**Phase transfer data of CAPRAM-AM1.0.**

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

**Aqueous-phase equilibriums of CAPRAM-AM1.0.**

| | Reaction | K | Ref. | $k_{f,298}$ | $k_{b,298}$ | Ref. |
|---|---|---|---|---|---|---|
| E1 | $C_6H_5OH \rightleftharpoons C_6H_5O^-$ | $1.0 \cdot 10^{-10}$ | [5] | $5.0 \cdot 10^{0}$ | $5.0 \cdot 10^{10}$ | est. |
| E2 | $C_6H_5OH^+ \rightleftharpoons C_6H_5O + H^+$ | $1.0 \cdot 10^{+2}$ | [12] | $5.0 \cdot 10^{12}$ | $5.0 \cdot 10^{10}$ | est. |
| E3 | $C_6H_5OH^+ + H_2O \rightleftharpoons PHENHCHD + H^+$ | $4.0 \cdot 10^{-2}$ | lower limit [13] | $2.0 \cdot 10^{7}$ | $5.0 \cdot 10^{8}$ | [14] |
| E4 | $Fe^{3+} + C_6H_5OH \rightleftharpoons FeC_6H_5O^{2+} + H^+$ | $1.67 \cdot 10^{-2}$ | [15] | $1.00 \cdot 10^{0}$ | $1.67 \cdot 10^{2}$ | [16] |
| E5 | $FeOH^{2+} + 1,2\text{-}C_6H_4(OH)_2 \rightleftharpoons FeC_6H_4O_2^+ + H^+$ | $4.35 \cdot 10^{-2}$ | [17] | $3.1 \cdot 10^{3}$ | $7.13 \cdot 10^{4}$ | |
| E6 | $C_7H_7OH \rightleftharpoons C_7H_7O^-$ | $7.4 \cdot 10^{-11}$ | [5] | $3.7 \cdot 10^{0}$ | $5.0 \cdot 10^{10}$ | est. |
| E7 | $C_7H_7OH^+ \rightleftharpoons C_7H_7O + H^+$ | $6.31 \cdot 10^{+1}$ | [12] | $2.0 \cdot 10^{5}$ | $3.17 \cdot 10^{3}$ | [18] |
| E8 | $C_7H_7OH^+ + H_2O \rightleftharpoons CRESCHD + H^+$ | $4.0 \cdot 10^{-2}$ | lower limit [13] | $2.0 \cdot 10^{7}$ | $5.0 \cdot 10^{8}$ | [14] |
| E9 | $C_6H_5CH_2OH^+ + H_2O \rightleftharpoons ALKHCHD + H^+$ | $2.40 \cdot 10^{-3}$ | est. [19] | $1.20 \cdot 10^{6}$ | $5.0 \cdot 10^{8}$ | [14] |
| E10 | $C_6H_5CH(OH)_2^+ + H_2O \rightleftharpoons ALDHCHD + H^+$ | $2.40 \cdot 10^{-3}$ | est. [19] | $1.20 \cdot 10^{6}$ | $5.0 \cdot 10^{8}$ | [14] |
| E11 | $C_6H_5CHO + H_2O \rightleftharpoons C_6H_5CH(OH)_2$ | $1.1 \cdot 10^{-2}$ | [20] | $5.5 \cdot 10^{8}$ | $5.0 \cdot 10^{10}$ | est. |
| E12 | $HOC_6H_4CHO + H_2O \rightleftharpoons HOC_6H_4CH(OH)_2$ | $1.1 \cdot 10^{-2}$ | est. | $5.5 \cdot 10^{8}$ | $5.0 \cdot 10^{10}$ | est. |
| E13 | $(HO)_2C_6H_3CHO + H_2O \rightleftharpoons (HO)_2C_6H_3CH(OH)_2$ | $1.1 \cdot 10^{-2}$ | est. | $5.5 \cdot 10^{8}$ | $5.0 \cdot 10^{10}$ | est. |
| E14 | $C_6H_5CO_2H \rightleftharpoons C_6H_5CO_2^-$ | $6.3 \cdot 10^{-5}$ | [21] | $3.2 \cdot 10^{6}$ | $5.0 \cdot 10^{10}$ | est. |
| E15 | $HOC_6H_4CO_2H \rightleftharpoons HOC_6H_4CO_2^-$ | $1.51 \cdot 10^{-3}$ | [22] | $7.57 \cdot 10^{7}$ | $5.0 \cdot 10^{10}$ | est. |
| E16 | $HOC_6H_4CO_2^- + Fe^{3+} \rightleftharpoons FeHOC_6H_4CO_2^{2+}$ | $2.51 \cdot 10^{4}$ | [22] | $1.26 \cdot 10^{15}$ | $5.0 \cdot 10^{10}$ | est. |
| E17 | $(HO)_2C_6H_3CO_2H \rightleftharpoons (HO)_2C_6H_3CO_2^-$ | $2.00 \cdot 10^{-3}$ | est. 2,3-dihydroxybenzoic acid, [23] | $1.00 \cdot 10^{8}$ | $5.0 \cdot 10^{10}$ | est. |
| E18 | $(HO)_2C_6H_3CO_2H + Fe^{3+} \rightleftharpoons (O)Fe(CO_2)C_6H_3OH^+ + 2\ H^+$ | $7.00 \cdot 10^{0}$ | [24] | $3.50 \cdot 10^{11}$ | $5.0 \cdot 10^{10}$ | est. |
| E19 | $(HO)_2C_6H_3CO_2^- + Fe^{3+} + H^+ \rightleftharpoons (O)Fe(CO_2)C_6H_3OH^+ + 2\ H^+$ | $3.50 \cdot 10^{3}$ | [24] | $1.75 \cdot 10^{14}$ | $5.0 \cdot 10^{10}$ | est. |
| E20 | $(O)Fe(CO_2)C_6H_3OH^+ \rightleftharpoons Fe^+(O)_2C_6H_3CO_2^- + H^+$ | $1.00 \cdot 10^{-6}$ | [24] | $5.00 \cdot 10^{4}$ | $5.0 \cdot 10^{10}$ | est. |
| E21 | $(HO)_3C_6H_2CO_2H \rightleftharpoons (HO)_3C_6H_2CO_2^-$ | $3.98 \cdot 10^{-5}$ | est. gallic acid, [25] | $1.99 \cdot 10^{6}$ | $5.0 \cdot 10^{10}$ | est. |
| E22 | $(HO)_3C_6H_2CO_2H + FeOH^{2+} \rightleftharpoons Fe(O)_2(HO)C_6H_2CO_2H^+ + H^+$ | $1.42 \cdot 10^{2}$ | [26] | $2.83 \cdot 10^{3}$ | $2.0 \cdot 10^{1}$ | |
| E23 | $2\text{-}HOC_6H_4O + O_2 \rightleftharpoons 1,2\text{-}C_6H_4O_2 + HO_2$ | $1.60 \cdot 10^{-2}$ | [27] | $1.6 \cdot 10^{6}$ | $1.0 \cdot 10^{8}$ | |
| E24 | $4\text{-}HOC_6H_4O + O_2 \rightleftharpoons 1,4\text{-}C_6H_4O_2 + HO_2$ | $1.60 \cdot 10^{-2}$ | [27] | $1.6 \cdot 10^{6}$ | $1.0 \cdot 10^{8}$ | |
| E25 | $2,4\text{-}C_6H_4N_2O_5 \rightleftharpoons 2,4\text{-}C_6H_3N_2O_5^- + H^+$ | $8.13 \cdot 10^{-5}$ | cal. | $4.06 \cdot 10^{6}$ | $5.0 \cdot 10^{10}$ | est. |
| E26 | $2,4\text{-}C_7H_6N_2O_5 \rightleftharpoons 2,4\text{-}C_6H_5N_2O_5^- + H^+$ | $3.55 \cdot 10^{-5}$ | cal. | $1.77 \cdot 10^{6}$ | $5.0 \cdot 10^{10}$ | est. |

