-Chlorophenol	2-$C_6H_3Cl_2OH$
2,6-Chlorophenol	4-$C_6H_3Cl_2OH$
2,4,6-Chlorophenol	2-$C_6H_2Cl_3OH$
2-Bromophenol	2-C_6H_4BrOH
4-Bromophenol	4-C_6H_4BrOH
2,4-Bromophenol	2-$C_6H_3Br_2OH$
2,6-Bromophenol	4-$C_6H_3Br_2OH$
2,4,6-Bromophenol	2-$C_6H_2Br_3OH$
Dinitrophenol	2,4-$C_6H_4N_2O_5$
Dinitrocresol	2,4-$C_7H_6N_2O_5$
Muconic acid	$C_6H_6O_4$
Methyl-muconic acid	$C_7H_8O_4$
2-(Hydroxymethyl)-1,4-benzoquinone	$C_7H_6O_7$
2-(Hydroxymethyl)-1,4-benzoquinone	$C_7H_6O_3$
3,6-Dioxo-1,4-cyclohexadiene-1-carbaldehyde	$C_7H_4O_3$
4,5-Dihydroxy-2-pentenoic acid	$C_5H_8O_4$
5-Hydroxy-4-oxo-2-pentenoic acid	$C_5H_6O_4$
4-oxo4ent-2-enoic acid	$C_5H_6O_3$
4-Hydroxy-2-pentenoic acid	$C_5H_6O_3$
4-oxopent-2-enal	$C_5H_7O_2$

Name	Molecular formular
5-pentenal-4-oxo-2-enoic acid	$C_5H_4O_4$
4-oxopent-2-enedial	$C_5H_4O_3$
Fumaric acid/Maleic acid	$C_4H_4O_4$
4-oxo-2-butenoic acid	$C_4H_4O_3$
Maldial	$C_4H_4O_2$
3-Hydroxy-2-oxopropanal	$C_3H_4O_3$
Methylglyoxal	$C_3H_4O_2$
Glycolic acid	$C_2H_2O_3$
Glyoxal	$C_2H_2O_2$

Table S5 Oxidation of the unsaturated organic compounds from oxidation of aromatic compounds by OH and O_3 for the separate core.

Reaction	k_{298}	$-E_A/R$	Comment	Reference
$C_5H_6O_3 + OH \rightarrow 0.5\ CH_3C(O)CH(OH)CH(O_2)COOH + 0.5\ CH_3C(O)CH(O_2)CH(OH)COOH$	$1.16 \cdot 10^{10}$			Minakata et al. [109]
$C_5H_5O_3^- + OH \rightarrow 0.5\ CH_3C(O)CH(OH)CH(O_2)COO^- + 0.5\ CH_3C(O)CH(O_2)CH(OH)COO^-$	$4.94 \cdot 10^{10}$			Minakata et al. [109]
$C_5H_6O_2 + OH \rightarrow 0.5\ CH_3C(O)CH(OH)CH(O_2)CHO + 0.5\ CH_3CH(OH)CH(O_2)C(O)CHO$	$3.04 \cdot 10^{10}$			Minakata et al. [109]
$C_5H_8O_3 + OH \rightarrow 0.5\ CH_3CH(OH)CH(OH)CH(O_2)COOH + 0.5\ CH_3CH(OH)CH(O_2)CH(OH)COOH$	$2.10 \cdot 10^{10}$			Minakata et al. [109]
$C_5H_7O_3^- + OH \rightarrow 0.5\ CH_3CH(OH)CH(OH)CH(O_2)COO^- + 0.5\ CH_3CH(OH)CH(O_2)CH(OH)COO^-$	$8.40 \cdot 10^{10}$			Minakata et al. [109]
$C_6H_4O_6 + OH \rightarrow HOOCC(O)CH(OH)CH(O_2)C(O)COOH$	$2.96 \cdot 10^{10}$			Minakata et al. [109]
$C_6H_3O_6^- + OH \rightarrow 0.5\ ^-OOCC(O)CH(OH)CH(O_2)C(O)COOH + 0.5\ HOOCC(O)CH(OH)CH(O_2)C(O)COO^-$	$2.96 \cdot 10^{10}$			Minakata et al. [109]
$C_6H_2O_6^{2-} + OH \rightarrow {}^-OOCC(O)CH(OH)CH(O_2)C(O)COO^-$	$2.96 \cdot 10^{10}$			Minakata et al. [109]
$C_5H_4O_5 + OH \rightarrow 0.5\ HOOCC(O)CH(OH)CH(O_2)COOH + 0.5\ HOOCC(O)CH(O_2)CH(OH)COOH$	$1.15 \cdot 10^{10}$			Minakata et al. [109]
$C_5H_3O_5^- + OH \rightarrow 0.5\ ^-OOCC(O)CH(OH)CH(O_2)COOH + 0.5\ ^-OOCC(O)CH(O_2)CH(OH)COOH$	$4.93 \cdot 10^{10}$			Minakata et al. [109]
$C_5H_2O_5^{2-} + OH \rightarrow 0.5\ ^-OOCC(O)CH(OH)CH(O_2)COO^- + 0.5\ ^-OOCC(O)CH(O_2)CH(OH)COO^-$	$4.93 \cdot 10^{10}$			Minakata et al. [109]
$C_5H_6O_4 + OH \rightarrow 0.5\ HOOCCH(OH)CH(O_2)CH(OH)CHO + 0.5\ HOOCCH(O_2)CH(OH)CH(OH)CHO$	$2.09 \cdot 10^{10}$			Minakata et al. [109]
$C_5H_5O_4^- + OH \rightarrow 0.5\ ^-OOCCH(OH)CH(O_2)CH(OH)CHO + 0.5\ ^-OOCCH(O_2)CH(OH)CH(OH)CHO$	$8.83 \cdot 10^{10}$			Minakata et al. [109]
$C_5H_8O_4 + OH \rightarrow 0.5\ HOCH_2CH(OH)CH(OH)CH(O_2)COOH + 0.5$	$2.15 \cdot 10^{10}$			Minakata et al. [109]

Reaction	k_{298}	$-E_A/R$	Comment	Reference
$HOCH_2CH(OH)CH(O_2)CH(OH)COOH$				
$C_5H_7O_4^- + OH \rightarrow HOCH_2CH(OH)CH(OH)CH(O_2)COO^- +$ $0.5\ HOCH_2CH(OH)CH(O_2)CH(OH)COO^-$	$8.44 \cdot 10^{10}$			Minakata et al. [109]
$C_6H_6O_4 + OH \rightarrow 0.5\ HOOCCH(OH)CH(O_2)CHCHCOOH$ $+ 0.5\ HOOCCH(O_2)CH(OH)CHCHCOOH$	$3.85 \cdot 10^{10}$			Minakata et al. [109]
$C_6H_5O_4^- + OH \rightarrow 0.5\ HOOCCH(OH)CH(O_2)CHCHCOO^- +$ $0.5\ HOOCCH(O_2)CH(OH)CHCHCOO^-$	$1.01 \cdot 10^{11}$			Minakata et al. [109]
$C_6H_4O_4^{2-} + OH \rightarrow 0.5\ {}^-OOCCH(OH)CH(O_2)CHCHCOO^- +$ $0.5\ {}^-OOCCH(O_2)CH(OH)CHCHCOO^-$	$1.64 \cdot 10^{11}$			Minakata et al. [109]
$C_7H_8O_4 + OH \rightarrow$ $0.2415\ CH_3C(COOH)=CHCH(OH)CH(O_2)COOH +$ $0.2415\ CH_3C(COOH)=CHCH(O_2)C(O)COOH +$ $0.25825\ CH_3CH(OH)(COOH)CH(O_2)CH=CHCOOH +$ $0.25825\ CH_3CH(O_2)(COOH)CH(OH)CH=CHCOOH$	$4.02 \cdot 10^{10}$			Minakata et al. [109]
$C_7H_7O_4^- + OH \rightarrow$ $0.08975\ CH_3C(COOH)=CHCH(OH)CH(O_2)COO^- +$ $0.08975\ CH_3C(COOH)=CHCH(O_2)C(O)COO^- +$ $0.40975\ CH_3CH(OH)(COOH)CH(O_2)CH=CHCOO^- +$ $0.40975\ CH_3CH(O_2)(COOH)CH(OH)CH=CHCOO^-$	$1.08 \cdot 10^{11}$			Minakata et al. [109]
$C_7H_6O_4^{2-} + OH \rightarrow$ $0.2415\ CH_3C(COO^-)=CHCH(OH)CH(O_2)COO^- +$ $0.2415\ CH_3C(COO^-)=CHCH(O_2)C(O)COO^- +$ $0.25825\ CH_3CH(OH)(COO^-)CH(O_2)CH=CHCOO^- +$ $0.25825\ CH_3CH(O_2)(COO^-)CH(OH)CH=CHCOO^-$	$1.71 \cdot 10^{11}$			Minakata et al. [109]
$C_5H_6O_3 + OH \rightarrow 0.5\ CH_3CH(OH)(COOH)C(O_2)CHO + 0.5$ $CH_3CH(O_2)(COOH)C(OH)CHO$	$1.34 \cdot 10^{10}$			Minakata et al. [109]
$C_5H_5O_3^- + OH \rightarrow 0.5\ CH_3C(OH)(COO^-)CH(O_2)CHO + 0.5$ $CH_3C(O_2)(COO^-)CH(OH)CHO$	$5.38 \cdot 10^{10}$			Minakata et al. [109]

Reaction	k_{298}	$-E_A/R$	Comment	Reference
$C_6H_8O_4 + OH \rightarrow$ 0.5 $CH_3C(OH)(COOH)CH(O_2)CH(OH)CHO$ + 0.5 $CH_3C(O_2)(COOH)CH(OH)CH(OH)CHO$	$2.26 \cdot 10^{10}$			Minakata et al. [109]
$C_6H_7O_4^- + OH \rightarrow$ 0.5 $CH_3C(OH)(COO^-)CH(O_2)CH(OH)CHO$ + 0.5 $CH_3C(O_2)(COO^-)CH(OH)CH(OH)CHO$	$8.99 \cdot 10^{10}$			Minakata et al. [109]
$C_6H_6O_6 + OH \rightarrow$ 0.5 $HOOCC(O)CH(OH)CH(OH)CH(O_2)COOH$ + 0.5 $HOOCC(O)CH(OH)CH(O_2)CH(OH)COOH$	$1.95 \cdot 10^{10}$			Minakata et al. [109]
$C_6H_5O_6^- + OH \rightarrow$ 0.5 $HOOCC(O)CH(OH)CH(OH)CH(O_2)COO^-$ + 0.5 $HOOCC(O)CH(OH)CH(O_2)CH(OH)COO^-$	$1.95 \cdot 10^{11}$			Minakata et al. [109]
$C_6H_4O_6^{2-} + OH \rightarrow$ 0.5 $^-OOCC(O)CH(OH)CH(OH)CH(O_2)COO^-$ + 0.5 $^-OOCC(O)CH(OH)CH(O_2)CH(OH)COO^-$	$8.25 \cdot 10^{10}$			Minakata et al. [109]
$C_5H_4O_4 + OH \rightarrow$ 0.5 $HOOCCH(OH)CH(O_2)C(O)CHO$ + 0.5 $HOOCCH(O_2)CH(OH)C(O)CHO$	$1.17 \cdot 10^{10}$			Minakata et al. [109]
$C_5H_3O_4^- + OH \rightarrow$ 0.5 $^-OOCCH(OH)CH(O_2)C(O)CHO$ + 0.5 $^-OOCCH(O_2)CH(OH)C(O)CHO$	$4.94 \cdot 10^{10}$			Minakata et al. [109]
$C_5H_4O_3 + OH \rightarrow$ 0.5 $OHCC(O)CH(OH)CH(O_2)CHO$ + 0.5 $OHCC(O)CH(O_2)CH(OH)CHO$	$3.04 \cdot 10^{10}$			Minakata et al. [109]
$C_5H_6O_3 + OH \rightarrow$ 0.5 $HOCH_2C(O)CH(OH)CH(O_2)CHO$ + 0.5 $HOCH_2C(O)CH(O_2)CH(OH)CHO$	$3.05 \cdot 10^{10}$			Minakata et al. [109]
$C_5H_6O_4 + OH \rightarrow$ 0.5 $HOCH_2C(O)CH(OH)CH(O_2)COOH$ + 0.5 $HOCH_2C(O)CH(OH)CH(O_2)COOH$	$1.17 \cdot 10^{10}$			Minakata et al. [109]
$C_5H_5O_4^- + OH \rightarrow$ 0.5 $HOCH_2C(O)CH(OH)CH(O_2)COO^-$ + 0.5 $HOCH_2C(O)CH(OH)CH(O_2)COO^-$	$4.95 \cdot 10^{10}$			Minakata et al. [109]
$C_5H_8O_4 + OH \rightarrow$	$1.96 \cdot 10^{10}$			Minakata et al. [109]

