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Supplement of

Acidity and the multiphase chemistry of atmospheric aqueous particles and clouds

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### Supplementary material to section 2

Table S1: Summary of the applied $H_A$ and $pK_a$ values for calculation of the LWC-acidity dependent aqueous fraction $X_{A_{aq}}$ presented in Figure 2, Figure 3 and Figure S1.

| Compound                      | $H_A$ (298K) M atm$^{-1}$ | Reference            | $pK_{a1}$ | $pK_{a2}$ | Reference            |
|-------------------------------|---------------------------|----------------------|-----------|-----------|----------------------|
| Sulfurous acid (dissolved SO$_2$) | 1.32                     | Sander (2015)        | 1.9       | 7.0       | Kolloff and Elving (1959) |
| Nitrous acid HONO            | 48.6                     | Park and Lee (1988)  | 3.29      | —         | Kolloff and Elving (1959) |
| Formic acid HCOOH            | 5530                     | Khan et al. (1992)   | 3.77      | —         | Braude et al. (1955)   |
| Acetic acid CH$_3$COOH       | 5471                     | Khan et al. (1992)   | 4.76      | —         | Haynes (1958)          |
| Glycolic acid CH$_2$OHCOOH   | 2.83·10$^4$              | Ip et al. (2009)     | 3.83      | —         | Zirchrom (2018)        |
| Phthalic acid C$_6$H$_4$(COOH)$_2$ | 4.96·10$^7$        | TOXNET (2015)        | 2.98      | 5.28      | Braude et al. (1955)   |
| 2-nitrophenol C$_6$H$_5$NO$_3$ | 1.47·10$^2$            | Guo and Brimblecombe (2007) | 7.21 | —         | Rappoport (1984)       |
| 2,4-dinitrophenol C$_6$H$_4$N$_2$O$_5$ | 1.11·10$^4$    | Tremp et al. (1993)  | 4.09      | —         | Rappoport (1984)       |
| Ammonia NH$_3$               | 59.8                     | Christie and Crisp (1967) | 9.24 | —         | Bjerrum et al. (1958)  |
| Dimetyhlamine CH$_3$)$_2$NH  | 56.5                     | Burkholder et al. (2015) | 10.4 | —         | Braude et al. (1955)   |
Supplementary material to section 4

Table S2. Rate constants and equilibrium constants for reaction of NO₂ with S(IV).

| T / K | $k_{10a}$ / L mol⁻¹ s⁻¹ | $k_{-10a}$ / s⁻¹ | $K_{10a}$ / L mol⁻¹ | $k_{10b}$ / L mol⁻¹ s⁻¹ | $k_{-10b}$ / s⁻¹ | $K_{10b}$ / L mol⁻¹ |
|-------|-------------------------|-------------------|---------------------|--------------------------|-------------------|----------------------|
| 288   | (1.5 ± 2) × 10⁷         | (8 ± 3) × 10⁵     | 1.9 × 10⁴           | (1⁻¹/₃) × 10⁶            | (1.7 ± 0.2) × 10² | 5.9 × 10³            |
| 298   | (1.2 ± 2) × 10⁷         | (9 ± 2) × 10⁵     | 1.3 × 10⁴           | (1⁻¹/₃) × 10⁶            | (2.3 ± 0.2) × 10² | 4.4 × 10³            |
| 308   | (1.7 ± 2) × 10⁷         | (1.2 ± 0.3) × 10³ | 1.4 × 10⁴           | (2⁻²/₃) × 10⁶            | (3.7 ± 0.3) × 10² | 5.4 × 10³            |
| 318   | (1.4 ± 2) × 10⁷         | (1.6 ± 0.2) × 10³ | 8.8 × 10³           | (4⁻⁴/₄) × 10⁶            | (5.8 ± 0.4) × 10² | 6.9 × 10³            |
| 328   | (1.2 ± 2) × 10⁷         | (2.2 ± 0.2) × 10³ | 5.5 × 10³           | (6⁻⁶/₁₃) × 10⁶           | (7 ± 1) × 10²    | 8.6 × 10³            |

Remarks: Since the measurement error of $k_{10a}$ does not allow to derive an Arrhenius expression, the temperatures were averaged from 288 K to 328 K, with a specified error calculated using the standard deviation. The reported errors of the Arrhenius expressions represent the statistical error using the Student’s t-distribution for a 95% confidence interval. The T-dependence of the equilibrium constant $K_{10b}$ of the NO₂ reaction with HSO₃⁻ was calculated without considering the result at $T = 288$ K.