| | Reaction | K | Ref. | $k_{f,298}$ | $k_{b,298}$ | Ref. |
|---|---|---|---|---|---|---|
| E27 | $4\text{-}C_6H_5NO_4 \rightleftharpoons 4\text{-}C_6H_4NO_4^- + H^+$ | $1.35 \cdot 10^{-7}$ | cal. | $6.74 \cdot 10^{3}$ | $5.0 \cdot 10^{10}$ | est. |
| E28 | $4\text{-}C_7H_7NO_4 \rightleftharpoons 4\text{-}C_7H_6NO_4^- + H^+$ | $1.38 \cdot 10^{-7}$ | cal. | $6.90 \cdot 10^{3}$ | $5.0 \cdot 10^{10}$ | est. |
| E29 | $2\text{-}C_6H_4ClOH \rightleftharpoons 2\text{-}C_6H_4ClO^-$ | $2.75 \cdot 10^{-9}$ | [28] | $1.38 \cdot 10^{2}$ | $5.0 \cdot 10^{10}$ | est. |
| E30 | $4\text{-}C_6H_4ClOH \rightleftharpoons 4\text{-}C_6H_4ClO^-$ | $3.72 \cdot 10^{-10}$ | [28] | $1.86 \cdot 10^{1}$ | $5.0 \cdot 10^{10}$ | est. |
| E31 | $2,4\text{-}C_6H_3Cl_2OH \rightleftharpoons 2,4\text{-}C_6H_3Cl_2O^-$ | $1.41 \cdot 10^{-8}$ | [28] | $7.05 \cdot 10^{2}$ | $5.0 \cdot 10^{10}$ | est. |
| E32 | $2,6\text{-}C_6H_3Cl_2OH \rightleftharpoons 2,6\text{-}C_6H_3Cl_2O^-$ | $1.07 \cdot 10^{-7}$ | [28] | $5.35 \cdot 10^{3}$ | $5.0 \cdot 10^{10}$ | est. |
| E33 | $2,4,6\text{-}C_6H_2Cl_3OH \rightleftharpoons 2,4,6\text{-}C_6H_2Cl_3O^-$ | $7.10 \cdot 10^{-7}$ | [28] | $3.55 \cdot 10^{4}$ | $5.0 \cdot 10^{10}$ | est. |
| E34 | $2\text{-}C_6H_4BrOH \rightleftharpoons 2\text{-}C_6H_4BrO^-$ | $3.55 \cdot 10^{-9}$ | [28] | $1.78 \cdot 10^{2}$ | $5.0 \cdot 10^{10}$ | est. |
| E35 | $4\text{-}C_6H_4BrOH \rightleftharpoons 4\text{-}C_6H_4BrO^-$ | $6.76 \cdot 10^{-10}$ | [28] | $3.38 \cdot 10^{1}$ | $5.0 \cdot 10^{10}$ | est. |
| E36 | $2,4\text{-}C_6H_3Br_2OH \rightleftharpoons 2,4\text{-}C_6H_3Br_2O^-$ | $1.41 \cdot 10^{-8}$ | [28] | $7.05 \cdot 10^{2}$ | $5.0 \cdot 10^{10}$ | est. |
| E37 | $2,6\text{-}C_6H_3Br_2OH \rightleftharpoons 2,6\text{-}C_6H_3Br_2O^-$ | $1.07 \cdot 10^{-7}$ | [28] | $5.35 \cdot 10^{3}$ | $5.0 \cdot 10^{10}$ | est. |
| E38 | $2,4,6\text{-}C_6H_2Br_3OH \rightleftharpoons 2,4,6\text{-}C_6H_2Br_3O^-$ | $7.10 \cdot 10^{-7}$ | [28] | $3.55 \cdot 10^{4}$ | $5.0 \cdot 10^{10}$ | est. |
| E39 | $2\text{-}ClC_6H_4CO_2H \rightleftharpoons 2\text{-}ClC_6H_5CO_2^-$ | $1.29 \cdot 10^{-3}$ | cal. | $6.44 \cdot 10^{7}$ | $5.0 \cdot 10^{10}$ | est. |
| E40 | $HOC_6H_3BrCO_2H \rightleftharpoons HOC_6H_3BrCO_2^-$ | $2.24 \cdot 10^{-3}$ | cal. | $1.12 \cdot 10^{8}$ | $5.0 \cdot 10^{10}$ | est. |

**Aqueous-phase reactions of CAPRAM-AM1.0.**

| | Reaction | $k_{298}$ | $-E_A/R$ | Comment | Reference |
|---|---|---|---|---|---|
| A1 | $C_6H_5OH + OH \rightarrow 0.92\ PHENHCHD + 0.08\ C_6H_5O$ | $8.41 \cdot 10^9$ | | [29] | [30] |
| A2 | $C_6H_5OH + NO_3 \rightarrow C_6H_5OH^+ + NO_3^-$ | $1.90 \cdot 10^9$ | -2100 | ETR | [31] |
| A3 | $C_6H_5OH + SO_4^- \rightarrow C_6H_5OH^+ + SO_4^{2-}$ | $8.80 \cdot 10^9$ | | ETR | [32] |
| A4 | $C_6H_5OH + Cl \rightarrow C_6H_5OH^+ + Cl^-$ | $2.50 \cdot 10^{10}$ | | ETR | [33] |
| A5 | $C_6H_5OH + Cl_2^- \rightarrow C_6H_5OH^+ + 2\ Cl^-$ | $3.20 \cdot 10^8$ | -878 | ETR after [34] | [35] |
| A6 | $C_6H_5OH + Br_2^- \rightarrow C_6H_5OH^+ + 2\ Br^-$ | $6.10 \cdot 10^6$ | -2080 | ETR | [35] |
| A7 | $C_6H_5OH + CO_3^- \rightarrow C_6H_5OH^+ + CO_3^{2-}$ | $2.20 \cdot 10^7$ | | ETR | [36] |
| A8 | $C_6H_5OH + NO_2 \rightarrow C_6H_5OH^+ + NO_2^-$ | $7.90 \cdot 10^2$ | | ETR | [37] |
| A9 | $C_6H_5O^- + NO_2 \rightarrow C_6H_5O + NO_2^-$ | $1.50 \cdot 10^7$ | -4126 | ETR | [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 | [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 [39] | [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 [39] | [40] |
| A13 | $HOCl + C_6H_5OH \rightarrow$ $0.8\ 2\text{-}C_6H_4ClOH + 0.2\ 4\text{-}C_6H_4ClOH + H_2O$ | $3.60 \cdot 10^{-1}$ | | | [41] |
| A14 | $HOCl + C_6H_5OH + H^+ \rightarrow$ $0.8\ 2\text{-}C_6H_4ClOH + 0.2\ 4\text{-}C_6H_4ClOH + H_2O + H^+$ | $3.52 \cdot 10^4$ | | | [41] |
| A15 | $HOCl + C_6H_5O^- \rightarrow$ $0.8\ 2\text{-}C_6H_4ClO^- + 0.2\ 4\text{-}C_6H_4ClO^- + H_2O$ | $2.19 \cdot 10^4$ | | | [41] |
| A16 | $HOBr + C_6H_5OH \rightarrow$ $0.67\ 2\text{-}C_6H_4BrOH + 0.33\ 4\text{-}C_6H_4BrOH + H_2O$ | $5.00 \cdot 10^2$ | | | [42] |
| A17 | $HOBr + C_6H_5O^- \rightarrow$ | $1.80 \cdot 10^8$ | | | [42] |