Reaction	k_{298}	$-E_A/R$	Comment	Reference
0.5 $CH_3C(O)CH(OH)CH(OH)CH(O_2)COOH$ + 0.5 $CH_3C(O)CH(OH)CH(O_2)CH(OH)COOH$				
$C_5H_7O_4^-$ + OH → 0.5 $CH_3C(O)CH(OH)CH(OH)CH(O_2)COO^-$ + 0.5 $CH_3C(O)CH(OH)CH(O_2)CH(OH)COO^-$	$8.25 \cdot 10^{10}$			Minakata et al. [109]
$C_5H_6O_6$ + OH → 0.134 $HOOCC(O)C(OH)(O_2)CH(OH)CHO$ + 0.426 $HOOCC(O)CH(OH)C(OH)(O_2)CHO$ + 0.44 $HOOCC(O)CH(OH)CH(OH)C(O)O_2$	$2.06 \cdot 10^{9}$			Minakata et al. [109]
$C_5H_5O_6^-$ + OH → 0.134 $^-OOCC(O)C(OH)(O_2)CH(OH)CHO$ + 0.426 $^-OOCC(O)CH(OH)C(OH)(O_2)CHO$ + 0.44 $^-OOCC(O)CH(OH)CH(OH)C(O)O_2$	$2.06 \cdot 10^{9}$			Minakata et al. [109]
$C_5H_8O_4$ + OH → 0.138 $CH_3C(O)C(OH)(O_2)CH(OH)CHO$ + 0.424 $CH_3C(O)C(OH)(OH)CH(O_2)CHO$ + 0.438 $CH_3C(O)CH(OH)CH(OH)C(O)O_2$	$2.12 \cdot 10^{9}$			Minakata et al. [109]
$C_7H_6O_7$ + OH → 0.5 $HOOCC(OH)(OH)CH(O_2)(COOH)CH=CHCOOH$ + 0.5 $HOOCC(OH)(O_2)CH(OH)(COOH)CH=CHCOOH$	$3.85 \cdot 10^{10}$			est. muconic acid
$C_7H_5O_7^-$ + OH → 0.5 $^-OOCC(OH)(OH)CH(O_2)(COOH)CH=CHCOOH$ + 0.5 $^-OOCC(OH)(O_2)CH(OH)(COOH)CH=CHCOOH$	$1.01 \cdot 10^{11}$			est. muconic acid
$C_7H_4O_7^{2-}$ + OH → 0.5 $^-OOCC(OH)(OH)CH(O_2)(COOH)CH=CHCOO^-$ + 0.5 $^-OOCC(OH)(O_2)CH(OH)(COOH)CH=CHCOO^-$	$1.64 \cdot 10^{11}$			est. muconic acid
$C_7H_4O_7^{3-}$ + OH → 0.5 $^-OOCC(OH)(OH)CH(O_2)(COO^-)CH=CHCOO^-$ + 0.5 $^-OOCC(OH)(O_2)CH(OH)(COO^-)CH=CHCOO^-$	$1.64 \cdot 10^{11}$			est. muconic acid

Reaction	k_{298}	$-E_A/R$	Comment	Reference
$C_6H_4O_4^{2-} + Cl_2^- \rightarrow C_4H_4O_3 + 2\ Cl^- + HO_2 + CO + CO_2 - 2\ O_2$	$2.10 \cdot 10^8$		products est.	Hasegawa and Neta [97]
$C_6H_6O_4 + O_3 \rightarrow C_4H_4O_3 + C_2H_2O_3 + H_2O_2 - H_2O$	$1.60 \cdot 10^4$		yields Leitzke and Sonntag [110]	Beltrán et al. [106]
$C_6H_5O_4^- + O_3 \rightarrow C_4H_4O_3 + C_2HO_3^- + H_2O_2 - H_2O$	$2.65 \cdot 10^4$			Leitzke and Sonntag [110]
$C_6H_4O_4^{2-} + O_3 \rightarrow C_4H_3O_3^- + C_2HO_3^- + H_2O_2 - H_2O$	$1.40 \cdot 10^5$		yields Leitzke and Sonntag [110]	Beltrán et al. [106]
$C_7H_8O_4 + O_3 \rightarrow 0.5\ C_4H_6O_5 + 0.5\ C_3H_4O_3 + 0.5\ C_4H_4O_3 + 0.5\ C_3H_5O_5 - H_2O$	$1.60 \cdot 10^4$		Leitzke and Sonntag [110]	est. muconic acid
$C_7H_7O_4^- + O_3 \rightarrow 0.5\ C_4H_6O_5 + 0.5\ C_3H_4O_3 + 0.5\ C_4H_4O_3 + 0.5\ C_3H_5O_5 - H_2O$	$2.65 \cdot 10^4$		Leitzke and Sonntag [110]	est. muconic acid
$C_7H_6O_4^{2-} + O_3 \rightarrow 0.5\ C_4H_6O_5 + 0.5\ C_3H_4O_3 + 0.5\ C_4H_4O_3 + 0.5\ C_3H_5O_5 - H_2O$	$1.40 \cdot 10^5$		Leitzke and Sonntag [110]	est. muconic acid
$C_5H_6O_3 + O_3 \rightarrow 0.5\ C_2H_2O_2 + 0.5\ C_3H_4O_4 + 0.5\ C_3H_4O_3 + 0.5\ C_2H_2O_3$	$1.00 \cdot 10^4$		est. lower limit	Herrmann et al. [111]
$C_5H_8O_4 + O_3 \rightarrow 0.5\ C_2H_2O_3 + 0.5\ C_3H_6O_4 + 0.5\ C_3H_6O_3 + 0.5\ C_2H_2O_4$	$1.00 \cdot 10^4$		est. lower limit	Herrmann et al. [111]
$C_5H_6O_4 + O_3 \rightarrow 0.5\ C_2H_2O_3 + 0.5\ C_3H_4O_4 + 0.5\ C_3H_4O_3 + 0.5\ C_2H_2O_4$	$1.00 \cdot 10^3$		est. lower limit	Herrmann et al. [111]
$C_5H_4O_3 + O_3 \rightarrow 0.5\ C_2H_2O_2 + 0.5\ C_3H_2O_4 + 0.5\ C_3H_2O_3 + 0.5\ C_2H_2O_3$	$1.00 \cdot 10^4$		est. lower limit	Herrmann et al. [111]
$C_5H_6O_4 + O_3 \rightarrow 0.5\ C_2H_2O_3 + 0.5\ C_3H_4O_4 + 0.5\ C_3H_4O_3 + 0.5\ C_2H_2O_4$	$1.00 \cdot 10^4$		est. lower limit	Herrmann et al. [111]
$C_5H_4O_4 + O_3 \rightarrow 0.5\ C_2H_2O_3 + 0.5\ C_3H_2O_4 + 0.5\ C_3H_2O_3 + 0.5\ C_2H_2O_4$	$1.00 \cdot 10^3$		est. lower limit	Herrmann et al. [111]
$C_7H_6O_7 + O_3 \rightarrow C_2H_2O_4 + C_5H_4O_5 + H_2O_2$	$1.60 \cdot 10^4$			est. muconic acid
$C_7H_5O_7^- + O_3 \rightarrow C_2HO_4^- + C_5H_4O_5 + H_2O_2$	$2.65 \cdot 10^4$			est. muconic acid
$C_7H_4O_7^{2-} + O_3 \rightarrow C_2HO_4^- + C_5H_3O_5^- + H_2O_2$	$1.40 \cdot 10^5$			est. muconic acid

Reaction	k_{298}	$-E_A/R$	Comment	Reference
$C_7H_3O_7^{3-} + O_3 \rightarrow C_2HO_4^- + C_5H_2O_5^{2-} + H_2O_2$	$1.40 \cdot 10^5$			est. muconic acid
$C_5H_6O_3 + O_3 \rightarrow 0.5\ C_3H_6O_4 + 0.5\ C_2H_2O_3 + 0.5\ C_2H_4O_5 + 0.5\ C_3H_4O_2$	$1.40 \cdot 10^3$			est. maleic acid
$C_5H_5O_3^- + O_3 \rightarrow 0.5\ C_3H_6O_4 + 0.5\ C_2H_1O_3^- + 0.5\ C_2H_3O_5^- + 0.5\ C_3H_4O_2$	$4.20 \cdot 10^3$			est. maleic acid
$C_5H_8O_3 + O_3 \rightarrow 0.5\ C_3H_8O_4 + 0.5\ C_2H_2O_3 + 0.5\ C_2H_6O_5 + 0.5\ C_3H_4O_2$	$1.40 \cdot 10^3$			est. maleic acid
$C_5H_7O_3^- + O_3 \rightarrow 0.5\ C_3H_8O_4 + 0.5\ C_2HO_3^- + 0.5\ C_2H_6O_5^- + 0.5\ C_3H_4O_2$	$4.20 \cdot 10^3$			est. maleic acid
$C_5H_6O_2 + O_3 \rightarrow 0.5\ C_3H_6O_4 + 0.5\ C_2H_2O_2 + 0.5\ C_2H_4O_4 + 0.5\ C_3H_4O_2$	$1.40 \cdot 10^3$			est. maleic acid
$C_5H_6O_3 + O_3 \rightarrow 0.5\ C_3H_6O_5 + 0.5\ C_2H_2O_2 + 0.5\ C_2H_4O_4 + 0.5\ C_3H_4O_3$	$1.40 \cdot 10^3$			est. maleic acid
$C_5H_8O_4 + O_3 \rightarrow 0.5\ C_3H_8O_5 + 0.5\ C_2H_2O_3 + 0.5\ C_2H_4O_5 + 0.5\ C_3H_6O_3$	$1.40 \cdot 10^3$			est. maleic acid
$C_5H_7O_4^- + O_3 \rightarrow 0.5\ C_3H_8O_5 + 0.5\ C_2HO_3^- + 0.5\ C_2H_3O_5^- + 0.5\ C_3H_6O_3$	$4.20 \cdot 10^3$			est. maleic acid
$C_5H_6O_4 + O_3 \rightarrow 0.5\ C_3H_6O_5 + 0.5\ C_2H_2O_3 + 0.5\ C_2H_4O_5 + 0.5\ C_3H_4O_3$	$1.40 \cdot 10^3$			est. maleic acid
$C_5H_5O_4^- + O_3 \rightarrow 0.5\ C_3H_6O_5 + 0.5\ C_2HO_3^- + 0.5\ C_2H_3O_5^- + 0.5\ C_3H_4O_3$	$4.20 \cdot 10^3$			est. maleic acid
$C_5H_4O_3 + O_3 \rightarrow 0.5\ C_3H_4O_5 + 0.5\ C_2H_2O_2 + 0.5\ C_2H_4O_4 + 0.5\ C_3H_2O_3$	$1.40 \cdot 10^3$			est. maleic acid
$C_5H_6O_4 + O_3 \rightarrow 0.5\ C_3H_6O_5 + 0.5\ C_2H_2O_3 + 0.5\ C_2H_4O_5 + 0.5\ C_3H_4O_3$	$1.40 \cdot 10^3$			est. maleic acid
$C_5H_5O_4^- + O_3 \rightarrow 0.5\ C_3H_6O_5 + 0.5\ C_2HO_3^- + 0.5\ C_2H_3O_5^- + 0.5\ C_3H_4O_3$	$4.20 \cdot 10^3$			est. maleic acid
$C_5H_4O_4 + O_3 \rightarrow 0.5\ C_3H_4O_5 + 0.5\ C_2H_2O_3 + 0.5\ C_2H_4O_5 +$	$1.40 \cdot 10^3$			est. maleic acid