Figure S1. Comparison of the calculated S(IV) oxidation rates by the NO₂ reaction pathway in mol L⁻¹ s⁻¹ using the different reaction rate constants of Lee and Schwartz (1983), Clifton et al. (1988) and Spindler et al. (2003) for the urban winter haze scenario of Cheng et al. (2016).
Determination of aqueous-phase concentrations of excited triplet states of photosensitizers (PS*)

To calculate initial S(IV) oxidation rates of PS* and compare their potential atmospheric relevance compared to other S(IV) to S(VI) conversion pathways under different environmental and acidity conditions, realistic aqueous-phase concentration levels of PS* were determined by means of multiphase chemistry simulations using the CAPRAM mechanism (Bräuer et al., 2019; Hoffmann et al., 2020; Ye et al., 2021). Simulations with CAPRAM mechanism have been performed for urban winter haze conditions (model period 4 (Dec. 27th-31st) based on (Ye et al., 2021)) as well as the CAPRAM standard summer remote and urban scenarios (Tilgner et al., 2013; Bräuer, 2015; Bräuer et al., 2019). A simple chemical mechanism scheme with 12 reactions was developed and applied in the SPACCIM model (see Fig. S2 below) considering the photochemical formation of the excited triplet states of photosensitizers (PS*) and their main loss processes.

![Chemical pathways of PS* considered in the reaction module.](image)

For the simulations, it was assumed that humic-like substances (HULIS) can act as potential photosensitizers. The initial photochemical formation of excited triplet states of photosensitizers (PS*) was implemented based on the photochemical data of m-methoxybenzaldehyde from recent measurements at TROPOS (Felber et al. (2021), photochemical implementation following the MCM, \( I = 1.72 \cdot 10^{-1} \text{ s}^{-1}, \ M = 0.765, \ N = 0.214 \)). Additionally, subsequent quenching reactions with water \( (k_{1st} = 1 \cdot 10^5 \text{ s}^{-1}) \) (Sharpless, 2012; Erickson et al., 2018; Ossola et al., 2019; Felber et al., 2020)), dissolved oxygen \( (k_{2nd} = 1 \cdot 10^9 \text{ M}^{-1} \text{ s}^{-1}) \) (Zepp et al., 1985; Canonica et al., 1995; Schweitzer and Schmidt, 2003; Montalti et al., 2006; Canonica, 2007; Erickson et al., 2018; Kaur and Anastasio, 2018; Felber et al., 2020) and dissolved organic matter \( (k_{2nd} = 1 \cdot 10^8 \text{ M}^{-1} \text{ s}^{-1}) \) (Canonica, 2007; Wenk et al., 2013; Erickson et al., 2018; Moor et al., 2019)) were included. The applied second-order quenching rate constants represents conservative estimates based on typical values reported in the literature given above. However, it should be noted that literature values especially for the quenching with dissolved organic matter show a huge
variation with typical values between $10^7$ and up to few $10^9$ M$^{-1}$ s$^{-1}$ (see above-mentioned references). Moreover, the simple mechanism scheme does not consider any triplet reactions with inorganics such as halides due to their very compound and triplet specific reactivity (see e.g. (Treinin and Hayon, 1976; Loeff et al., 1992; Loeff et al., 1993; Tinel et al., 2014)). Consequently, the calculated concentrations represent upper limit values for the steady-state concentrations of PS$^*$. Finally, daytime mean concentrations were calculated for urban winter haze, rural aerosol and rural/urban cloud conditions based on the modelled PS$^*$ concentration profiles (see Table 1 in the main manuscript text) and applied for the comparison of the different S(IV) to S(VI) conversion pathways (see Fig 7). The obtained daytime mean concentrations, ranging from about few $10^{-11}$ mol L$^{-1}$ under deliquesced aerosol conditions to $10^{-13} – 10^{-12}$ mol L$^{-1}$ under cloud conditions, are in a reasonable agreement with reported triplet concentrations in aerosols ($2.3 \cdot 10^{-13} – 1.6 \cdot 10^{-10}$ mol L$^{-1}$ estimated by Wang et al. (2020)), in fog samples ($0.07 – 1.5 \cdot 10^{-13}$ (Kaur and Anastasio, 2018)) and in natural surface waters ($10^{-14} – 10^{-13}$ (Zepp et al., 1985; Canonica et al., 1995)).
Supplementary material to section 5

Table S3. Overview of determined hydration equilibrium constants $K_{\text{Hyd.}}$ of aldehydes and ketones. Recommended values are in bold.