| | Reaction | $k_{298}$ | $-E_A/R$ | Comment | Reference |
|---|---|---|---|---|---|
| | 0.67 2-$C_6H_4BrO^-$ + 0.33 4-$C_6H_4BrO^-$ + $H_2O$ | | | | |
| A18 | $C_6H_5OH + HONO \rightarrow 4\text{-}C_6H_5NO_2 + H_2O$ | $9.20 \cdot 10^{-3}$ | | | [37] |
| A19 | $4\text{-}C_6H_5NO_2 \rightarrow 4\text{-}C_6H_5NO_3$ | $3.00 \cdot 10^{-5}$ | | | [37] |
| A20 | $C_6H_5OH^+ + Fe^{2+} \rightarrow C_6H_5OH + Fe^{3+}$ | $6.00 \cdot 10^{8}$ | | est. same as for Anisole | [43] |
| A21 | $C_6H_5O + HO_2 \rightarrow C_6H_5OH + O_2$ | $2.00 \cdot 10^{9}$ | | | [34] |
| A22 | $C_6H_5O + O_2^- \rightarrow 1,4\text{-}C_6H_4O_2 - H^+ - H_2O$ | $1.00 \cdot 10^{9}$ | | | [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 | [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 | [45] |
| A25 | $C_6H_5O + NO_2 \rightarrow 0.67\ 2\text{-}C_6H_5NO_3 + 0.33\ 4\text{-}C_6H_5NO_3$ | $3.00 \cdot 10^{9}$ | | | [46] |
| A26 | $C_6H_5O + C_6H_5O \rightarrow C_{12}H_{10}O_2$ | $2.45 \cdot 10^{9}$ | | | [39] |
| A27 | $2\text{-}C_6H_5NO_3 + h\nu \rightarrow C_6H_4(OH)_2 + HONO - H_2O$ | $1.896 \cdot 10^{-06}$ | $\cos(\chi)^{0.670}\exp(-0.081/\cos(\chi))$ | | [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 [48] | [49] |
| A29 | PHENHCHD + $Fe^{3+} \rightarrow$ 0.5 1,2-$C_6H_4(OH)_2$ + 0.5 1,4-$C_6H_4(OH)_2$ + $Fe^{2+}$ + $H^+$ | $7.00 \cdot 10^{3}$ | | | [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, [51] | [49] |
| A31 | $PHENHCHD + NO_2 \rightarrow 0.5\ 2\text{-}C_6H_5NO_3 + 0.5\ 4\text{-}C_6H_5NO_3$ | $8.20 \cdot 10^{9}$ | | | [48] |
| A32 | $1,2\text{-}C_6H_4(OH)_2 + OH \rightarrow 1,2\text{-}C_6H_4O_2 + HO_2 - O_2 + H_2O$ | $4.70 \cdot 10^{9}$ | | [52] | mean from [53] |
| A33 | $1,2\text{-}C_6H_4(OH)_2 + NO_3 \rightarrow 2\text{-}HOC_6H_4O + NO_3^- + H^+$ | $5.20 \cdot 10^{8}$ | -4691 | H-abstraction | [54] |
| A34 | $1,2\text{-}C_6H_4(OH)_2 + SO_4^- \rightarrow 2\text{-}HOC_6H_4O + SO_4^{2-} + H^+$ | $5.20 \cdot 10^{8}$ | -4691 | H-abstraction | est. after [55] |
| A35 | $1,2\text{-}C_6H_4(OH)_2 + HO_2 \rightarrow 2\text{-}HOC_6H_4O + H_2O_2$ | $4.70 \cdot 10^{4}$ | | H-abstraction | [56] |
| A36 | $1,2\text{-}C_6H_4(OH)_2 + O_2^- \rightarrow 2\text{-}HOC_6H_4O + H_2O_2 - H^+$ | $2.70 \cdot 10^{5}$ | | H-abstraction | [56] |
| A37 | $1,2\text{-}C_6H_4(OH)_2 + O_3 \rightarrow C_6H_6O_4 + H_2O_2 - H_2O$ | $5.20 \cdot 10^{5}$ | | est. | [39] |
| A38 | $1,2\text{-}C_6H_4(OH)_2 + 2\ HONO \rightarrow 1,2\text{-}C_6H_4O_2 + 2\ NO + 2\ H_2O$ | $4.51 \cdot 10^{0}$ | | | [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. $Fe(OH)_2^{2+}$ [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. $Fe(OH)_2^+$ [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 [52] | [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 | [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 [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 | [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 | [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. | [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 [52] | [62] |
| A48 | $1,2\text{-}C_6H_4O_2 + NO_2^- \rightarrow NO_2C_6H_3(OH)_2 + OH^- - H_2O$ | $1.16 \cdot 10^{1}$ | | | [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 [52] | [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 [55] |
| A51 | $1,4\text{-}C_6H_4O_2 + SO_4^- \rightarrow C_4H_4O_4 + C_2H_2O_2 + HO_2 + SO_4^{2-} + H^+ - 2\ O_2$ | $1.00 \cdot 10^{8}$ | | | [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 $4\text{-}HOC_6H_4O$ | [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 $4\text{-}HOC_6H_4O$ | [64] |
| A54 | $2\ 2\text{-}HOC_6H_4O \rightarrow 1,2\text{-}C_6H_4(OH)_2 + 1,2\text{-}C_6H_4O_2$ | $1.09 \cdot 10^{9}$ | | | [65] |
| A55 | $4\text{-}HOC_6H_4O + Fe^{2+} + H^+ \rightarrow 1,4\text{-}C_6H_4(OH)_2 + Fe^{3+}$ | $1.50 \cdot 10^{5}$ | | | [64] |
| A56 | $4\text{-}HOC_6H_4O + Fe^{3+} \rightarrow 1,4\text{-}C_6H_4O_2 + Fe^{2+} + H^+$ | $7.00 \cdot 10^{5}$ | | | [64] |
| A57 | $2\ 4\text{-}HOC_6H_4O \rightarrow 1,4\text{-}C_6H_4(OH)_2 + 1,4\text{-}C_6H_4O_2$ | $1.09 \cdot 10^{9}$ | | | [65] |
| A58 | $HOCl + 2\text{-}C_6H_4ClO^- \rightarrow 0.7\ 2,6\text{-}C_6H_3Cl_2O^- + 0.3\ 2,4\text{-}C_6H_3Cl_2O^- + H_2O$ | $2.42 \cdot 10^{3}$ | | | [66] |
| A59 | $HOCl + 4\text{-}C_6H_4ClOH \rightarrow 2,4\text{-}C_6H_3Cl_2OH + H_2O$ | $2.00 \cdot 10^{-2}$ | | | [66] |
| A60 | $HOCl + 4\text{-}C_6H_4ClO^- \rightarrow 2,4\text{-}C_6H_3Cl_2O^- + H_2O$ | $2.67 \cdot 10^{3}$ | | | [66] |
| A61 | $HOCl + 2,6\text{-}C_6H_3Cl_2O^- \rightarrow 2,4,6\text{-}C_6H_2Cl_3O^- + H_2O$ | $1.94 \cdot 10^{2}$ | | | [66] |
| A62 | $HOCl + 2,4\text{-}C_6H_3Cl_2O^- \rightarrow 2,4,6\text{-}C_6H_2Cl_3O^- + H_2O$ | $3.03 \cdot 10^{2}$ | | | [66] |
| A63 | $HOBr + 2\text{-}C_6H_4BrO^- \rightarrow$ | $6.40 \cdot 10^{6}$ | | | [67] |