Reaction	k_{298}	$-E_A/R$	Comment	Reference
$0.5\ C_3H_2O_3$				
$C_5H_3O_4^- + O_3 \rightarrow 0.5\ C_3H_4O_5 + 0.5\ C_2HO_3^- + 0.5\ C_2H_3O_5^- + 0.5\ C_3H_2O_3$	$4.20 \cdot 10^3$			est. maleic acid
$C_5H_4O_5 + O_3 \rightarrow 0.5\ C_3H_4O_6 + 0.5\ C_2H_2O_3 + 0.5\ C_2H_4O_5 + 0.5\ C_3H_2O_4$	$1.40 \cdot 10^3$			est. maleic acid
$C_5H_3O_5^- + O_3 \rightarrow 0.5\ C_3H_3O_6^- + 0.5\ C_2H_2O_3 + 0.5\ C_2H_4O_5 + 0.5\ C_3HO_4^-$	$4.20 \cdot 10^3$			est. maleic acid
$C_5H_2O_5^{2-} + O_3 \rightarrow 0.5\ C_3H_3O_6^- + 0.5\ C_2HO_3^- + 0.5\ C_2H_3O_5^- + 0.5\ C_3HO_4^-$	$7.00 \cdot 10^3$			est. maleic acid
$C_6H_4O_6 + O_3 \rightarrow C_3H_2O_4 + C_3H_4O_6$	$1.40 \cdot 10^3$			est. maleic acid
$C_6H_3O_6^- + O_3 \rightarrow C_3HO_4^- + C_3H_4O_6$	$4.20 \cdot 10^3$			est. maleic acid
$C_5H_2O_6^{2-} + O_3 \rightarrow C_3HO_4^- + C_3H_3O_6^-$	$7.00 \cdot 10^3$			est. maleic acid
$C_5H_6O_3 + O_3 \rightarrow 0.5\ C_3H_6O_5 + 0.5\ C_2H_2O_2 + 0.5\ C_2H_4O_4 + 0.5\ C_3H_4O_3$	$1.40 \cdot 10^3$			est. maleic acid
$C_5H_5O_3^- + O_3 \rightarrow 0.5\ C_3H_5O_5^- + 0.5\ C_2H_2O_2 + 0.5\ C_2H_4O_4 + 0.5\ C_3H_3O_3^-$	$4.20 \cdot 10^3$			est. maleic acid
$C_6H_8O_4 + O_3 \rightarrow 0.5\ C_3H_4O_3 + 0.5\ C_3H_6O_5 + 0.5\ C_3H_6O_5 + 0.5\ C_3H_4O_3$	$1.40 \cdot 10^3$			est. maleic acid
$C_6H_7O_4^- + O_3 \rightarrow 0.5\ C_3H_4O_3 + 0.5\ C_3H_5O_5^- + 0.5\ C_3H_6O_5 + 0.5\ C_3H_3O_3^-$	$4.20 \cdot 10^3$			est. maleic acid
$C_6H_6O_6 + O_3 \rightarrow 0.5\ C_2H_2O_3 + 0.5\ C_4H_6O_7 + 0.5\ C_3H_4O_5 + 0.5\ C_4H_4O_5$	$1.60 \cdot 10^4$			est. muconic acid
$C_6H_5O_6^- + O_3 \rightarrow 0.5\ C_2H_2O_3 + 0.5\ C_4H_5O_7^- + 0.5\ C_3H_4O_5 + 0.5\ C_4H_3O_5^-$	$2.65 \cdot 10^4$			est. muconic acid
$C_6H_4O_6^{2-} + O_3 \rightarrow 0.5\ C_2HO_3^- + 0.5\ C_4H_5O_7^- + 0.5\ C_3H_3O_5^- + 0.5\ C_4H_3O_5^-$	$1.40 \cdot 10^5$			est. muconic acid
$C_6H_8O_4 + O_3 \rightarrow 0.5\ C_2H_2O_3 + 0.5\ C_4H_8O_5 + 0.5\ C_2H_4O_5 + 0.5\ C_4H_6O_3$	$1.40 \cdot 10^3$			est. maleic acid

Reaction	k_{298}	$-E_A/R$	Comment	Reference
$C_6H_7O_4^- + O_3 \rightarrow 0.5\ C_2HO_3^- + 0.5\ C_4H_8O_5 + 0.5\ C_2H_3O_5^- + 0.5\ C_4H_6O_3$	$4.20 \cdot 10^3$			est. maleic acid

Table S6 Emission values of the two urban environments used in the simulations. Strong emission scenario based on the values in Ervens et al. [112] is done using the ratios given in Middleton et al. [113].

Compound	moderate emission rate (molecules cm^{-2} s^{-1})	strong emission rate[112] (molecules cm^{-2} s^{-1})	Comment
Inorganics			
CO	$2.04 \cdot 10^{12}$	$8.99 \cdot 10^{12}$	
NH_3	$9.03 \cdot 10^{10}$	$3.03 \cdot 10^{11}$	
NO	$8.56 \cdot 10^{11}$	$1.01 \cdot 10^{12}$	
NO_2	$7.10 \cdot 10^{10}$	-	
SO_2	$8.94 \cdot 10^{11}$	$3.27 \cdot 10^{12}$	
HCl	$5.25 \cdot 10^{10}$	-	cal. from UK Emission Inventory
Organics			
Alkanes			
Methane	$1.47 \cdot 10^{12}$	-	
Ethane	$6.48 \cdot 10^{11}$	$1.54 \cdot 10^{11}$	
Propane	$1.61 \cdot 10^{9}$	$1.23 \cdot 10^{10}$	
n-Butane	$1.87 \cdot 10^{10}$	$1.89 \cdot 10^{11}$	
i-Butena	$5.08 \cdot 10^{8}$	$5.13 \cdot 10^{9}$	
n-Pentane	$2.33 \cdot 10^{9}$	$6.65 \cdot 10^{10}$	
i-Pentane	$4.13 \cdot 10^{9}$	$1.18 \cdot 10^{11}$	
n-Hexane	$1.97 \cdot 10^{9}$	$6.73 \cdot 10^{10}$	
3-Methylpentane	$5.77 \cdot 10^{8}$	$1.97 \cdot 10^{10}$	
2,2-Dimethylbutane	$3.54 \cdot 10^{8}$	$1.21 \cdot 10^{10}$	
2-Methylpentane	$8.99 \cdot 10^{9}$	$3.16 \cdot 10^{10}$	
n-Heptane	$2.88 \cdot 10^{10}$	$1.29 \cdot 10^{11}$	
i-Heptane	$5.36 \cdot 10^{9}$	$2.40 \cdot 10^{10}$	

Compound	moderate emission rate (molecules cm^{-2} s^{-1})	strong emission rate[112] (molecules cm^{-2} s^{-1})	Comment
Octane	$5.42 \cdot 10^{9}$	$2.76 \cdot 10^{10}$	
Nonane	$2.02 \cdot 10^{9}$	$1.16 \cdot 10^{10}$	
Decane	$1.33 \cdot 10^{9}$	$8.46 \cdot 10^{9}$	
Undecane	$3.32 \cdot 10^{9}$	$2.31 \cdot 10^{10}$	
Cyclohexane	$5.33 \cdot 10^{9}$	$2.00 \cdot 10^{10}$	
Alkenes			
Ethene	$1.65 \cdot 10^{10}$	$2.61 \cdot 10^{11}$	
Propene	$9.19 \cdot 10^{9}$	$3.09 \cdot 10^{10}$	
n-Butene	$1.47 \cdot 10^{9}$	$6.60 \cdot 10^{9}$	
i-Butene	$3.29 \cdot 10^{7}$	$1.48 \cdot 10^{8}$	
n-Pentene	$7.90 \cdot 10^{8}$	$4.43 \cdot 10^{9}$	
3-Methylbutene	$1.41 \cdot 10^{8}$	$7.88 \cdot 10^{8}$	
2-Methylbutene	$8.78 \cdot 10^{6}$	$4.92 \cdot 10^{7}$	
n-Hexene	$9.44 \cdot 10^{8}$	$4.20 \cdot 10^{9}$	
Trimethylethylene	$7.47 \cdot 10^{8}$	-	
trans-2-Butene	$5.85 \cdot 10^{8}$	-	
cis-2-Butene	$4.29 \cdot 10^{8}$	-	
trans-Pentene	$5.58 \cdot 10^{8}$	-	
cis-Pentene	$3.42 \cdot 10^{8}$	-	
cis-Hexene	$1.42 \cdot 10^{8}$	-	
Dialkenes			
Butadiene	$1.11 \cdot 10^{9}$	$1.24 \cdot 10^{11}$	
Isoprene	$3.52 \cdot 10^{7}$	$1.54 \cdot 10^{10}$	
Alkynes			
Ethyne	$8.92 \cdot 10^{9}$	$4.04 \cdot 10^{10}$	
Aromatics			

Compound	moderate emission rate (molecules cm^{-2} s^{-1})	strong emission rate[112] (molecules cm^{-2} s^{-1})	Comment
Benzene	$9.41 \cdot 10^{8}$	$1.89 \cdot 10^{10}$	
Styrene	$5.21 \cdot 10^{8}$	$9.02 \cdot 10^{9}$	
Toluene	$6.01 \cdot 10^{9}$	$1.42 \cdot 10^{11}$	
Ethyl benzene	$5.69 \cdot 10^{7}$	$1.55 \cdot 10^{9}$	
n-Propyl benzene	$1.46 \cdot 10^{7}$	$4.50 \cdot 10^{8}$	
i-Propyl benzene	$4.01 \cdot 10^{6}$	$1.24 \cdot 10^{8}$	
o-Xylene	$4.64 \cdot 10^{8}$	$2.04 \cdot 10^{10}$	
p-Xylene	$6.24 \cdot 10^{8}$	$2.74 \cdot 10^{10}$	
1,2,4-Trimethylbenzene	$3.51 \cdot 10^{8}$	$1.75 \cdot 10^{10}$	
1,3,5-Trimethylbenzene	$3.24 \cdot 10^{8}$	$1.61 \cdot 10^{10}$	
m-Xylene	$1.70 \cdot 10^{8}$	$7.46 \cdot 10^{9}$	
1,2,3-Trimethylbenzene	$9.96 \cdot 10^{7}$	$4.95 \cdot 10^{9}$	
o-Ethyl toluene	$6.22 \cdot 10^{7}$	$3.09 \cdot 10^{9}$	
m-Ethyl toluene	$3.99 \cdot 10^{7}$	$1.98 \cdot 10^{9}$	
Aldehydes			
Methanal	$1.74 \cdot 10^{10}$	$2.58 \cdot 10^{10}$	
Ethanal	$3.56 \cdot 10^{9}$	$3.53 \cdot 10^{10}$	
Propanal	$1.34 \cdot 10^{8}$	$1.74 \cdot 10^{9}$	
Butanal	$1.08 \cdot 10^{8}$	$1.74 \cdot 10^{9}$	
Acrolein	$6.22 \cdot 10^{8}$	$7.85 \cdot 10^{9}$	
Crotonaldehyde	$5.53 \cdot 10^{7}$	$8.72 \cdot 10^{8}$	
Benzaldehyde	$2.19 \cdot 10^{8}$	$5.23 \cdot 10^{9}$	
p-Tolualdehyde	$9.69 \cdot 10^{7}$	$2.62 \cdot 10^{9}$	
Glyoxal	$1.67 \cdot 10^{8}$	$2.18 \cdot 10^{9}$	
Methylglyoxal	$1.08 \cdot 10^{8}$	$1.74 \cdot 10^{9}$	
Organic acids			