| $K_{\text{Hyd.}}$ | T /K | Comment | Reference                        |
|------------------|------|---------|----------------------------------|
| **Aldehydes**    |      |         |                                  |
| **Formaldehyde** |      |         |                                  |
| 2000             | 298  | Review  | Bell (1966)                      |
| 2000             | 298  | Review  | Ogata and Kawasaki (1970)        |
| 2190             | 293  | UV/VIS, T-dependent, pH = 5 – 9 | Zavitsas et al. (1970)          |
| 2220             | 295  | Chemical trapping, pH = 4 – 7   | Sutton and Downes (1972)        |
| 2420             | 298  | UV/VIS, p-dependent              | Lewis and Wolfenden (1973)      |
| 2270             | 298  | UV/VIS, NMR spectroscopy         | McDonald and Martin (1979)      |
| 2000             | 298  | Review                           | Doussin and Monod (2013)        |
| 2100             | 293  | NMR spectroscopy, pH = 1 – 8, T-dep. | Rivlin et al. (2015) |
| **Acetaldehyde** |      |         |                                  |
| 1.43             | 298  | Review  | Bell (1966)                      |
| 1.06             | 298  | UV/VIS, T-dependent               | Kurz (1967)                     |
| 1.2              | 296  | UV/VIS, NMR spectroscopy          | Ahrens and Strehlow (1965); Bell (1966) |
| 1.2              | 298  | UV/VIS, p-dependent               | Lewis and Wolfenden (1973)      |
| 1.2              | 298  | UV/VIS, Chemical trapping         | Sørensen and Jencks (1987)      |
| 1.19             | 298  | Review                            | Tur’yán (2000)                  |
| **1.2**          | **298** | Review                         | **Doussin and Monod (2013)**    |
| **Propanal (Propionaldehyde)** |      |         |                                  |
| 0.71             | 298  | Review                            | Greenzaid et al. (1967a)        |
| 0.71             | 298  | NMR spectroscopy                  | Greenzaid et al. (1967a)        |
| 0.708            | 308.65 | NMR spectroscopy               | Socrates (1969)                 |
| 0.714            | 298  | UV/VIS, p-dependent               | Lewis and Wolfenden (1973)      |
| 0.83             | 298  | Stopped flow measurement, pH = 1 – 6 | Buschmann et al. (1982)        |
| **0.85**         | **298** | Review                         | **Doussin and Monod (2013)**    |
| **Butanal**      |      |         |                                  |
| 0.43             | 298  | Review                            | Bell (1966)                      |
| 0.48             | 298  | NMR spectroscopy                  | Greenzaid et al. (1967a)        |
| 0.426            | 298  | UV/VIS, p-dependent               | Lewis and Wolfenden (1973)      |
| **0.60**         | **298** | Review                         | **Doussin and Monod (2013)**    |
| **Pivaldehyde**  |      |         |                                  |
| 0.1              | 298  | UV/VIS, pH = 4.6                  | Lienhard and Jencks (1966)      |
| 0.24             | 298  | NMR spectroscopy                  | Greenzaid et al. (1967a)        |
| 0.244            | 298  | UV/VIS, p-dependent               | Lewis and Wolfenden (1973)      |
| **0.23**         | **298** | Review                         | **Doussin and Monod (2013)**    |
| **Glyoxal (1st hydration)** |     |         |                                  |
| 207              | 298  | Review                            | Doussin and Monod (2013)        |
| Compound                                      | Temperature | Method                          | Reference                                      |
|-----------------------------------------------|-------------|---------------------------------|-----------------------------------------------|
| Glyoxal (2nd hydration)                        | 20000       | Review                          | Doussin and Monod (2013)                      |
| Methylglyoxal (1st hydration)                  | 2700        | Polarography                    | Wasa and Musha (1970)                         |
|                                               | 565         | Terminal gem-diol, NMR spectroscopy | Creighton et al. (1988)                     |
|                                               | 1279        | Polarography                    | Montoya and Mellado (1994)                    |
|                                               | 2000        | Review                          | Doussin and Monod (2013)                      |
|                                               | 1515        | Review, average from 3 values   | This work                                     |
| Methylglyoxal (2nd hydration)                  | 0.5         | Second gem-diol, NMR spectroscopy | Creighton et al. (1988)                      |
| Glycolaldehyde                                | 25          | Review                          | Bell (1966)                                   |
|                                               | 15.7        | Review                          | Doussin and Monod (2013)                      |
| Acetone                                       | 0.002       | Review                          | Bell (1966)                                   |
|                                               | 0.002       | NMR spectroscopy                | Greenzaid et al. (1967a)                      |
|                                               | 0.002       | Review                          | Doussin and Monod (2013)                      |
| Diacetyl, (2,3-butandione)                     | 3.3         | Review                          | Bell (1966)                                   |
|                                               | 0.244       | UV/VIS, p-dependent             | Lewis and Wolfenden (1973)                    |
|                                               | 2           | Stopped flow measurement, pH = 1 – 3 | Buschmann et al. (1982)                     |
|                                               | 2           | Review                          | Doussin and Monod (2013)                      |
| 2-imidazol-carboxaldehyde                     | 125         | pH = 1.5, NMR spectroscopy, pH-dep. | Ackendorf et al. (2017)                      |
|                                               | 0.043       | pH = 9, NMR spectroscopy, pH-dep. | Ackendorf et al. (2017)                      |
Table S4. Overview of determined hydration equilibrium constants $K_{\text{Hyd.}}$ of $\alpha$-oxocarboxylic acids.