| | Reaction | $k_{298}$ | $-E_A/R$ | Comment | Reference |
|---|---|---|---|---|---|
| | 0.7 2,6-$C_6H_3Br_2O^-$ + 0.3 2,4-$C_6H_3Br_2O^-$ + $H_2O$ | | | | |
| A64 | HOBr + 4-$C_6H_4BrO^-$ → 2,4-$C_6H_3Br_2O^-$ + $H_2O$ | $4.80 \cdot 10^6$ | | | [67] |
| A65 | HOBr + 2,6-$C_6H_3Br_2OH$ → 2,4,6-$C_6H_2Br_3OH$ + $H_2O$ | $1.70 \cdot 10^4$ | | | [68] |
| A66 | HOBr + 2,6-$C_6H_3Br_2O^-$ → 2,4,6-$C_6H_2Br_3O^-$ + $H_2O$ | $4.80 \cdot 10^5$ | | | [68] |
| A67 | HOBr + 2,4-$C_6H_3Br_2OH$ → 2,4,6-$C_6H_2Br_3OH$ + $H_2O$ | $1.20 \cdot 10^4$ | | | [68] |
| A68 | HOBr + 2,4-$C_6H_3Br_2O^-$ → 2,4,6-$C_6H_2Br_3O^-$ + $H_2O$ | $8.90 \cdot 10^5$ | | | [68] |
| A69 | $C_7H_7OH$ + OH → $C_7H_6(OH)_2$ | $1.10 \cdot 10^{10}$ | | product [69] | [70] |
| A70 | $C_7H_7OH$ + $NO_3$ → $C_7H_7OH^+$ + $NO_3^-$ | $1.10 \cdot 10^9$ | | | [31] |
| A71 | $C_7H_7OH$ + $SO_4^-$ → $C_7H_7OH^+$ + $SO_4^{2-}$ | $3.40 \cdot 10^9$ | | | [18] |
| A72 | $C_7H_7OH$ + $Cl_2^-$ → $C_7H_7OH^+$ + 2 $Cl^-$ | $4.30 \cdot 10^7$ | | | [71] |
| A73 | $C_7H_7OH$ + $Br_2^-$ → $C_7H_7OH^+$ + 2 $Br^-$ | $4.30 \cdot 10^6$ | | | est. one order of magnitude lower as $Cl_2^-$ |
| A74 | $C_7H_7O^-$ + $NO_2$ → $C_7H_7O$ + $NO_2^-$ | $3.40 \cdot 10^7$ | | | [72] |
| A75 | $C_7H_7OH$ + $NO_2^+$ → 2-$C_7H_7NO_3$ + $H^+$ | $4.07 \cdot 10^5$ | | est. same as for guaiacol | [73] |
| A76 | $C_7H_7OH$ + $O_3$ → $C_7H_6(OH)_2$ + $O_2$ | $5.48 \cdot 10^4$ | -5300 | | [74] |
| A77 | $C_7H_7OH$ + HONO → 2-$C_7H_7NO_2$ | $9.20 \cdot 10^{-3}$ | | est. same as for phenol | [37] |
| A78 | 2-$C_7H_7NO_2$ → 2-$C_7H_7NO_3$ | $3.00 \cdot 10^{-5}$ | | est. same as for nitrosophenol | [37] |
| A79 | $C_7H_7OH^+$ + $Fe^{2+}$ → $C_7H_7OH$ + $Fe^{3+}$ | $6.00 \cdot 10^8$ | | est. same as for Anisole | [43] |
| A80 | CRESCHD + $O_2$ → 0.4 $C_7H_6(OH)_2$ + 0.4 $HO_2$ + 0.6 CRESO2 | $2.00 \cdot 10^6$ | | yields from calculations in [75] | PSSA [76] |
| A81 | CRESCHD + $Fe^{3+}$ → $C_7H_6(OH)_2$ + $Fe^{2+}$ + $H^+$ | $7.00 \cdot 10^3$ | | est. like PHENHCHD | [50] |
| A82 | CRESCHD + $NO_2$ → 2-$C_7H_7NO_3$ | $8.20 \cdot 10^9$ | | est. same as for PHENHCHD | [48] |
| A83 | 2 CRESCHD → $C_7H_6(OH)_2$ + $C_7H_7OH$ | $1.00 \cdot 10^8$ | | as HCHD, [51] | [49] |
| A84 | 2 CRESO2 → 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 | [77] |
| A85 | CRESO2 → | $2.00 \cdot 10^2$ | | $HO_2$ elimination | [78] |

| | Reaction | $k_{298}$ | $-E_A/R$ | Comment | Reference |
|---|---|---|---|---|---|
| | 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 $HO_2$ | | | | |
| A86 | $C_7H_7O + HO_2 \rightarrow C_7H_7OH$ | $2.0 \cdot 10^9$ | | | [34] |
| A87 | $C_7H_7O + O_2^- \rightarrow C_7H_6O_2 - H^+ - H_2O$ | $1.00 \cdot 10^9$ | | | [39] |
| A88 | $C_7H_7O + NO_2 \rightarrow 2\text{-}C_7H_7NO_3$ | $3.00 \cdot 10^9$ | | est. same as for $C_6H_5O$ | [46] |
| A89 | $C_7H_7O + C_7H_7O \rightarrow C_{14}H_{12}O_2$ | $2.45 \cdot 10^9$ | | | [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 [69] | [79] |
| A91 | $C_7H_6O_2 + OH \rightarrow C_7H_8O_4 + HO_2 - O_2 - H_2O$ | $2.00 \cdot 10^{10}$ | | | [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 [80] | [81] |
| A93 | $4\text{-}C_6H_5NO_3 + NO_3 \rightarrow$ NIPHENHCHD + $NO_3^-$ + $H^+$ | $7.70 \cdot 10^8$ | | | [82] |
| A94 | $4\text{-}C_6H_5NO_3 + SO_4^- \rightarrow$ NIPHENHCHD + $SO_4^{2-}$ + $H^+$ | $7.70 \cdot 10^8$ | | | est. after [55] |
| A95 | $4\text{-}C_6H_5NO_3 + HOBr \rightarrow C_6H_4NO_3Br + H_2O$ | $9.20 \cdot 10^3$ | | | [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 [84] | [85] |
| A97 | $2\text{-}C_6H_5NO_3 + NO_3 \rightarrow$ NIPHENHCHD + $H^+$ + $NO_3^-$ | $8.30 \cdot 10^8$ | | | [86] |
| A98 | $2\text{-}C_6H_5NO_3 + SO_4^- \rightarrow$ NIPHENHCHD + $SO_4^{2-}$ + $H^+$ | $8.30 \cdot 10^8$ | | | est. after [55] |
| A99 | $4\text{-}C_6H_5NO_4 + OH \rightarrow$ NICATHCHD | $1.00 \cdot 10^{10}$ | | | [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 [84] | [87] |
| A101 | $2,4\text{-}C_6H_4N_2O_5 + h\nu \rightarrow 4\text{-}C_6H_5NO_4$ + HONO | $1.675 \cdot 10^{-06}\cos(\chi)^{0.846}\exp(-0.096/\cos(\chi))$ | | | [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 [84] | [87] |
| A103 | $2,4\text{-}C_6H_3N_2O_5^- + h\nu \rightarrow 4\text{-}C_6H_4NO_4^-$ + HONO | $1.0 \cdot 10^{-05}\cos(\chi)^{0.546}\exp(-0.117/\cos(\chi))$ | | | [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 | [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 | [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 [55] |
| A107 | $2\text{-}C_7H_7NO_3 + Cl_2^- \rightarrow$ NICRESHCHD + $H^+$ + 2 $Cl^-$ | $1.50 \cdot 10^8$ | | | [89] |

| | Reaction | $k_{298}$ | $-E_A/R$ | Comment | Reference |
|---|---|---|---|---|---|
| A108 | 2-$C_7H_7NO_3$ + h$\nu$ → $C_7H_6(OH)_2$ + 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 [90] | PSSA [76] |
| A110 | NIPHENHCHD + $Fe^{3+}$ → 4-$C_6H_5NO_4$ + $Fe^{2+}$ + $H^+$ | $7.00 \cdot 10^{3}$ | | | [50] |
| A111 | NIPHENHCHD + $NO_2$ → 2,4-$C_6H_4N_2O_5$ | $1.00 \cdot 10^{7}$ | | | est. according to [85] |
| A112 | 2 NIPHENHCHD → 4-$C_6H_5NO_4$ + 4-$C_6H_5NO_3$ | $5.00 \cdot 10^{8}$ | | as HCHD, [51] | [50] |
| A113 | NICATHCHD + $O_2$ → NICATO2 | $2.00 \cdot 10^{6}$ | | | PSSA [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 | [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. | [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 [76] |
| A117 | NICRESHCHD + $Fe^{3+}$ → 2-$C_7H_7NO_4$ + $Fe^{2+}$ + $H^+$ | $7.00 \cdot 10^{3}$ | | | [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, [51] | [49] |
| A120 | 2,4-$C_7H_6N_2O_5$ + h$\nu$ → 2-$C_7H_7NO_4$ + HONO | $1.675 \cdot 10^{-06}\cos(\chi)^{0.846}\exp(-0.096/\cos(\chi))$ | | | est. |
| A121 | 2,4-$C_7H_5N_2O_5^-$ + h$\nu$ → 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. | [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. | [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 $H_2O$ | $6.40 \cdot 10^{9}$ | | | [19] |
| A125 | $C_6H_5CH_2OH$ + $NO_3$ → $C_6H_5CHOH$ + $NO_3^-$ + $H^+$ | $4.50 \cdot 10^{8}$ | | | [91] |
| A126 | $C_6H_5CH_2OH$ + $SO_4^-$→ $C_6H_5CH_2OH^+$ + $SO_4^{2-}$ | $3.20 \cdot 10^{9}$ | | | [19] |
| A127 | ALKHCHD + $O_2$ → 0.4 $HOC_6H_4CH_2OH$ + 0.4 $HO_2$ + 0.6 ALKHCHDOX | $2.00 \cdot 10^{6}$ | | [19], [51] | PSSA [76] |
| A128 | ALKHCHD + $Fe^{3+}$ → $HOC_6H_5CH_2OH$ + $Fe^{2+}$ + $H^+$ | $7.00 \cdot 10^{3}$ | | [19] | [50] |
| A129 | 2 ALKHCHD → $C_6H_5CH_2OH$ + $HOC_6H_4CH_2OH$ | $1.00 \cdot 10^{8}$ | | as HCHD, [51] | [49] |