Compound	moderate emission rate (molecules cm^{-2} s^{-1})	strong emission rate[112] (molecules cm^{-2} s^{-1})	Comment
Formic acid	$1.83 \cdot 10^{6}$	-	
Acetic acid	$2.80 \cdot 10^{7}$	$8.44 \cdot 10^{9}$	
Benzoic acid	$6.89 \cdot 10^{5}$	-	
Ketones			
Propanone	$1.36 \cdot 10^{10}$	$5.11 \cdot 10^{10}$	
Butanone	$1.01 \cdot 10^{10}$	$4.71 \cdot 10^{10}$	
Hexanone	$6.66 \cdot 10^{7}$	$4.32 \cdot 10^{8}$	
Cyclohexanone	$6.80 \cdot 10^{7}$	$4.32 \cdot 10^{8}$	
Alcohols			
Methanol	$5.21 \cdot 10^{8}$	$1.16 \cdot 10^{11}$	
Ethanol	$1.83 \cdot 10^{10}$	$4.03 \cdot 10^{11}$	
Propanol	$1.22 \cdot 10^{7}$	$4.27 \cdot 10^{8}$	
i-Propanol	$4.82 \cdot 10^{9}$	$1.15 \cdot 10^{11}$	
Butanol	$8.00 \cdot 10^{7}$	$2.35 \cdot 10^{9}$	
i-Butanol	$7.28 \cdot 10^{7}$	$2.41 \cdot 10^{8}$	
Glycol	$1.65 \cdot 10^{9}$	$4.57 \cdot 10^{10}$	
Propylene glycol	$3.97 \cdot 10^{9}$	$1.35 \cdot 10^{10}$	
Cyclohexanol	$5.38 \cdot 10^{7}$	$2.41 \cdot 10^{8}$	
Phenol	$7.06 \cdot 10^{8}$	$1.09 \cdot 10^{11}$	
Ether			
Dimethyl ether	$1.49 \cdot 10^{9}$	$1.19 \cdot 10^{10}$	
Diethyl ether	$5.09 \cdot 10^{8}$	$1.68 \cdot 10^{9}$	
Methyl glycol	$7.23 \cdot 10^{9}$	$2.45 \cdot 10^{10}$	
Ethylene oxide	$4.73 \cdot 10^{7}$	$3.62 \cdot 10^{8}$	
Ethyl ethanoate	$1.61 \cdot 10^{8}$	$2.46 \cdot 10^{9}$	
Methyl acetate	$8.44 \cdot 10^{7}$	$1.09 \cdot 10^{9}$	

Compound	moderate emission rate (molecules cm^{-2} s^{-1})	strong emission rate[112] (molecules cm^{-2} s^{-1})	Comment
Isopropylacetate	$6.84 \cdot 10^{8}$	$1.21 \cdot 10^{10}$	
Butyl acetate	$8.35 \cdot 10^{8}$	$3.84 \cdot 10^{10}$	
Propyl acetate	$2.64 \cdot 10^{8}$	$1.07 \cdot 10^{10}$	
Monoterpenes			
α-Pinene	$4.40 \cdot 10^{7}$	$1.88 \cdot 10^{10}$	
β-Pinene	$4.17 \cdot 10^{7}$	-	
Limonene	$5.02 \cdot 10^{6}$	$1.88 \cdot 10^{10}$	
Halogenated organics			
Chloromethane	$9.15 \cdot 10^{9}$	$1.10 \cdot 10^{9}$	
Dichloromethane	$3.25 \cdot 10^{9}$	$2.05 \cdot 10^{10}$	
Trichloromethane	$2.67 \cdot 10^{8}$	$1.30 \cdot 10^{8}$	McCulloch et al. [114]
Trichlororethane	$2.37 \cdot 10^{9}$	$6.44 \cdot 10^{7}$	
1,2-Dichloroethane	$5.12 \cdot 10^{6}$	$5.12 \cdot 10^{6}$	
Chloroethene	$3.36 \cdot 10^{8}$	$8.32 \cdot 10^{9}$	
Trichloroethene	$8.01 \cdot 10^{8}$	$3.25 \cdot 10^{8}$	
Tetrachloroethene	$9.55 \cdot 10^{8}$	$8.63 \cdot 10^{8}$	
Vinyltrichloride	$5.60 \cdot 10^{8}$	$5.60 \cdot 10^{8}$	
Bromomethane	$1.44 \cdot 10^{7}$	$1.44 \cdot 10^{7}$	Yokouchi et al. [115]

Table S7 Contribution of different oxidants to the oxidation of aromatic compounds in gas and aqueous phase in the moderately polluted urban environment. If oxidants contribute more than 10% to aqueous-phase oxidation they are marked bold.

	Gas phase			Aqueous phase						
	OH	NO_3	O_3	OH	NO_3	O_3	Cl	Cl_2^-	SO_4^-	HO_2
Phenol										
Overall	33.6%	57.7%	-	4.3%	1.3%	0.0%	0.7%	0.1%	2.3%	-
Cloud	19.7%	24.9%	-	**27.5%**	8.3%	0.1%	4.6%	0.5%	14.4%	-
Non-cloud	36.1%	63.9%	-	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	-
Catechol										
Overall	20.9%	49.8%	1.7%	7.7%	0.3%	**14.0%**	-	-	0.1%	5.6%
Cloud	0.6%	3.5%	0.1%	**26.8%**	1.0%	**48.6%**	-	-	0.3%	**19.2%**
Non-cloud	29.1%	68.5%	2.3%	0.0%	0.0%	0.1%	-	-	0.0%	0.0%
Nitrophenol										
Overall	22.6%	56.9%	-	**12.5%**	6.8%	-	-	-	1.2%	-
Cloud	7.8%	17.3%	-	**45.7%**	**24.9%**	-	-	-	4.3%	-
Non-cloud	28.1%	71.9%	-	0.0	0.0%	-	-	-	0.0%	-
Dinitrophenol										
Overall	1.2%	2.1%	-	**95.7%**	-	-	-	-	-	-
Cloud	0.1%	0.2%	-	**99.7%**	-	-	-	-	-	-
Non-cloud	35.8%	64.2%	-	0.1%	-	-	-	-	-	-
Nitrocatechol										
Overall	2.4%	44.1%	-	**53.5%**	-	-	-	-	-	-
Cloud	0.0%	0.0%	-	**100.0%**	-	-	-	-	-	-
Non-cloud	5.1%	93.6%	-	1.4%	-	-	-	-	-	-
Cresol										
Overall	33.9%	61.1%	-	4.3%	0.4%	0.1%	-	0.0%	0.3%	-
Cloud	24.1%	40.9%	-	**29.4%**	3.1%	0.7%	-	0.0%	1.9%	-
Non-cloud	35.5%	64.5%	-	0.0%	0.0%	0.0%	-	0.0%	0.0%	-

	Gas phase			Aqueous phase						
	OH	NO_3	O_3	OH	NO_3	O_3	Cl	Cl_2^-	SO_4^-	HO_2
Methylcatechol										
Overall	22.4%	50.3%	3.0%	**24.3%**	-	-	-	-	-	-
Cloud	1.7%	7.2%	0.6%	**90.5%**	-	-	-	-	-	-
Non-cloud	30.0%	66.1%	3.9%	0.0%	-	-	-	-	-	-
Nitrocresol										
Overall	22.8%	76.8%	-	0.3%	0.0%	-	-	0.0%	0.0%	-
Cloud	24.5%	71.4%	-	3.8%	0.2%	-	-	0.1%	0.0%	-
Non-cloud	22.6%	77.4%	-	0.0%	0.0%	-	-	0.0%	0.0%	-
Benzoic acid										
Overall	8.3%	-	-	**44.9%**	**10.4%**	-	**34.7%**	0.0%	1.7%	-
Cloud	0.6%	-	-	**48.7%**	**11.2%**	-	**37.6%**	0.0%	6.0%	-
Non-cloud	99.8%	-	-	0.0%	0.0%	-	0.2%	0.0%	0.0%	-

Table S8 Contribution of different oxidants to the oxidation of aromatic compounds in gas and aqueous phase in the strongly polluted urban environment. If oxidants contribute more than 10% to aqueous-phase oxidation they are marked bold.

	Gas phase			Aqueous phase						
	OH	NO_3	O_3	OH	NO_3	O_3	Cl	Cl_2^-	SO_4^-	HO_2
Phenol										
Overall	21.1%	76.0%	-	0.3%	2.0%	0.0%	0.0%	0.0%	0.6%	-
Cloud	11.3%	61.5%	-	2.7%	**18.6%**	0.2%	0.2%	0.0%	5.5%	-
Non-cloud	22.2%	77.8%	-	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	-
Catechol										
Overall	11.5%	68.3%	1.9%	0.3%	0.3%	**13.3%**	-	-	0.0%	4.4%
Cloud	0.2%	5.8%	0.2%	1.8%	1.5%	**68.1%**	-	-	0.1%	**22.4%**
Non-cloud	14.2%	83.4%	2.3%	0.0%	0.0%	0.1%	-	-	0.0%	0.0%
Nitrophenol										
Overall	14.7%	75.3%	-	0.5%	9.3%	-	-	-	0.2%	-
Cloud	3.8%	40.2%	-	2.7%	**51.8%**	-	-	-	1.3%	-
Non-cloud	17.0%	83.0%	-	0.0	0.0%	-	-	-	0.0%	-
Dinitrophenol										
Overall	10.8%	42.6%	-	**38.6%**	-	-	-	-	-	-
Cloud	0.8%	7.2%	-	**76.4%**	-	-	-	-	-	-
Non-cloud	21.1%	78.8%	-	0.0%	-	-	-	-	-	-
Nitrocatechol										
Overall	3.5%	84.9%	-	**11.6%**	-	-	-	-	-	-
Cloud	0.0%	0.2%	-	**99.8%**	-	-	-	-	-	-
Non-cloud	3.9%	95.4%	-	0.7%	-	-	-	-	-	-
Cresol										
Overall	24.3%	74.7%	-	0.2%	0.5%	0.1%	-	0.0%	0.1%	-
Cloud	12.4%	78.5%	-	2.1%	5.1%	1.3%	-	0.0%	0.7%	-
Non-cloud	25.7%	74.3%	-	0.0%	0.0%	0.0%	-	0.0%	0.0%	-

	Gas phase			Aqueous phase						
	OH	NO_3	O_3	OH	NO_3	O_3	Cl	Cl_2^-	SO_4^-	HO_2
Methylcatechol										
Overall	15.0%	78.8%	4.2%	1.9%	-	-	-	-	-	-
Cloud	3.7%	61.6%	4.8%	**29.9%**	-	-	-	-	-	-
Non-cloud	15.8%	80.0%	4.2%	0.0%	-	-	-	-	-	-
Nitrocresol										
Overall	13.7%	86.3%	-	0.0%	0.0%	-	-	0.0%	0.0%	-
Cloud	7.0%	92.7%	-	0.1%	0.2%	-	-	0.0%	0.0%	-
Non-cloud	14.3%	85.7%	-	0.0%	0.0%	-	-	0.0%	0.0%	-
Benzoic acid										
Overall	30.8%	-	-	9.5%	**52.2%**	-	6.1%	0.0%	1.5%	-
Cloud	0.6%	-	-	**13.4%**	**74.3%**	-	8.7%	0.0%	2.0%	-
Non-cloud	100.0%	-	-	0.0%	0.0%	-	0.2%	0.0%	0.0%	-