| $K_{\text{Hyd.}}$ | T /K | Comment | Reference |
|------------------|------|---------|-----------|
| Glyoxylate       |      |         |           |
| Glyoxylic acid   |      |         |           |
| 1100             | 298  | Review  | Tur’yan (1998) |
| 1100             | 298  | Review  | Doussin and Monod (2013) |
| Glyoxylate       |      |         |           |
| 19               | 298  | NMR spectroscopy, in D$_2$O, pH = 6 | Copper and Redfield (1975) |
| 67               | 298  | Review  | Tur’yan (1998) |
| 54.6             |      | NMR spectroscopy, room temperature | Leitzke et al. (2001) |
| 67               | 298  | Review  | Doussin and Monod (2013) |
| Pyruvic acid     |      |         |           |
| 2.38             | 298  | Review referring Strehlow (1962) | Bell (1966) |
| 2.4              | 298  | Review  | Tur’yan (1999) |
| 1.4              | 298  | Review  | Doussin and Monod (2013) |
| 2.35             | 298  | NMR spectroscopy, in 10% D$_2$O, pH = 0, ionic strength 0.15, pH = 0 – 6 (cf. Fig. 11) | Lopalco et al. (2016) |
| 1.0, 1.3, 1.5    | 296  | NMR spectroscopy, in 0.02, 0.05 and 0.1 M pyruvic acid, pH = 2.06 | Reed Harris et al. (2014) |
| 0.98             | 296  | in 0.01 M pyruvic acid, pH = 2.2, NMR spectroscopy, in 0.0005 M pyruvic acid, pH = 3.5 | Rapf et al. (2017b) |
| 0.29             |      |         |           |
| 0.89             | 296  | in 0.01 M pyruvic acid, at pH = 2.2, NMR spectroscopy, pH-dep. (cf. Fig. 11) | Rapf et al. (2017a) |
| 2.4              | 298  | pH = 0 (cf. Tur’yan (1999) and Lopalco et al. (2016)) | This work |
| Pyruvate         |      |         |           |
| not hydrated     |      | IR spectroscopy, pH = neutral | Jencks and Carriuolo (1958) |
| 0.054            | 298  | NMR spectroscopy, in 2 M pyruvic acid | Becker (1964) |
| not hydrated     | 298  | UV/VIS, pH = 5.2 | Lienhard and Jencks (1966) |
| 0.054            | 298  | NMR spectroscopy | Greenzaid et al. (1967a) |
| 0.011            | 303  | in 10% D$_2$O, NMR spectroscopy | Öjelund et al. (1967) |
| 0.053            |      | in 20% D$_2$O, NMR spectroscopy | |
| 0.09             | 298  | Pulse polarography | Fonds et al. (1969) |
| 0.04             | 296.7| NMR spectroscopy, pH = 6.5 | Patting and Strehlow (1969) |
| 0.087            | 298  | NMR spectroscopy, in D$_2$O, pH = 6 | Copper and Redfield (1975) |
| 0.075            | 311  | NMR spectroscopy, in 0.5 M pyruvic acid in D$_2$O | Kokesh (1976) |
| 0.06             | 298  | Review | Doussin and Monod (2013) |
| 0.087            | 298  | NMR spectroscopy, in 10% D$_2$O, pH = 6, ionic strength 0.15, pH = 0 – 6 (cf. Fig. 11) | Lopalco et al. (2016) |
| 0.13             | 296  | in 0.01 M pyruvic acid, at pH = 7, pH-dep. | Rapf et al. (2017a) |
| 0.08             | 298  | Average of all values at 298 K at pH = 6 | This work |
| Mesoxalic acid   |      |         |           |
| (α-Keto acid)    |      |         |           |
| 100              | 298  | Pressure jump method, 0.1 M mesoxalic acid in H$_2$O | Strehlow (1962) |
| 99               | 298  | Review  | Doussin and Monod (2013) |
| $K_{\text{hydration}}$ | T/K | Comment | Reference |
|----------------------|-----|---------|-----------|
| 100                  | 298 | Average value | This work |
| **α-Ketobutyric acid** |     |         |           |
| 1.703                | 298 | NMR spectroscopy, 0.1 M in D$_2$O, pH = 0.5 | Copper and Redfield (1975) |
| 0.075                | 298 | NMR spectroscopy, 0.1 M in D$_2$O, pH = 6 | Copper and Redfield (1975) |
| 1.38                 | 311 | NMR spectroscopy, 0.5 M in D$_2$O, pH = 0.5 | Kokesh (1976) |
| 0.075                | 311 | NMR spectroscopy, 0.55 M in D$_2$O, pH = 0.5 | Kokesh (1976) |