| | Reaction | $k_{298}$ | $-E_A/R$ | Comment | Reference |
|---|---|---|---|---|---|
| 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 | [78] |
| A131 | $C_6H_5CH_2OH^+ \rightarrow C_6H_5CHOH + H^+$ | $5.00 \cdot 10^7$ | | lower limit | [19] |
| A132 | $C_6H_5CHOH + O_2 \rightarrow C_6H_5CHO + HO_2$ | $2.00 \cdot 10^9$ | | CAPRAM Standard | [78] |
| A133 | $HOC_6H_4CH_2OH + OH \rightarrow$ 0.14 $HOC_6H_4CHOH$ + 0.14 $H_2O$ + 0.86 ALKOHHCHD | $5.27 \cdot 10^9$ | | | [92] |
| A134 | $HOC_6H_4CH_2OH + Cl_2^- \rightarrow$ ALKOHHCHD + 2 $Cl^-$ + $H^+$ | $2.80 \cdot 10^8$ | | products est. | [92] |
| A135 | $HOC_6H_4CHOH + O_2 \rightarrow HOC_6H_4CHO + HO_2$ | $2.00 \cdot 10^9$ | | CAPRAM Standard | [78] |
| A136 | ALKOHHCHD + $O_2$ → 0.4 $(HO)_2C_6H_3CH_2OH$ + 0.4 $HO_2$ + 0.6 ALKOHHCHDOX | $2.00 \cdot 10^6$ | | [19], [51] | PSSA [76] |
| A137 | ALKOHHCHD + $Fe^{3+}$ → 0.4 $(HO)_2C_6H_4CH_2OH$ + $Fe^{2+}$ + $H^+$ | $7.00 \cdot 10^3$ | | [19] | [50] |
| A138 | 2 ALKOHHCHD → $C_6H_5CH_2OH$ + $(HO)_2C_6H_4CH_2OH$ | $1.00 \cdot 10^8$ | | as HCHD, [51] | [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 | [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 | [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 | [78] |
| A143 | $C_6H_5CHO + OH \rightarrow$ 0.75 ALDHCHD + 0.25 $C_6H_5O_2$ + 0.25 $H_2O$ + 0.25 CO | $2.60 \cdot 10^9$ | | yields [93] | [70] |
| A144 | $C_6H_5CH(OH)_2 + OH \rightarrow C_6H_5C(OH)_2 + H_2O$ | $2.60 \cdot 10^9$ | | yields [93] | [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 [93] | est. after [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 [93] | [93] |
| A147 | ALDHCHD + $O_2$ → 0.4 $HOC_6H_4CHO$ + 0.4 $HO_2$ + 0.6 ALDHCHDOX | $2.00 \cdot 10^6$ | | yields [93] | PSSA [76] |

| | Reaction | $k_{298}$ | $-E_A/R$ | Comment | Reference |
|---|---|---|---|---|---|
| A148 | ALDHCHD + $Fe^{3+}$ → $HOC_6H_4CHO$ + $Fe^{2+}$ + $H^+$ | $7.00 \cdot 10^3$ | | yields [93] | [50] |
| A149 | 2 ALDHCHD → $C_6H_5CHO$ + $HOC_6H_4CHO$ | $1.00 \cdot 10^8$ | | [51] | [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 | [78] |
| A151 | $C_6H_5CH(OH)_2^+$ → $C_6H_5CH(OH)_2$ + $H^+$ | $5.00 \cdot 10^7$ | | est. $C_6H_5CH_2OH^+$ | [19] |
| A152 | $C_6H_5C(OH)_2$ + $O_2$ → $C_6H_5CO_2H$ + $HO_2$ | $2.00 \cdot 10^9$ | | CAPRAM Standard | [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 | [94] |
| A154 | $HOC_6H_4CH(OH)_2$ + OH → $HOC_6H_4CH(OH)_2$ | $1.21 \cdot 10^{10}$ | | est. p-hydroxybenzaldehyde | [94] |
| A155 | $HOC_6H_4CHO$ + $NO_3$ → $HOC_6H_4CHO^+$ + $NO_3^-$ | $5.90 \cdot 10^9$ | | est. p-hydroxybenzaldehyde | est. after [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 [55] |
| A157 | $HOC_6H_4CHO$ + $SO_4^-$ → $HOC_6H_4CHO^+$ + $SO_4^{2-}$ | $5.90 \cdot 10^9$ | | est. p-hydroxybenzaldehyde | [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 | [94] |
| A159 | $HOC_6H_4CHO^+$ → $HOC_6H_4O_2$ + CO + $H^+$ | $5.00 \cdot 10^7$ | | est. $C_6H_5CH_2OH^+$ | [19] |
| A160 | $HOC_6H_4CH(OH)_2^+$ → $HOC_6H_4CH(OH)_2$ + $H^+$ | $5.00 \cdot 10^7$ | | est. $C_6H_5CH_2OH^+$ | [19] |
| A161 | $HOC_6H_4CH(OH)_2$ + $O_2$ → $HOC_6H_4CO_2H$ + $HO_2$ | $2.00 \cdot 10^9$ | | CAPRAM Standard | [78] |
| A162 | ALDOHHCHD + $O_2$ → 0.4 $(HO)_2C_6H_3CHO$ + 0.4 $HO_2$ + 0.6 ALDOHHCHDOX | $2.00 \cdot 10^6$ | | [94] | PSSA [76] |
| A163 | ALDOHHCHD + $Fe^{3+}$ → $(HO)_2C_6H_4CHO$ + $Fe^{2+}$ + $H^+$ | $7.00 \cdot 10^3$ | | [93] | [50] |
| A164 | 2 ALDOHHCHD → $HOC_6H_5CHO$ + $(HO)_2C_6H_4CHO$ | $1.00 \cdot 10^8$ | | [51] | [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 | [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 | [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 | [78] |
| A169 | $C_6H_5CO_2H$ + OH → ACIDHCHD | $1.80 \cdot 10^9$ | | | [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 | | [31] |
| A171 | $C_6H_5CO_2H + SO_4^- \rightarrow$ ACIDHCHD + $H^+ + SO_4^{2-}$ - $H_2O$ | $6.50 \cdot 10^7$ | -1300 | | est. after [55] |
| A172 | $C_6H_5CO_2H + Cl \rightarrow$ ACIDCLCHD | $1.80 \cdot 10^{10}$ | | | [44] |
| A173 | $C_6H_5CO_2H + Cl_2^- \rightarrow$ ACIDCLCHD + $Cl^-$ | $2.00 \cdot 10^5$ | | | [44] |
| A174 | $C_6H_5CO_2^- + OH \rightarrow$ 0.93 $ACIDHCHD^-$ + 0.07 $C_6H_5O_2$ + 0.07 $CO_2$ + 0.07 $OH^-$ | $5.90 \cdot 10^9$ | | [95] | [70] |
| A175 | $C_6H_5CO_2^- + NO_3 \rightarrow C_6H_5O_2 + NO_3^-$ | $1.20 \cdot 10^9$ | | ETR assumed | est. after [55] |
| A176 | $C_6H_5CO_2^- + SO_4^- \rightarrow C_6H_5O_2 + SO_4^{2-}$ | $1.20 \cdot 10^9$ | | ETR assumed | [96] |
| A177 | $C_6H_5CO_2^- + Cl_2^- \rightarrow C_6H_5O_2$ + 2 $Cl^-$ | $2.00 \cdot 10^6$ | | ETR assumed | [97] |
| A178 | ACIDHCHD + $O_2 \rightarrow HOC_6H_4CO_2H + HO_2$ | $2.00 \cdot 10^6$ | | [98], [75] | PSSA [76] |
| A179 | ACIDHCHD + $Fe^{3+} \rightarrow$ 0.93 $HOC_6H_4CO_2H$ + 0.07 $C_6H_5OH$ + 0.07 $CO_2$ + 0.07 $H_2O$ + $Fe^{2+}$ + $H^+$ | $7.00 \cdot 10^3$ | | [98] | [50] |
| A180 | 2 ACIDHCHD $\rightarrow C_6H_5CO_2H + HOC_6H_4CO_2H + H_2O$ | $3.95 \cdot 10^8$ | | [98] | [50] |
| A181 | $ACIDHCHD^- + O_2 \rightarrow HOC_6H_4CO_2^- + HO_2$ | $2.00 \cdot 10^6$ | | [98], [75] | PSSA [76] |
| A182 | $ACIDHCHD^- + Fe^{3+} \rightarrow$ 0.93 $HOC_6H_4CO_2^-$ + 0.07 $C_6H_5O^-$ + 0.07 $CO_2$ + 0.07 $H_2O$ + $Fe^{2+}$ + $H^+$ | $7.00 \cdot 10^3$ | | [98] | [50] |
| A183 | 2 $ACIDHCHD^- \rightarrow C_6H_5CO_2^- + HOC_6H_4CO_2^- + H_2O$ | $3.95 \cdot 10^8$ | | [98] | [50] |
| A184 | ACIDCLCHD + $O_2 \rightarrow$ 2-$ClC_6H_4CO_2H + HO_2$ | $2.00 \cdot 10^6$ | | | PSSA [76] |
| A185 | ACIDCLCHD + $Fe^{3+} \rightarrow$ 2-$ClC_6H_4CO_2H + Fe^{2+} + H^+$ | $7.00 \cdot 10^3$ | | | [50] |
| A186 | 2 ACIDCLCHD $\rightarrow C_6H_5CO_2H$ + 2-$ClC_6H_4CO_2H$ + HCl | $1.00 \cdot 10^8$ | | as HCHD, [51] | [49] |
| A187 | 2 $C_6H_5O_2 \rightarrow$ 2 $C_6H_5O + O_2$ | $1.00 \cdot 10^6$ | | | [77] |
| A188 | $HOC_6H_4CO_2H + OH \rightarrow$ SAHCHD | $2.20 \cdot 10^{10}$ | | est. Salicylic acid [99] | [70] |
| A189 | $HOC_6H_4CO_2H + NO_3 \rightarrow$ SAHCHD + $H^+ + NO_3^-$ - $H_2O$ | $1.50 \cdot 10^9$ | | | [86] |
| A190 | $HOC_6H_4CO_2H + SO_4^- \rightarrow$ SAHCHD + $H^+ + SO_4^{2-}$ - $H_2O$ | $1.50 \cdot 10^9$ | | | est. after [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 | [97] |
| A192 | $HOC_6H_4CO_2H + Br_2 \rightarrow HOC_6H_3BrCO_2H + Br^- + H^+$ | $4.42 \cdot 10^9$ | -4030 | est. Salicylic acid | [100] |