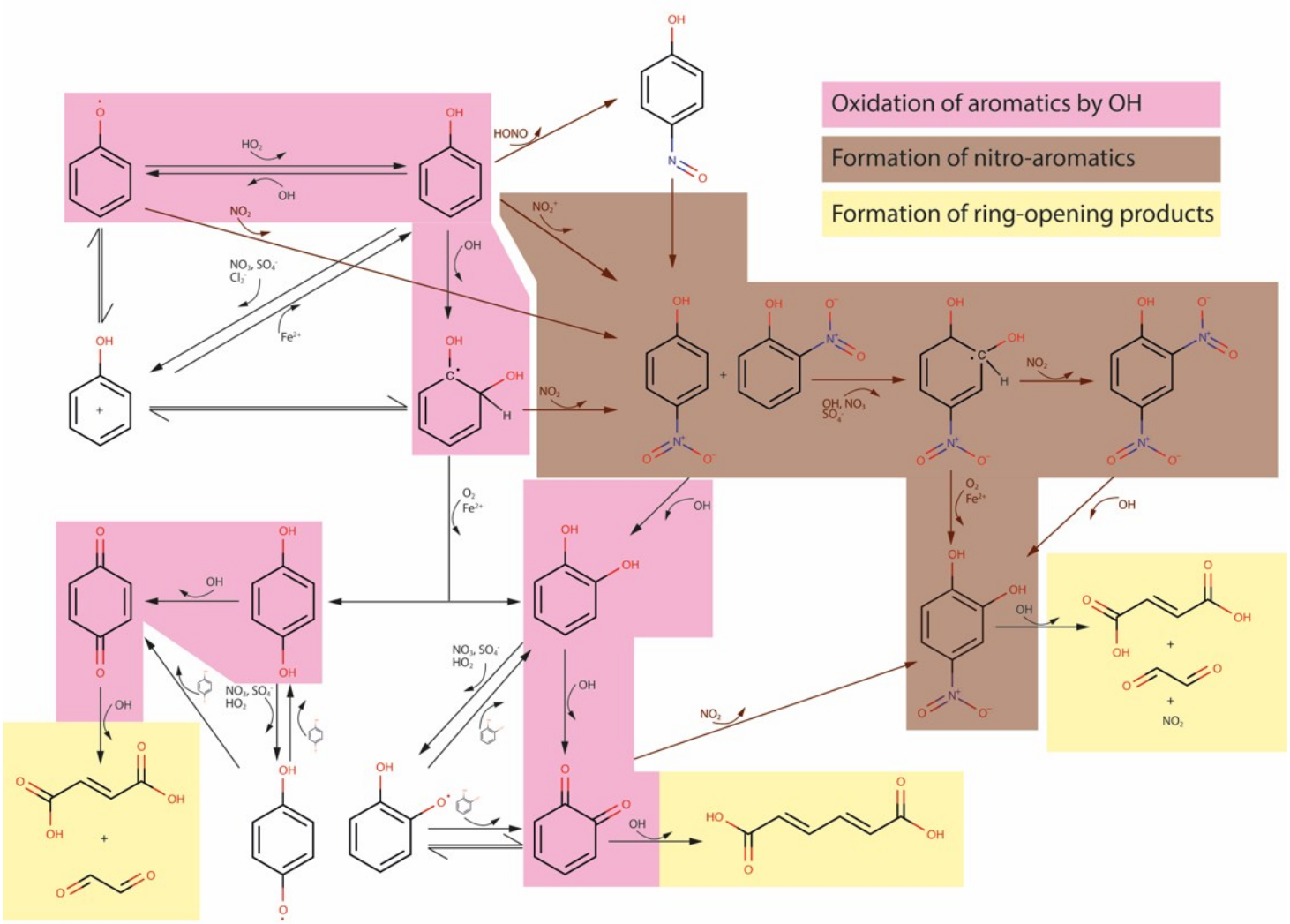

Figure S1 Schematic description of the oxidation of phenol implemented in the AM1.0 into nitrated aromatics as well as ring-opening products.

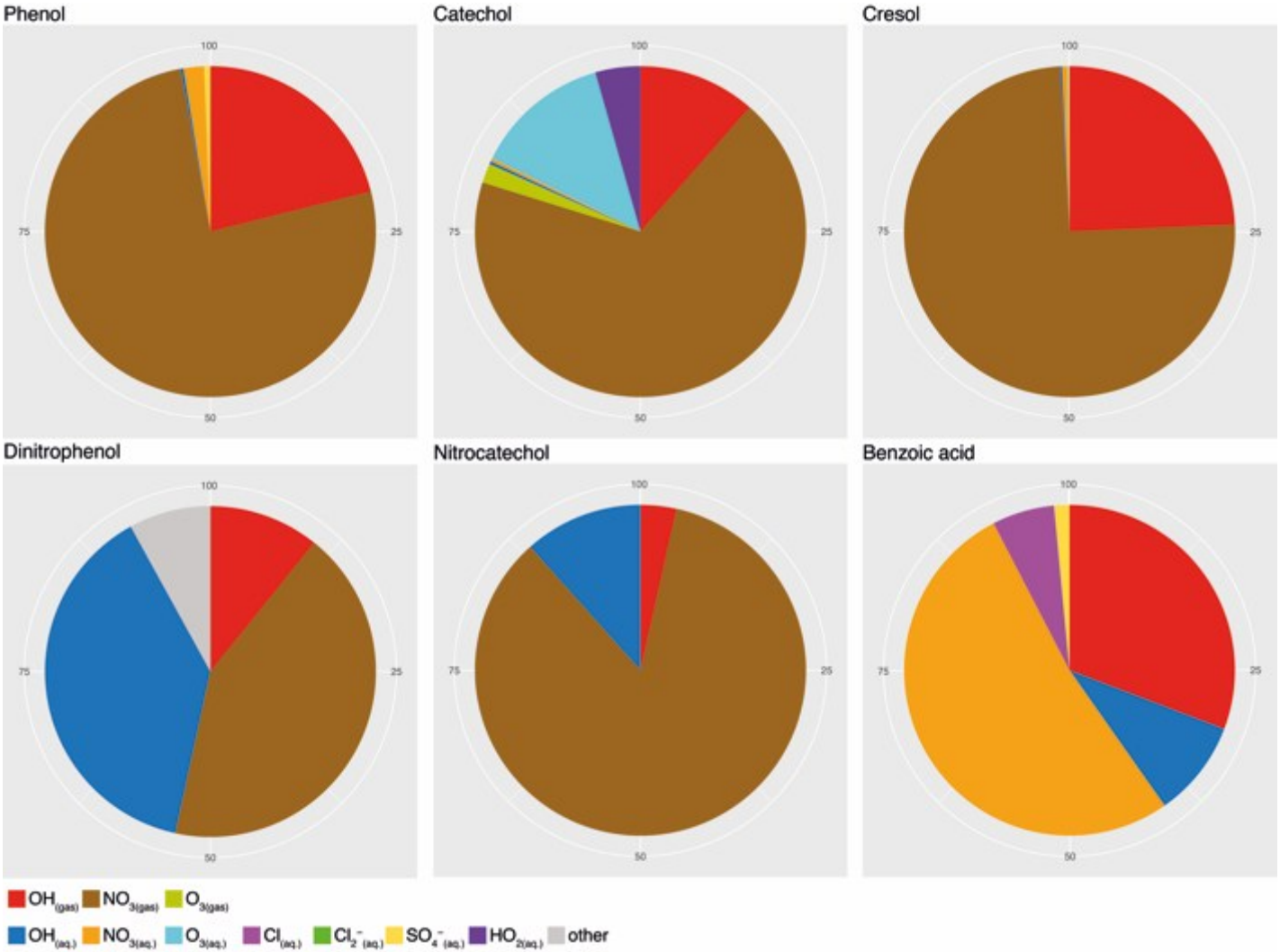

Figure S2 Depiction of the contribution of different oxidants to the degradation of specific substituted aromatic compounds in gas and aqueous phase at the 'strongly polluted' environmental scenario. The contribution is calculated for the whole simulation time using the overall mean of the different oxidants.

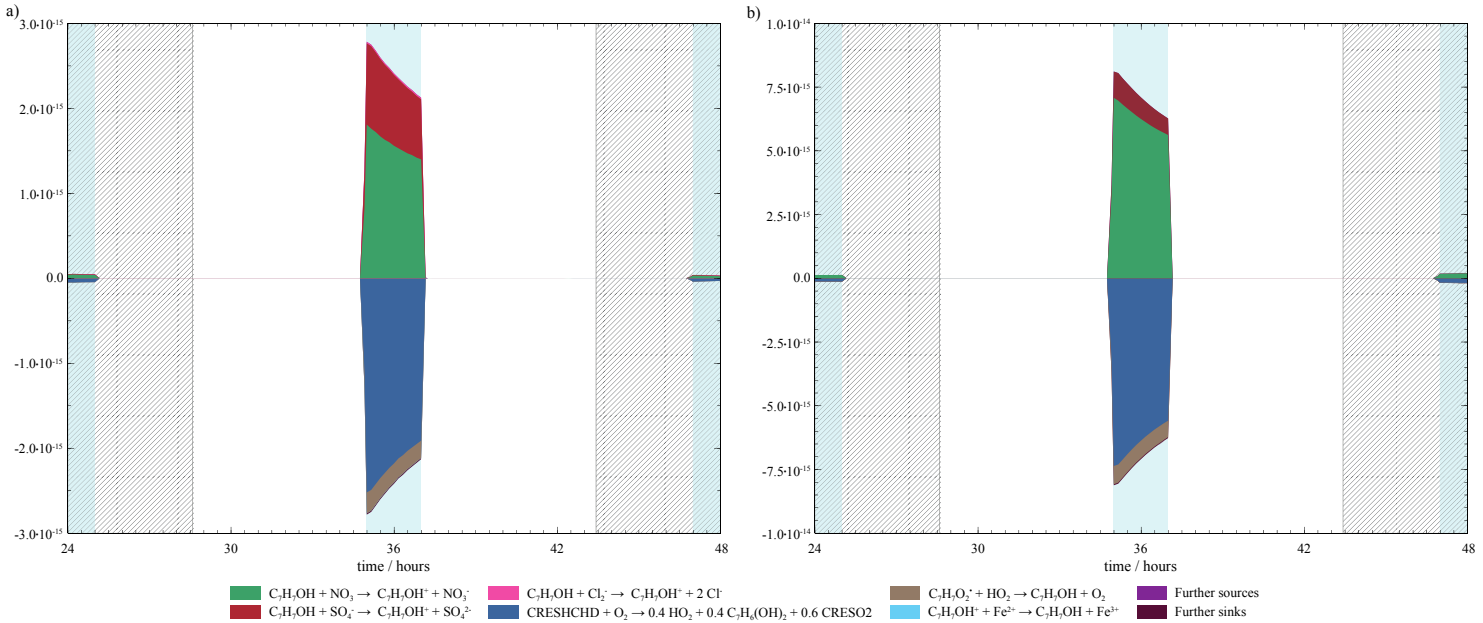

Figure S3 Modelled time-resolved sink and source fluxes of the 'moderately polluted' (a) and the 'strongly polluted' (b) environmental scenario at summer conditions. Positive Fluxes describe formation and negative fluxes contribute to the degradation of CRESHCHD, the radical cation, and the phenoxyl radical in the aqueous phase. The sink and source fluxes are given for the second model day. Grey shaded bars denote the night periods and light blue bars the cloud periods.