| **Oxaloacetic acid (2-Butanedioic acid, Oxobutanedioic acid)** |     |         |           |
| 6.05                 | 311 | NMR spectroscopy, 1.4 M in H$_2$O, pH = 1.3 (6.2% enol form) | Kokesh (1976) |
| 0.5                  | 311 | NMR spectroscopy, 1.4 M in H$_2$O, anion | Kokesh (1976) |
| 0.06                 | 311 | NMR spectroscopy, 1.4 M in H$_2$O, pH = 6.89 (7.4% enol form) | Kokesh (1976) |
| 1.7                  | 298 | Polarography, diacid | Kozlowski and Zuman (1992) |
| 0.06                 | 298 | Polarography, dianion | Kozlowski and Zuman (1992) |
| **2-Ketopentanoic acid (α-Ketovaleric acid, 2-Oxopentanoic acid)** |     |         |           |
| 1.6                  | 298 | Estimated value, stopped flow measurement, pH = 1.1 – 1.7 | Buschmann et al. (1982) |
| **Dimethylpyruvic acid (α-Ketoisovaleric acid, 3-Methyl-2-oxobutanoic acid)** |     |         |           |
| 1.703                | 298 | NMR spectroscopy, 0.1 M in D$_2$O, pH = 0.5 | Copper and Redfield (1975) |
| 0.075                | 298 | NMR spectroscopy, 0.1 M in D$_2$O, pH = 6 | Copper and Redfield (1975) |
| 1.786                | 298 | NMR spectroscopy, in 10% D$_2$O, pH = 0, pH – dep. measurement | Lopalco et al. (2016) |
| 0.037                | 298 | NMR spectroscopy, in 10% D$_2$O, pH = 6, pH – dep. measurement | Lopalco et al. (2016) |
| 1.75                 | 298 | Dianion, average of 2 values at 298 K | This work |
| 0.06                 | 298 | Dicacid, average of 2 values at 298 K | This work |
| **Trimethylpyruvic acid (3,3-Dimethyl-2-oxobutanoic acid)** |     |         |           |
| 0.46                 | 298 | Polarography, c = 0.025 M, pH = 5 | Wasa and Musha (1970) |
| **(dl-α-Keto-β-methylvaleric acid, 4-Methyl-2-oxopentanoic acid)** |     |         |           |
| 1.5                  | 298 | NMR spectroscopy, 0.1 M in D$_2$O, pH = 0.5 | Copper and Redfield (1975) |
| 0.285                | 298 | NMR spectroscopy, in 10% D$_2$O, pH = 0, pH – dep. measurement | Lopalco et al. (2016) |
| 0.006                | 298 | NMR spectroscopy, in 10% D$_2$O, pH = 6, pH – dep. measurement | Lopalco et al. (2016) |
| **(α-Ketoisocaproic acid)** |     |         |           |
| 0.111                | 298 | NMR spectroscopy, 0.1 M in D$_2$O, pH = 0.5 | Copper and Redfield (1975) |
| >0.01                | 298 | NMR spectroscopy, 0.1 M in D$_2$O, pH = 6 | Copper and Redfield (1975) |
| **(α-Ketoglutaric acid)** |     |         |           |
| 1.128                | 298 | NMR spectroscopy, 0.1 M in D$_2$O, pH = 0.5 | Copper and Redfield (1975) |
| 0.064                | 298 | NMR spectroscopy, 0.1 M in D$_2$O, pH = 6 | Copper and Redfield (1975) |
| 1.35                 | 298 | NMR spectroscopy | Jen and Knoche (1969) |
| $K_{hyd}$ | T /K | Comment | Reference |
|-----------|------|---------|-----------|
| 0.03      | 298  | NMR spectroscopy, pH = 5.3  | Jen and Knoche (1969) |
| 1.79      | 298  | Polarography, diacid | Kozlowski and Zuman (1992) |
| 0.26      | 298  | Polarography, dianion | Kozlowski and Zuman (1992) |
| **1.4**   | **298** | Diacid, average of all values at 298 K | This work |
| **0.12**  | **298** | Dianion, average of 2 values at 298 K | This work |
| (α-Ketoadipinic acid) | | | |
| 1.128     | 298  | NMR spectroscopy, 0.1 M in D_2O, pH = 0.5 | Copper and Redfield (1975) |
| **0.064** | **298** | NMR spectroscopy, 0.1 M in D_2O, pH = 6 | Copper and Redfield (1975) |
| 1.13      | 298  | Estimated value, stopped flow measurement, pH = 1.1 – 1.6 | Buschmann et al. (1982) |
| **1.129** | **298** | Diacid, average of 2 values at 298 K | This work |
| Acetopyruvic acid | | | |
| **4.4**   | **301** | NMR spectroscopy, pH = dep. measurement | Guthrie (1972) |