| | Reaction | $k_{298}$ | $-E_A/R$ | Comment | Reference |
|---|---|---|---|---|---|
| A193 | $HOC_6H_4CO_2H + O_3 \rightarrow (HO)_2C_6H_3CO_2H + O_2$ | $2.00 \cdot 10^2$ | | est. | [101] |
| A194 | $HOC_6H_4CO_2^- + OH \rightarrow 0.93\ SAHCHD^- + 0.07\ COO^- + 0.07\ 1,4\text{-}C_6H_4(OH)_2$ | $1.60 \cdot 10^{10}$ | | [102] | [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 [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 | [103] |
| A197 | $HOC_6H_4CO_2^- + O_3 \rightarrow (HO)_2C_6H_3CO_2^- + O_2$ | $1.78 \cdot 10^5$ | | est. | [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. $Fe(OH)^{2+}$ [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 [52] | PSSA [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 [52] | [50] |
| A201 | $2\ SAHCHD \rightarrow HOC_6H_4CO_2H + 0.75\ HOC_6H_4O_2 + 0.75\ CO_2 + 0.25\ (HO)_2C_6H_3CO_2H$ | $1.00 \cdot 10^8$ | | [51] | [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 [52] | PSSA [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 [52] | [50] |
| A204 | $2\ SAHCHD^- \rightarrow HOC_6H_4CO_2^- + 0.75\ HOC_6H_4O_2 + 0.75\ CO_2 + 0.25\ (HO)_2C_6H_3CO_2^-$ | $1.00 \cdot 10^8$ | | [51] | [49] |
| A205 | $2\ HOC_6H_4O_2 \rightarrow 2\text{-}HOC_6H_4O + 2\text{-}HOC_6H_4O + O_2$ | $1.00 \cdot 10^6$ | | | [78] |
| A206 | $(HO)_2C_6H_3CO_2H + OH \rightarrow TRIACIDHCHD$ | $8.00 \cdot 10^9$ | | | [104] |
| A207 | $(HO)_2C_6H_3CO_2H + HO_2 \rightarrow TRIACIDHCHD + H_2O_2 - H^+$ | $3.90 \cdot 10^4$ | | est. | [56] |
| A208 | $TRIACIDHCHD + O_2 \rightarrow$ | $2.00 \cdot 10^6$ | | products est. [104] | PSSA [76] |

| | Reaction | $k_{298}$ | $-E_A/R$ | Comment | Reference |
|---|---|---|---|---|---|
| | 0.4 $(HO)_3C_6H_2CO_2H$ + 0.4 $HO_2$ + 0.6 TRIACIDHCHDOX | | | | |
| A209 | TRIACIDHCHD + $Fe^{3+}$ → $(HO)_3C_6H_4CO_2H$ + $Fe^{2+}$ + $H^+$ | $7.00 \cdot 10^3$ | | products est. [104] | [50] |
| A210 | 2 TRIACIDHCHD → $(HO)_2C_6H_4CO_2H$ + $(HO)_3C_6H_4CO_2H$ | $1.00 \cdot 10^8$ | | [51] | [49] |
| A211 | $(HO)_3C_6H_2CO_2H$ + OH → $(HO)_3C_6H_2O_2$ | $6.40 \cdot 10^9$ | | est. [102] | [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 [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 | [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 | [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. [106] | [106] |
| A216 | $(HO)_3C_6H_2CO_2^-$ + OH → $(HO)_3C_6H_2O_2$ + $CO_2$ + $OH^-$ | $1.10 \cdot 10^{10}$ | | ETR assumed | [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 [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 | [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 | [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. [106] | [107] |
| A221 | 2 $(HO)_3C_6H_2O_2$ → $(HO)_3C_6H_2O$ | $1.00 \cdot 10^6$ | | | [78] |
| A222 | 2 $(HO)_3C_6H_2O$ → $(HO)_2C_6H_2(O)_2$ + $C_6H_2(OH)_4$ | $1.09 \cdot 10^9$ | | | [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. [108] | [108] |