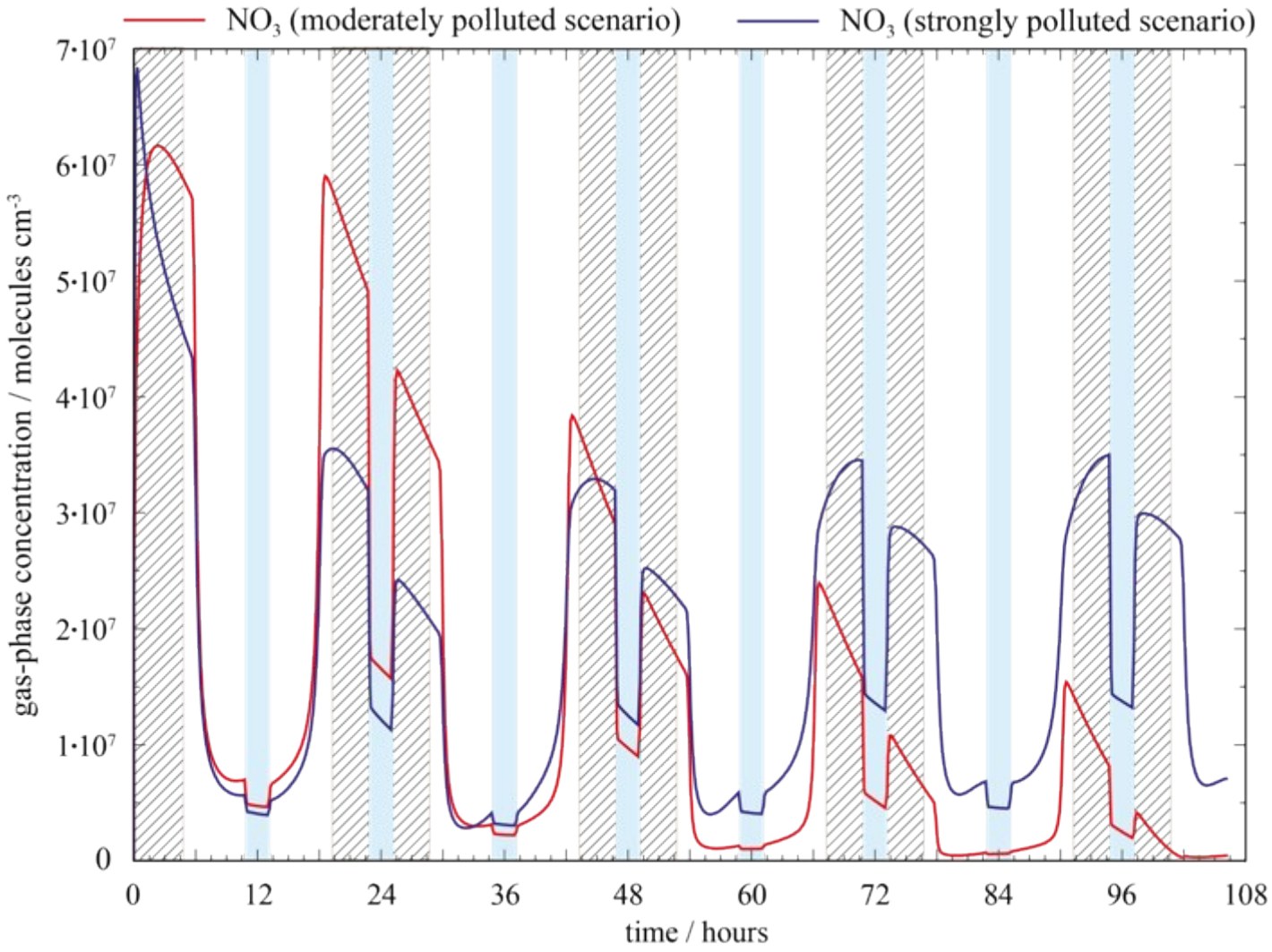

Figure S4 Gas-phase concentration time profile of the NO_3 radical over the whole simulation time under summer conditions for both urban environments.

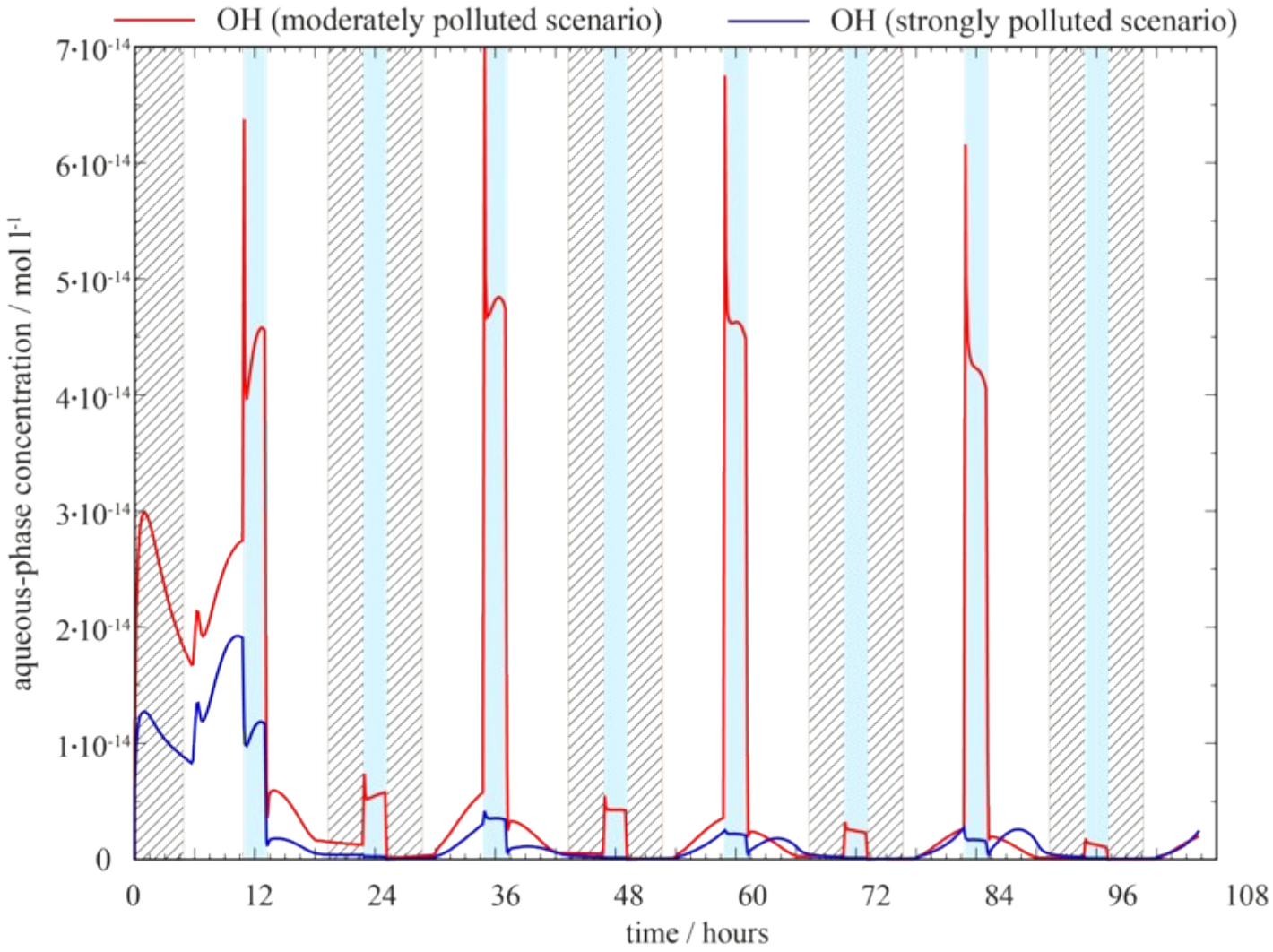

Figure S5 Aqueous-phase concentration time profile of the OH radical over the whole simulation time under summer conditions for both urban environments.

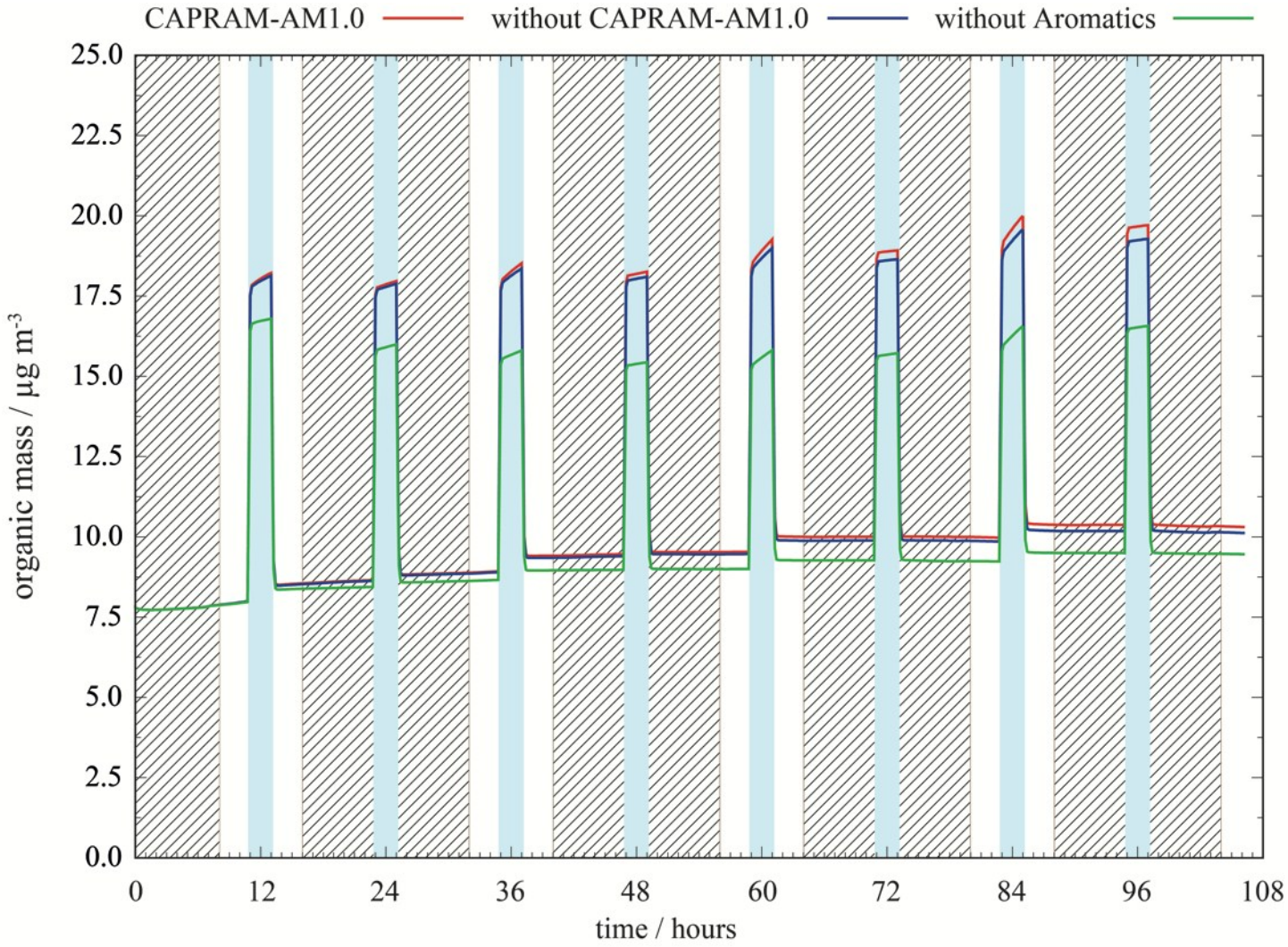

Figure S6 Evolution of organic mass in the aqueous phase in the 'moderately polluted' urban environment at wintertime over the whole simulation time in µg m^{-3}.