In the following paragraphs, the data compiled in Tables S3 and S4 are briefly discussed. It should be noted that individual data which have been already been compiled in former reviews are generally not repeated here.

**Formaldehyde**

The evaluation of the hydration constant of formaldehyde has been done several times (Bell, 1966; Ogata and Kawasaki, 1970; Doussin and Monod, 2013). Nevertheless, some studies were not included in these reviews. The values obtained $K_{hyd.} = 2190$ at T = 293 K by Zavitsas et al. (1970), $K_{hyd.} = 2220$ at T = 295 K by (Sutton and Downes, 1972), $K_{hyd.} = 2420$ at T = 298 K by Lewis and Wolfenden (1973) and $K_{hyd.} = 2270$ at T = 298 K by McDonald and Martin (1979) are slightly higher than the last recommended value $K_{hyd.} = 2000$ at T = 298 K by Doussin and Monod (2013). Except the investigation of formaldehyde by Rivlin et al. (2015) with $K_{hyd.} = 2100$ at T = 293 K no further recent measured value of the hydration equilibrium constant was added. Since there is no significant change in the recent reported values, the last recommendation suggested by Doussin and Monod (2013) should be applied.

**Acetaldehyde**

In contrast to formaldehyde, acetaldehyde has a significant smaller hydration equilibrium constant by a factor of $10^3$, due to the electronic influence of the CH$_3$ group. The value recommended $K_{hyd.} = 1.43$ at T = 298 K by Bell (1966) was suggested by a review of Tur'yan (2000) appears to be lower with $K_{hyd.} = 1.2$ at T = 298 K. Further studies (Kurz, 1967; Lewis and Wolfenden, 1973; Sorensen and Jencks, 1987) which were not included in Tur'yan (2000) or Doussin and Monod (2013) indicated the same $K_{hyd.}$ value. The last recent review by Doussin and Monod (2013) suggested the use of the recommended value from Tur'yan (2000), which as well be the recommendation from the present work.


Propanal

Table S3 summarizes the given $K_{\text{hydr.}}$ values from Bell (1966) and the references therein, Greenzaid et al. (1967b); Lewis and Wolfenden (1973); Buschmann et al. (1982) as well as Doussin and Monod (2013) and the references therein. The recommended value $K_{\text{hydr.}} = 0.85$ from Doussin and Monod (2013) refers to a slightly higher value based on studies from the 1980’s. Overall, it is recommended to use the suggested value from Doussin and Monod (2013).

Butanal

The hydration of butanal ($K_{\text{hydr.}} = 0.43$) was first revised by Bell (1966). Similar values have been determined by Greenzaid et al. (1967b); Lewis and Wolfenden (1973) compiled in Table S3. The recent evaluation by Doussin and Monod (2013) considering more recent investigations, which indicated higher values. The recommendation from Doussin and Monod (2013) as well as our recommendation can be given with $K_{\text{hydr.}} = 0.60$.

Pivaldehyde

The investigation compiled by Greenzaid et al. (1967b); Lewis and Wolfenden (1973) as well as references included in Doussin and Monod (2013) supports the recommended value. A smaller value was found by Lienhard and Jencks (1966), but it has to be mentioned that the derived values tends to be too low in this study.