**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 |
|---|---|---|---|---|
| $C_5H_6O_3 + OH \rightarrow 0.5\ CH_3C(O)CH(OH)CH(O_2)COOH + 0.5\ CH_3C(O)CH(O_2)CH(OH)COOH$ | $1.16 \cdot 10^{10}$ | | | 109 |
| $C_5H_5O_3^- + OH \rightarrow 0.5\ CH_3C(O)CH(OH)CH(O_2)COO^- + 0.5\ CH_3C(O)CH(O_2)CH(OH)COO^-$ | $4.94 \cdot 10^{10}$ | | | 109 |
| $C_5H_6O_2 + OH \rightarrow 0.5\ CH_3C(O)CH(OH)CH(O_2)CHO + 0.5\ CH_3CH(OH)CH(O_2)C(O)CHO$ | $3.04 \cdot 10^{10}$ | | | 109 |
| $C_5H_8O_3 + OH \rightarrow 0.5\ CH_3CH(OH)CH(OH)CH(O_2)COOH + 0.5\ CH_3CH(OH)CH(O_2)CH(OH)COOH$ | $2.10 \cdot 10^{10}$ | | | 109 |
| $C_5H_7O_3^- + OH \rightarrow 0.5\ CH_3CH(OH)CH(OH)CH(O_2)COO^- + 0.5\ CH_3CH(OH)CH(O_2)CH(OH)COO^-$ | $8.40 \cdot 10^{10}$ | | | 109 |
| $C_6H_4O_6 + OH \rightarrow HOOCC(O)CH(OH)CH(O_2)C(O)COOH$ | $2.96 \cdot 10^{10}$ | | | 109 |
| $C_6H_3O_6^- + OH \rightarrow 0.5\ ^-OOCC(O)CH(OH)CH(O_2)C(O)COOH + 0.5\ HOOCC(O)CH(OH)CH(O_2)C(O)COO^-$ | $2.96 \cdot 10^{10}$ | | | 109 |
| $C_6H_2O_6^{2-} + OH \rightarrow\ ^-OOCC(O)CH(OH)CH(O_2)C(O)COO^-$ | $2.96 \cdot 10^{10}$ | | | 109 |
| $C_5H_4O_5 + OH \rightarrow 0.5\ HOOCC(O)CH(OH)CH(O_2)COOH + 0.5\ HOOCC(O)CH(O_2)CH(OH)COOH$ | $1.15 \cdot 10^{10}$ | | | 109 |
| $C_5H_3O_5^- + OH \rightarrow 0.5\ ^-OOCC(O)CH(OH)CH(O_2)COOH + 0.5\ ^-OOCC(O)CH(O_2)CH(OH)COOH$ | $4.93 \cdot 10^{10}$ | | | 109 |
| $C_5H_2O_5^{2-} + OH \rightarrow 0.5\ ^-OOCC(O)CH(OH)CH(O_2)COO^- + 0.5\ ^-OOCC(O)CH(O_2)CH(OH)COO^-$ | $4.93 \cdot 10^{10}$ | | | 109 |
| $C_5H_6O_4 + OH \rightarrow 0.5\ HOOCCH(OH)CH(O_2)CH(OH)CHO + 0.5\ HOOCCH(O_2)CH(OH)CH(OH)CHO$ | $2.09 \cdot 10^{10}$ | | | 109 |
| $C_5H_5O_4^- + OH \rightarrow 0.5\ ^-OOCCH(OH)CH(O_2)CH(OH)CHO + 0.5\ ^-OOCCH(O_2)CH(OH)CH(OH)CHO$ | $8.83 \cdot 10^{10}$ | | | 109 |

| Reaction | $k_{298}$ | $-E_A/R$ | Comment | Reference |
|---|---|---|---|---|
| $C_5H_8O_4 + OH \rightarrow 0.5$ $HOCH_2CH(OH)CH(OH)CH(O_2)COOH + 0.5$ $HOCH_2CH(OH)CH(O_2)CH(OH)COOH$ | $2.15 \cdot 10^{10}$ | | | [109] |
| $C_5H_7O_4^- + OH \rightarrow HOCH_2CH(OH)CH(OH)CH(O_2)COO^- +$ $0.5\ HOCH_2CH(OH)CH(O_2)CH(OH)COO^-$ | $8.44 \cdot 10^{10}$ | | | [109] |
| $C_6H_6O_4 + OH \rightarrow 0.5\ HOOCCH(OH)CH(O_2)CHCHCOOH$ $+ 0.5\ HOOCCH(O_2)CH(OH)CHCHCOOH$ | $3.85 \cdot 10^{10}$ | | | [109] |
| $C_6H_5O_4^- + OH \rightarrow 0.5\ HOOCCH(OH)CH(O_2)CHCHCOO^- +$ $0.5\ HOOCCH(O_2)CH(OH)CHCHCOO^-$ | $1.01 \cdot 10^{11}$ | | | [109] |
| $C_6H_4O_4^{2-} + OH \rightarrow 0.5\ ^-OOCCH(OH)CH(O_2)CHCHCOO^- +$ $0.5\ ^-OOCCH(O_2)CH(OH)CHCHCOO^-$ | $1.64 \cdot 10^{11}$ | | | [109] |
| $C_7H_8O_4 + OH \rightarrow$ $0.2415\ CH_3C(COOH)=CHCH(OH)CH(O_2)COOH +$ $0.2415\ CH_3C(COOH)=CHCH(O_2)C(O)COOH +$ $0.25825\ CH_3CH(OH)(COOH)CH(O_2)CH=CHCOOH +$ $0.25825\ CH_3CH(O_2)(COOH)CH(OH)CH=CHCOOH$ | $4.02 \cdot 10^{10}$ | | | [109] |
| $C_7H_7O_4^- + OH \rightarrow$ $0.08975\ CH_3C(COOH)=CHCH(OH)CH(O_2)COO^- +$ $0.08975\ CH_3C(COOH)=CHCH(O_2)C(O)COO^- +$ $0.40975\ CH_3CH(OH)(COOH)CH(O_2)CH=CHCOO^- +$ $0.40975\ CH_3CH(O_2)(COOH)CH(OH)CH=CHCOO^-$ | $1.08 \cdot 10^{11}$ | | | [109] |
| $C_7H_6O_4^{2-} + OH \rightarrow$ $0.2415\ CH_3C(COO^-)=CHCH(OH)CH(O_2)COO^- +$ $0.2415\ CH_3C(COO^-)=CHCH(O_2)C(O)COO^- +$ $0.25825\ CH_3CH(OH)(COO^-)CH(O_2)CH=CHCOO^- +$ $0.25825\ CH_3CH(O_2)(COO^-)CH(OH)CH=CHCOO^-$ | $1.71 \cdot 10^{11}$ | | | [109] |
| $C_5H_6O_3 + OH \rightarrow 0.5\ CH_3CH(OH)(COOH)C(O_2)CHO + 0.5$ $CH_3CH(O_2)(COOH)C(OH)CHO$ | $1.34 \cdot 10^{10}$ | | | [109] |

| Reaction | $k_{298}$ | $-E_A/R$ | Comment | Reference |
|---|---|---|---|---|
| $C_5H_5O_3^- + OH \rightarrow 0.5\ CH_3C(OH)(COO^-)CH(O_2)CHO + 0.5\ CH_3C(O_2)(COO^-)CH(OH)CHO$ | $5.38 \cdot 10^{10}$ | | | [109] |
| $C_6H_8O_4 + OH \rightarrow 0.5\ CH_3C(OH)(COOH)CH(O_2)CH(OH)CHO + 0.5\ CH_3C(O_2)(COOH)CH(OH)CH(OH)CHO$ | $2.26 \cdot 10^{10}$ | | | [109] |
| $C_6H_7O_4^- + OH \rightarrow 0.5\ CH_3C(OH)(COO^-)CH(O_2)CH(OH)CHO + 0.5\ CH_3C(O_2)(COO^-)CH(OH)CH(OH)CHO$ | $8.99 \cdot 10^{10}$ | | | [109] |
| $C_6H_6O_6 + OH \rightarrow 0.5\ HOOCC(O)CH(OH)CH(OH)CH(O_2)COOH + 0.5\ HOOCC(O)CH(OH)CH(O_2)CH(OH)COOH$ | $1.95 \cdot 10^{10}$ | | | [109] |
| $C_6H_5O_6^- + OH \rightarrow 0.5\ HOOCC(O)CH(OH)CH(OH)CH(O_2)COO^- + 0.5\ HOOCC(O)CH(OH)CH(O_2)CH(OH)COO^-$ | $1.95 \cdot 10^{11}$ | | | [109] |
| $C_6H_4O_6^{2-} + OH \rightarrow 0.5\ ^-OOCC(O)CH(OH)CH(OH)CH(O_2)COO^- + 0.5\ ^-OOCC(O)CH(OH)CH(O_2)CH(OH)COO^-$ | $8.25 \cdot 10^{10}$ | | | [109] |
| $C_5H_4O_4 + OH \rightarrow 0.5\ HOOCCH(OH)CH(O_2)C(O)CHO + 0.5\ HOOCCH(O_2)CH(OH)C(O)CHO$ | $1.17 \cdot 10^{10}$ | | | [109] |
| $C_5H_3O_4^- + OH \rightarrow 0.5\ ^-OOCCH(OH)CH(O_2)C(O)CHO + 0.5\ ^-OOCCH(O_2)CH(OH)C(O)CHO$ | $4.94 \cdot 10^{10}$ | | | [109] |
| $C_5H_4O_3 + OH \rightarrow 0.5\ OHCC(O)CH(OH)CH(O_2)CHO + 0.5\ OHCC(O)CH(O_2)CH(OH)CHO$ | $3.04 \cdot 10^{10}$ | | | [109] |
| $C_5H_6O_3 + OH \rightarrow 0.5\ HOCH_2C(O)CH(OH)CH(O_2)CHO + 0.5\ HOCH_2C(O)CH(O_2)CH(OH)CHO$ | $3.05 \cdot 10^{10}$ | | | [109] |
| $C_5H_6O_4 + OH \rightarrow 0.5\ HOCH_2C(O)CH(OH)CH(O_2)COOH + 0.5\ HOCH_2C(O)CH(OH)CH(O_2)COOH$ | $1.17 \cdot 10^{10}$ | | | [109] |