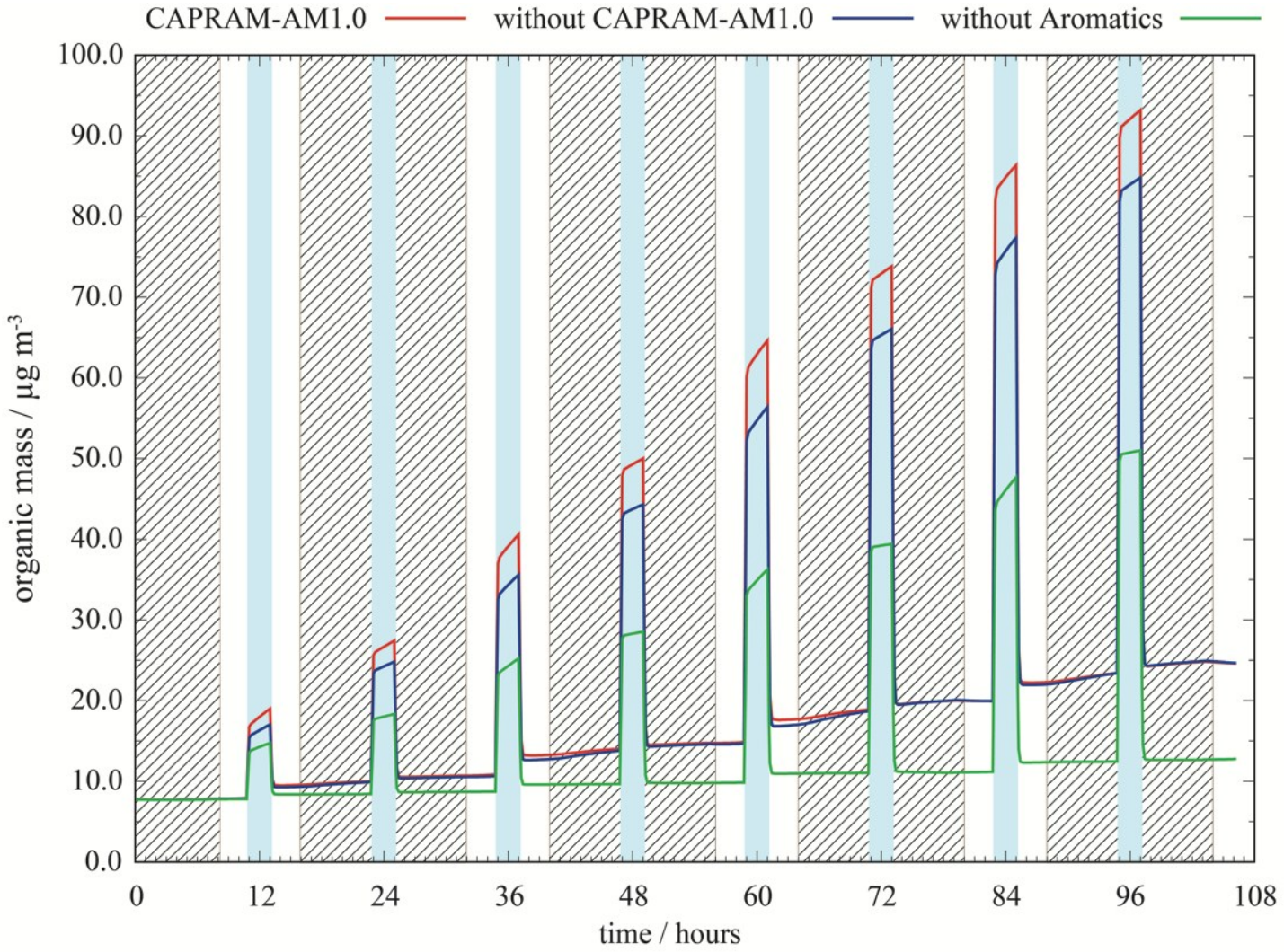

Figure S7 Evolution of organic mass in the aqueous phase in the 'strongly polluted' urban environment at wintertime over the whole simulation time in µg m^{-3}.

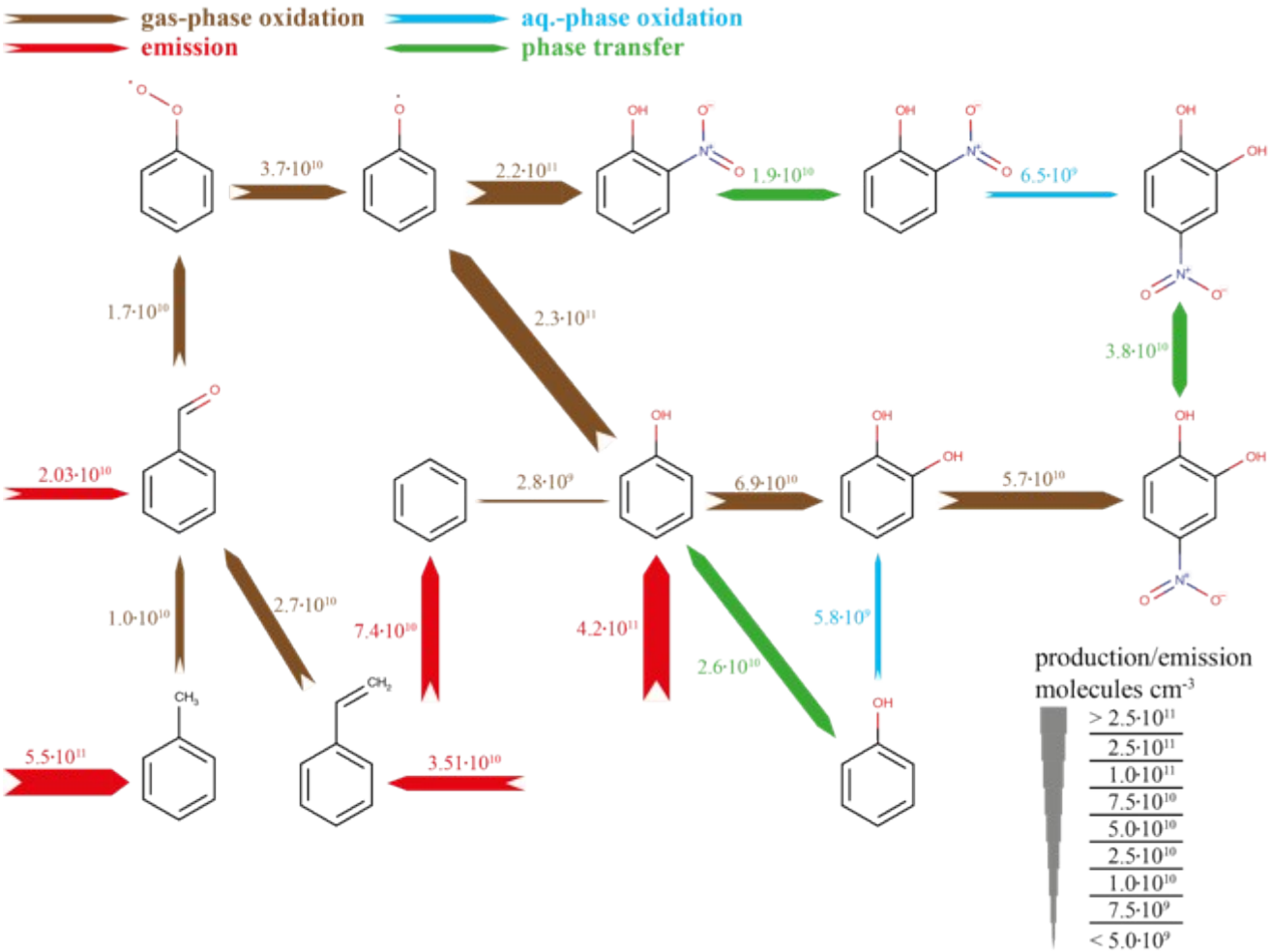

Figure S8 Depiction of multiphase source and sink fluxes (in 10^{11} molecules cm^{-3} s^{-1}) leading to the formation of nitrocatechol over the full simulation time of the moderately polluted urban environment. Only oxidation fluxes exceeding 5% of the total flux are included. The width of arrows indicates the magnitude of the mass flux. Red arrows represent emission fluxes, brown arrows represent gas-phase oxidation, blue arrows aqueous-phase oxidation, and green arrows corresponding phase transfer processes.

References

1. V. Feigenbrugel, S. Le Calvé, P. Mirabel and F. Louis, *Atmospheric Environment*, 2004, 38, 5577-5588.
2. M. R. Heal, M. J. Pilling, P. E. Titcombe and B. J. Whitaker, *Geophys Res Lett*, 1995, 22, 3043-3046.
3. E. N. Fuller, Schettle.Pd and J. C. Giddings, *Ind. Eng. Chem.*, 1966, 58, 19-27.
4. R. Sander, *Atmospheric Chemistry and Physics*, 2015, 15, 4399-4981.
5. N. Lahoutifard, M. Ammann, L. Gutzwiller, B. Ervens and C. George, *Atmospheric Chemistry and Physics*, 2002, 2, 215-226.
6. J. Altschuh, R. Bruggemann, H. Santl, G. Eichinger and O. G. Piringer, *Chemosphere*, 1999, 39, 1871-1887.
7. L. Allou, L. El Maimouni and S. Le Calvé, *Atmospheric Environment*, 2011, 45, 2991-2998.
8. H. X. Li, D. Ellis and D. Mackay, *J Chem Eng Data*, 2007, 52, 1580-1584.
9. X. X. Guo and P. Brimblecombe, *Chemosphere*, 2007, 68, 436-444.
10. G. Leyssens, F. Louis and J. P. Sawerysyn, *J Phys Chem A*, 2005, 109, 1864-1872.
11. J. Tremp, P. Mattrel, S. Fingler and W. Giger, *Water Air Soil Poll*, 1993, 68, 113-123.
12. W. T. Dixon and D. Murphy, *J Chem Soc Perk T 2*, 1975, DOI: DOI 10.1039/p29750000850, 850-853.
13. K. Sehested and J. Holcman, *J Phys Chem-Us*, 1978, 82, 651-653.
14. K. Sehested, J. Holcman and E. J. Hart, *J Phys Chem-Us*, 1977, 81, 1363-1367.
15. R. M. Milburn, *J Am Chem Soc*, 1955, 77, 2064-2067.
16. K. Nakamura, T. Tsuchida, Yamagish.A and M. Fujimoto, *B Chem Soc Jpn*, 1973, 46, 456-459.
17. E. Mentasti and E. Pelizzetti, *J Chem Soc Dalton*, 1973, DOI: DOI 10.1039/dt9730002605, 2605-2608.
18. S. C. Choure, M. M. M. Bamatraf, B. S. M. Rao, R. Das, H. Mohan and J. P. Mittal, *J Phys Chem A*, 1997, 101, 9837-9845.
19. S. Steenken and R. Ramaraj, *J Chem Soc Perk T 2*, 2001, DOI: DOI 10.1039/b102515p, 1613-1619.
20. P. Greenzaid, *J Org Chem*, 1973, 38, 3164-3167.
21. C. K. Remucal and D. Manley, *Environ Sci-Wat Res*, 2016, 2, 565-579.
22. M. V. Park, *J Chem Soc A*, 1966, DOI: DOI 10.1039/j19660000816, 816-&.
23. A. Avdeef, S. R. Sofen, T. L. Bregante and K. N. Raymond, *J Am Chem Soc*, 1978, 100, 5362-5370.
24. J. H. Xu and R. B. Jordan, *Inorg Chem*, 1988, 27, 1502-1507.
25. P. Dwibedy, G. R. Dey, D. B. Naik, K. Kishore and P. N. Moorthy, *Physical Chemistry Chemical Physics*, 1999, 1, 1915-1918.
26. M. J. Hynes and M. O Coinceanainn, *J Inorg Biochem*, 2001, 85, 131-142.
27. L. Valgimigli, R. Amorati, M. G. Fumo, G. A. DiLabio, G. F. Pedulli, K. U. Ingold and D. A. Pratt, *J Org Chem*, 2008, 73, 1830-1841.
28. M. Deborde and U. von Gunten, *Water Research*, 2008, 42, 13-51.
29. N. V. Raghavan and S. Steenken, *J Am Chem Soc*, 1980, 102, 3495-3499.
30. J. Bonin, I. Janik, D. Janik and D. M. Bartels, *J Phys Chem A*, 2007, 111, 1869-1878.