Methylglyoxal

A further hydration constant of the dicarbonyl compound was found in the literature, which was not considered by the evaluation in Doussin and Monod (2013). The $K_{\text{hydr.}}$ of methylglyoxal was reported with a value of 2700 (Wasa and Musha, 1970), 1279 (Montoya and Mellado, 1994) and 565 (Creighton et al., 1988). The new recommended value is suggested to be the average value of all three studies, with a derived $K_{\text{hydr.}} = 1512$. Nevertheless, even with this value the majority (>99.9%) of the methylglyoxal is present in its gem-diol.

Glycolaldehyde

Bell (1966) recommend for glycolaldehyde a $K_{\text{hydr.}} = 25$. The revision from Doussin and Monod (2013) considers more recent and higher values. The recommendation based on the reference in Doussin and Monod (2013) yield with $K_{\text{hydr.}} = 15.7$. Our study follows this recommended value.

Acetone

In case of acetone, the reported values agree very well. Bell (1966) recommended a very low hydration equilibrium constant for acetone, which was also obtained by an investigation of Greenzaid et al. (1967b).
Diacetyl

The recommendation from Doussin and Monod (2013) for Diacetyl was based on more recent results from the references therein. A higher value $K_{\text{hyd.}} = 3.3$ was earlier suggested by Bell (1966). Later on a smaller value was obtained by Lewis and Wolfenden (1973) ($K_{\text{hyd.}} = 0.244$) and by Buschmann et al. (1982) ($K_{\text{hyd.}} = 2.1$). Therefore, we also recommend the given value from Doussin and Monod (2013).

Further hydration constants for simple aldehydes and ketones have been evaluated in Doussin and Monod (2013). Since there are no further recent studies found in the literature, in many cases these available recommended values can be followed.

Glyoxylic acid

The study of Tur'yan (1998) compiled and reviewed the hydration equilibrium constants of glyoxylic acid as well as the deprotonated glyoxylate. The $K_{\text{hyd.}}$ values of this compound have been determined by UV/VIS spectroscopy (Strehlow, 1962; Ahrens, 1968; Sørensen et al., 1974), NMR spectroscopy (Cooper and Redfield, 1975; Rendina et al., 1984; Gunshore et al., 1985) and electrochemical methods (Kúta and Valenta, 1963; Fonds et al., 1969; Tur'yan, 1998). The obtained range of $K_{\text{hyd.}} > 99 – 1700$, results in an uncertainty of less than 1% for the appearance of the keto form of the protonated glyoxylic acid. Tur'yan (1998) recommended a value $K_{\text{hyd.}} = 1100$ by measuring and evaluating the rate constant of the dehydration and recombination reaction of the glyoxylic acid. The variety of glyoxylate values is similar. The values reported in the literature change from $K_{\text{hyd.}} > 15 – 260$, results in 6.3% respectively 0.4% for the keto form of glyoxylate. The suggested recommended value $K_{\text{hyd.}} = 67$ by Tur'yan (1998) indicates that only a small fraction of 1.5% of the glyoxylate is not hydrated, which is in good agreement with the directly reported fraction of 1.8% (Leitzke et al., 2001). Several $pK_a$ values to describe the dissociation equilibrium of the keto form of glyoxylic acid at various ionic strength have been reported: $pK_a = 1.72$ (Leussing and Hanna, 1966), $pK_a = 1.68$ (Fonds et al., 1969) and $pK_a = 1.70 – 1.75$ (Tur'yan, 1998). In contrast the hydrated form of the glyoxylic acid (dihydroxyethanoic acid) has a slightly higher $pK_a$ value: $pK_a = 2.92$ (Leussing and Hanna, 1966), $pK_a = 3.06$ (Fonds et al., 1969) and $pK_a = 2.89 – 2.96$ (Tur'yan, 1998). Further reported values do not distinguish between the keto form of the carbonyl group and the diol form ($pK_a = 3.3$ (Strehlow, 1962), $pK_a = 3.46$ (Öjelund et al., 1967).

Since the revision compiled by Tur'yan (1998) no recent determination of hydration constants of glyoxylic acid was found, with exception for the deprotonated glyoxylate from Leitzke et al. (2001). Nevertheless, Doussin and Monod (2013) and the present work follow the recommendation given by Tur'yan (1998).