| Reaction | $k_{298}$ | $-E_A/R$ | Comment | Reference |
|---|---|---|---|---|
| $C_5H_5O_4^- + OH \rightarrow 0.5\ HOCH_2C(O)CH(OH)CH(O_2)COO^- + 0.5\ HOCH_2C(O)CH(OH)CH(O_2)COO^-$ | $4.95 \cdot 10^{10}$ | | | [109] |
| $C_5H_8O_4 + OH \rightarrow 0.5\ CH_3C(O)CH(OH)CH(OH)CH(O_2)COOH + 0.5\ CH_3C(O)CH(OH)CH(O_2)CH(OH)COOH$ | $1.96 \cdot 10^{10}$ | | | [109] |
| $C_5H_7O_4^- + OH \rightarrow 0.5\ CH_3C(O)CH(OH)CH(OH)CH(O_2)COO^- + 0.5\ CH_3C(O)CH(OH)CH(O_2)CH(OH)COO^-$ | $8.25 \cdot 10^{10}$ | | | [109] |
| $C_5H_6O_6 + OH \rightarrow 0.134\ HOOCC(O)C(OH)(O_2)CH(OH)CHO + 0.426\ HOOCC(O)CH(OH)C(OH)(O_2)CHO + 0.44\ HOOCC(O)CH(OH)CH(OH)C(O)O_2$ | $2.06 \cdot 10^{9}$ | | | [109] |
| $C_5H_5O_6^- + OH \rightarrow 0.134\ ^-OOCC(O)C(OH)(O_2)CH(OH)CHO + 0.426\ ^-OOCC(O)CH(OH)C(OH)(O_2)CHO + 0.44\ ^-OOCC(O)CH(OH)CH(OH)C(O)O_2$ | $2.06 \cdot 10^{9}$ | | | [109] |
| $C_5H_8O_4 + OH \rightarrow 0.138\ CH_3C(O)C(OH)(O_2)CH(OH)CHO + 0.424\ CH_3C(O)C(OH)(OH)CH(O_2)CHO + 0.438\ CH_3C(O)CH(OH)CH(OH)C(O)O_2$ | $2.12 \cdot 10^{9}$ | | | [109] |
| $C_7H_6O_7 + OH \rightarrow 0.5\ HOOCC(OH)(OH)CH(O_2)(COOH)CH=CHCOOH + 0.5\ HOOCC(OH)(O_2)CH(OH)(COOH)CH=CHCOOH$ | $3.85 \cdot 10^{10}$ | | est. muconic acid | |
| $C_7H_5O_7^- + OH \rightarrow 0.5\ ^-OOCC(OH)(OH)CH(O_2)(COOH)CH=CHCOOH + 0.5\ ^-OOCC(OH)(O_2)CH(OH)(COOH)CH=CHCOOH$ | $1.01 \cdot 10^{11}$ | | est. muconic acid | |
| $C_7H_4O_7^{2-} + OH \rightarrow 0.5\ ^-OOCC(OH)(OH)CH(O_2)(COOH)CH=CHCOO^- + 0.5\ ^-OOCC(OH)(O_2)CH(OH)(COOH)CH=CHCOO^-$ | $1.64 \cdot 10^{11}$ | | est. muconic acid | |

| Reaction | $k_{298}$ | $-E_A/R$ | Comment | Reference |
|---|---|---|---|---|
| $C_7H_4O_7^{3-} + OH \rightarrow$ 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 |
| $C_6H_4O_4^{2-} + Cl_2^- \rightarrow C_4H_4O_3 + 2\ Cl^- + HO_2 + CO + CO_2 - 2\ O_2$ | $2.10 \cdot 10^8$ | | products est. | [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 [110] | [106] |
| $C_6H_5O_4^- + O_3 \rightarrow C_4H_4O_3 + C_2HO_3^- + H_2O_2 - H_2O$ | $2.65 \cdot 10^4$ | | | [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 [110] | [106] |
| $C_7H_8O_4 + O_3 \rightarrow 0.5\ C_4H_6O_5 + 0.5\ C_3H_4O_3 + 0.5\ C_4H_4O_3 + 0.5\ C_3H_5O_5 - H_2O$ | $1.60 \cdot 10^4$ | | [110] | est. muconic acid |
| $C_7H_7O_4^- + O_3 \rightarrow 0.5\ C_4H_6O_5 + 0.5\ C_3H_4O_3 + 0.5\ C_4H_4O_3 + 0.5\ C_3H_5O_5 - H_2O$ | $2.65 \cdot 10^4$ | | [110] | est. muconic acid |
| $C_7H_6O_4^{2-} + O_3 \rightarrow 0.5\ C_4H_6O_5 + 0.5\ C_3H_4O_3 + 0.5\ C_4H_4O_3 + 0.5\ C_3H_5O_5 - H_2O$ | $1.40 \cdot 10^5$ | | [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 | [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 | [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 | [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 | [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 | [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 | [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 |

| Reaction | $k_{298}$ | $-E_A/R$ | Comment | Reference |
|---|---|---|---|---|
| $C_7H_4O_7^{2-} + O_3 \rightarrow C_2HO_4^- + C_5H_3O_5^- + H_2O_2$ | $1.40 \cdot 10^5$ | | | est. muconic acid |
| $C_7H_3O_7^{3-} + O_3 \rightarrow C_2HO_4^- + C_5H_2O_5^{2-} + H_2O_2$ | $1.40 \cdot 10^5$ | | | 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 |

| Reaction | $k_{298}$ | $-E_A/R$ | Comment | Reference |
|---|---|---|---|---|
| $C_5H_4O_4 + O_3 \rightarrow 0.5\ C_3H_4O_5 + 0.5\ C_2H_2O_3 + 0.5\ C_2H_4O_5 + 0.5\ C_3H_2O_3$ | $1.40 \cdot 10^3$ | | | est. maleic acid |
| $C_5H_3O_4^- + O_3 \rightarrow 0.5\ C_3H_4O_5 + 0.5\ C_2HO_3^- + 0.5\ C_2H_3O_5^- + 0.5\ C_3H_2O_3$ | $4.20 \cdot 10^3$ | | | 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 |

| Reaction | $k_{298}$ | $-E_A/R$ | Comment | Reference |
|---|---|---|---|---|
| $C_6H_8O_4 + O_3 \rightarrow 0.5\ C_2H_2O_3 + 0.5\ C_4H_8O_5 + 0.5\ C_2H_4O_5 + 0.5\ C_4H_6O_3$ | $1.40 \cdot 10^3$ | | | est. maleic acid |
| $C_6H_7O_4^- + O_3 \rightarrow 0.5\ C_2HO_3^- + 0.5\ C_4H_8O_5 + 0.5\ C_2H_3O_5^- + 0.5\ C_4H_6O_3$ | $4.20 \cdot 10^3$ | | | est. maleic acid |

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