31. T. Umschlag, R. Zellner and H. Herrmann, *Physical Chemistry Chemical Physics*, 2002, 4, 2975-2982.
32. J. Ziajka and W. Pasiuk-Bronikowska, *Atmospheric Environment*, 2005, 39, 1431-1438.
33. Z. B. Alfassi, S. Mosseri and P. Neta, *J Phys Chem-Us*, 1989, 93, 1380-1385.
34. D. Vione, V. Maurino, C. Minero, P. Calza and E. Pelizzetti, *Env. Sci. Tech.*, 2005, 39, 5066-5075.
35. Z. B. Alfassi, R. E. Huie, P. Neta and L. C. T. Shoute, *J Phys Chem-Us*, 1990, 94, 8800-8805.
36. S. N. Chen and M. Z. Hoffman, *Radiat Res*, 1973, 56, 40-47.
37. D. Vione, S. Belmondo and L. Carnino, *Environ Chem Lett*, 2004, 2, 135-139.
38. M. R. Heal, M. A. J. Harrison and J. N. Cape, *Atmospheric Environment*, 2007, 41, 3515-3520.
39. E. Mvula and C. von Sonntag, *Org Biomol Chem*, 2003, 1, 1749-1756.
40. J. Hoigne and H. Bader, *Water Research*, 1983, 17, 173-183.
41. H. Gallard and U. Von Gunten, *Env. Sci. Tech.*, 2002, 36, 884-890.
42. H. Gallard, F. Pellizzari, J. P. Croue and B. Legube, *Water Research*, 2003, 37, 2883-2892.
43. C. Walling, D. M. Camaioni and S. S. Kim, *J Am Chem Soc*, 1978, 100, 4814-4818.
44. D. O. Martire, J. A. Rosso, S. Bertolotti, G. C. Le Roux, A. M. Braun and M. C. Gonzalez, *J Phys Chem A*, 2001, 105, 5385-5392.
45. P. Calza, V. Maurino, C. Minero, E. Pelizzetti, M. Sega and A. Vincenti, *J Photoch Photobio A*, 2005, 170, 61-67.
46. D. Vione, B. Sur, B. K. Dutta, V. Maurino and C. Minero, *J Photoch Photobio A*, 2011, 224, 68-70.
47. A. Alif, J. F. Pilichowski and P. Boule, *J Photoch Photobio A*, 1991, 59, 209-219.
48. P. Barzaghi and H. Herrmann, *Physical Chemistry Chemical Physics*, 2002, 4, 3669-3675.
49. E. Mvula, M. N. Schuchmann and C. von Sonntag, *J Chem Soc Perk T 2*, 2001, DOI: DOI 10.1039/b008434o, 264-268.
50. D. I. Metelitsa, *Russian Chemical Reviews*, 1971, 40, 563-580.
51. A. Mantaka, D. G. Marketos and G. Stein, *J Phys Chem-Us*, 1971, 75, 3886-&.
52. C. K. Scheck and F. H. Frimmel, *Water Research*, 1995, 29, 2346-2352.
53. J. D. Smith, H. Kinney and C. Anastasio, *Physical Chemistry Chemical Physics*, 2015, 17, 10227-10237.
54. P. Barzaghi and H. Herrmann, *Physical Chemistry Chemical Physics*, 2004, 6, 5379.
55. H. Herrmann, D. Hoffmann, T. Schaefer, P. Brauer and A. Tilgner, *Chemphyschem*, 2010, 11, 3796-3822.
56. B. H. J. Bielski, D. E. Cabelli, R. L. Arudi and A. B. Ross, *Journal of Physical and Chemical Reference Data*, 1985, 14, 1041-1100.
57. L. Khalafi and M. Rafiee, *Journal of Hazardous Materials*, 2010, 174, 801-806.
58. T. Arakaki, K. Saito, K. Okada, H. Nakajima and Y. Hitomi, *Chemosphere*, 2010, 78, 1023-1027.
59. M. A. Oturan, J. Peiroten, P. Chartrin and A. J. Acher, *Env. Sci. Tech.*, 2000, 34, 3474-3479.
60. A. D. Nadezhdin and H. B. Dunford, *Can J Chem*, 1979, 57, 3017-3022.
61. P. S. Rao and E. Hayon, *J Phys Chem-Us*, 1975, 79, 397-402.
62. M. N. Schuchmann, E. Bothe, J. von Sonntag and C. von Sonntag, *J Chem Soc Perk T 2*, 1998, DOI: DOI 10.1039/a708772a, 791-796.

63. J. Criquet and N. K. V. Leitner, *Radiation Physics and Chemistry*, 2015, 106, 307-314.
64. P. Neta and J. Grodkowski, *Journal of Physical and Chemical Reference Data*, 2005, 34, 109-199.
65. G. E. Adams and B. D. Michael, *T Faraday Soc*, 1967, 63, 1171-&.
66. H. Gallard and U. von Gunten, *Water Research*, 2002, 36, 65-74.
67. S. Echigo and R. A. Minear, *Water Sci Technol*, 2006, 53, 235-243.
68. J. L. Acero, P. Piriou and U. von Gunten, *Water Research*, 2005, 39, 2979-2993.
69. T. Q. Zhang, L. Cheng, L. Ma, F. C. Meng, R. G. Arnold and A. E. Saez, *Chemosphere*, 2016, 161, 349-357.
70. G. V. Buxton, C. L. Greenstock, W. P. Helman and A. B. Ross, *Journal of Physical and Chemical Reference Data*, 1988, 17, 513-886.
71. H. Herrmann, Essen, 1997.
72. Z. B. Alfassi, R. E. Huie and P. Neta, *J Phys Chem-Us*, 1986, 90, 4156-4158.
73. A. Kroflic, M. Grilc and I. Grgic, *Env. Sci. Tech.*, 2015, 49, 9150-9158.
74. Y. Zheng and C. H. Kuo, *Chem Eng Commun*, 1996, 145, 33-51.
75. G. Merga, H. P. Schuchmann, B. S. M. Rao and C. vonSonntag, *J Chem Soc Perk T 2*, 1996, DOI: DOI 10.1039/p29960001097, 1097-1103.
76. X. W. Fang, X. M. Pan, A. J. Rahmann, H. P. Schuchmann and C. Vonsonntag, *Chem-Eur J*, 1995, 1, 423-429.
77. A. Tilgner and H. Herrmann, *Atmospheric Environment*, 2010, 44, 5415-5422.
78. P. Bräuer, Leipzig, 2015.
79. M. Gohn and N. Getoff, *J Chem Soc Farad T 1*, 1977, 73, 1207-1215.
80. K. Eiben, Schultef.D, C. Suarez and H. Zorn, *Int J Radiat Phys Ch*, 1971, 3, 409-&.
81. B. Cercek and M. Ebert, *Adv Chem Ser*, 1968, 210-+.
82. D. Hoffmann, PhD, Leipzig, 2007.
83. M. B. Heeb, J. Criquet, S. G. Zimmermann-Steffens and U. von Gunten, *Water Research*, 2014, 48, 15-42.
84. K. Tanaka, W. Luesaiwong and T. Hisanaga, *J Mol Catal a-Chem*, 1997, 122, 67-74.
85. D. Vione, V. Maurino, C. Minero, M. Duncianu, R. I. Olariu, C. Arsene, M. Sarakha and G. Mailhot, *Atmospheric Environment*, 2009, 43, 2321-2327.
86. C. Weller, D. Hoffmann, T. Schaefer and H. Herrmann, *Z Phys Chem*, 2010, 224, 1261-1287.
87. A. Albinet, C. Minero and D. Vione, *Chemosphere*, 2010, 80, 753-758.
88. B. Rindone, J. Hjorth, M. Pilling, H. Herrmann, W. Behnke and C. Zetzsch, *Uptake and nitration of aromatics in the tropospheric aqueous phase (UNARO)*, Universita' di Milano, 1999.
89. A. Walter, Diploma, Leipzig, 2000.
90. C. vonSonntag, P. Dowideit, X. W. Fang, R. Mertens, X. M. Pan, M. N. Schuchmann and H. P. Schuchmann, *Water Sci Technol*, 1997, 35, 9-15.
91. O. Ito, S. Akiho and M. Iino, *B Chem Soc Jpn*, 1989, 62, 1606-1611.

92. S. B. Dhiman and D. B. Naik, *J Phys Org Chem*, 2010, 23, 48-55.
93. S. B. Sharma, M. Mudaliar, B. S. M. Rao, H. Mohan and J. P. Mittal, *J Phys Chem A*, 1997, 101, 8402-8408.
94. S. Geeta, S. B. Sharma, B. S. M. Rao, H. Mohan, S. Dhanya and J. P. Mittal, *J Photoch Photobio A*, 2001, 140, 99-107.
95. Y. W. Deng, K. Zhang, H. Chen, T. X. Wu, M. Krzyaniak, A. Wellons, D. Bolla, K. Douglas and Y. G. Zuo, *Atmospheric Environment*, 2006, 40, 3665-3676.
96. P. Neta, V. Madhavan, H. Zemel and R. W. Fessenden, *J Am Chem Soc*, 1977, 99, 163-164.
97. K. Hasegawa and P. Neta, *J Phys Chem-Us*, 1978, 82, 854-857.
98. G. W. Klein, K. Bhatia, V. Madhavan and R. H. Schuler, *J Phys Chem-Us*, 1975, 79, 1767-1774.
99. X. Huang, X. Li, B. Pan, H. Li, Y. Zhang and B. Xie, *Water Res*, 2015, 73, 9-16.
100. D. B. Patil, G. J. Thakur and P. M. Shende, *Asian J Chem*, 2010, 22, 5072-5076.
101. F. J. Benitez, J. Beltran-Heredia, J. A. Peres and J. R. Dominguez, *Journal of Hazardous Materials*, 2000, 73, 161-178.
102. P. S. M. Santos, M. R. M. Domingues and A. C. Duarte, *Chemosphere*, 2016, 154, 599-603.
103. K. Kishore and T. Mukherjee, *Radiation Physics and Chemistry*, 2006, 75, 14-19.
104. C. K. Duesteberg and T. D. Waite, *Env. Sci. Tech.*, 2007, 41, 4103-4110.
105. P. Caregnato, P. M. D. Gara, G. N. Bosio, M. C. Gonzalez, N. Russo, M. D. C. Michelini and D. O. Martire, *J Phys Chem A*, 2008, 112, 1188-1194.
106. F. J. Beltrán, O. Gimeno, F. J. Rivas and M. Carbajo, *Journal of Chemical Technology & Biotechnology*, 2006, 81, 1787-1796.
107. F. J. Beltran, J. F. Garcia-Araya, F. J. Rivas, P. Alvarez and E. Rodriguez, *Ozone-Sci Eng*, 2000, 22, 167-183.
108. E. Mousset, L. Frunzo, G. Esposito, E. D. van Hullebusch, N. Oturan and M. A. Oturan, *Appl Catal B-Environ*, 2016, 180, 189-198.
109. D. Minakata, K. Li, P. Westerhoff and J. Crittenden, *Env. Sci. Tech.*, 2009, 43, 6220-6227.
110. A. Leitzke and C. v. Sonntag, *Ozone: Science & Engineering*, 2009, 31, 301-308.
111. H. Herrmann, T. Schaefer, A. Tilgner, S. A. Styler, C. Weller, M. Teich and T. Otto, *Chem Rev*, 2015, 115, 4259-4334.
112. B. Ervens, C. George, J. E. Williams, G. V. Buxton, G. A. Salmon, M. Bydder, F. Wilkinson, F. Dentener, P. Mirabel, R. Wolke and H. Herrmann, *J Geophys Res-Atmos*, 2003, 108.
113. P. Middleton, W. R. Stockwell and W. P. L. Carter, *Atmos Environ a-Gen*, 1990, 24, 1107-1133.
114. A. McCulloch, M. L. Aucott, T. E. Graedel, G. Kleiman, P. M. Midgley and Y. F. Li, *J Geophys Res-Atmos*, 1999, 104, 8417-8427.
115. Y. Yokouchi, F. Hasebe, M. Fujiwara, H. Takashima, M. Shiotani, N. Nishi, Y. Kanaya, S. Hashimoto, P. Fraser, D. Toom-Sauntry, H. Mukai and Y. Nojiri, *J Geophys Res-Atmos*, 2005, 110.
116. D. Stone, L. K. Whalley and D. E. Heard, *Chem Soc Rev*, 2012, 41, 6348-6404.