Pyruvic acid

As in the previous case, many methods have been used to study the hydration equilibrium of pyruvic acid, such as pressure (Strehlow, 1962; Buschmann et al., 1982) or temperature jump relaxation (Ahrens, 1968), UV/VIS spectrometry (Knoche et al., 1985; Fischer and Warneck, 1991), NMR spectroscopy (Becker, 1964; Gold et al., 1964; Leussing and Stanfield, 1964;
Greenzaid et al., 1967b; Griffiths and Socrates, 1967; Öjelund et al., 1967; Socrates, 1967; Patting and Strehlow, 1969; Pocker et al., 1969; Hellström and Almqvist, 1970; Cooper and Redfield, 1975; Kokesh, 1976; Reed Harris et al., 2014; Lopalco et al., 2016; Rapf et al., 2017a; Rapf et al., 2017b), as well as electrochemical methods (Fonds et al., 1969; Fleury et al., 1977; Kozlowski and Zuman, 1987; Tur'yan, 1999). The values obtained from these studies are in a range from $K_{\text{Hyd.1}} = 0.6 – 3.2$.

The majority of the studies were undertaken at high pyruvic acid concentrations (> 2 mol L$^{-1}$), while the pH values were not adjusted or measured (cf. Table S4). Patting and Strehlow (1969) investigated the concentration dependency of the hydration equilibria from 0.14 – 10 mol L$^{-1}$ at different temperatures. The results of these authors indicate that the hydration equilibrium constant is concentration-dependent. The value of the pyruvic acid for infinitive dilution at $T = 298$ K can be calculated with $K_{\text{hyd.1}} = 2.53$ from their temperature-dependent studies. However, the evaluation of the hydration equilibrium constant $K_{\text{hyd.1}}$ is dependent on the used dissociation constant. In the literature, several $pK_a$ values of the keto form respectively diol form of pyruvic acid can be found. Becker (1964) reported the $pK_a$ values of the dehydrated and hydrate acid with $pK_a = 2.07$ and 3.6. Smaller values of have been reported by Hellström and Almqvist (1970) $pK_a = 1.5$ and 3.0, (Fischer et al., 1988) $pK_a = 1.55$ and 2.79. Fischer and Warneck (1991) reinvestigated the temperature dependent dissociation equilibria of pyruvic acid with the $pK_a$ values 1.8 and 3.71. Lopalco et al. (2016) yield for the hydrated acid $pK_a = 1.76$ and in case of the dehydrated acid $pK_a = 3.24$. The use of the different dissociation constants can explain many of the uncertainties of the derived hydration constants. The pH-dependency of the equilibria was investigated by Pocker et al. (1969) using the $pK_a$ values 2.18 (Strehlow, 1962) and 3.6 (Becker, 1964). Tur'yan (1999) reinvestigated the hydration equilibria by polarography.

In this study, many values of $K_{\text{hyd.1}}$ have been corrected by using the $pK_a$ from Fischer and Warneck (1991), deriving a recommended value of $K_{\text{hyd.1}} = 2.4$ at pH = 0 and $T = 298$ K (cf. Table S4). The more recent pH dependent measurements employed by Lopalco et al. (2016) and Rapf et al. (2017a) agree quite well with the recommended value from Tur'yan (1999), although Rapf et al. (2017a) used the $pK_a$ values as in the study of Pocker et al. (1969) to describe the dissociation equilibria. In conclusion for pyruvic acid, the recommended value for the hydration equilibrium constant of pyruvic acid of $K_{\text{hyd.1}} = 1.4$ given by Doussin and Monod (2013) appears too low when considering the recently published values (Lopalco et al., 2016; Rapf et al., 2017a). Our present review suggests to follow the recommendation of $K_{\text{hyd.1}} = 2.4$ given by Tur'yan (1998).

**Pyruvate**

The variability of the hydration equilibrium constant $K_{\text{hyd.2}}$ of the pyruvate is reported in the literature in a range of $K_{\text{hyd.2}} < 0.1$ at $T = 298$ K. The present study recommends a $K_{\text{hyd.}} = 0.08$ of pyruvate, as an average value from the data at $T = 298$ K in Table S4. This value is slightly higher than recommendation by Doussin and Monod (2013).

**Mesoxalic acid**

In case of the mesoxalic acid only the fully protonated dicarboxylic acid equilibrium constant was reported by Strehlow (1962) ($K_{\text{hyd.}} = 100$) and by Le Henaff (1968) ($K_{\text{hyd.}} = 99$). The derived recommended value $K_{\text{Hyd.}} = 100$ suggested from this present
review is very close to the value of $K_{\text{hyd.}} = 99$ suggested by Doussin and Monod (2013). Unfortunately, there are no further data reported concerning the pH dependency of mesoxalic acid.

**Other $\alpha$-oxocarboxylic acids**

In case of other $\alpha$-oxocarboxylic acids a few more hydration equilibrium constants have been reported in the literature by Jen and Knoche (1969); Wasa and Musha (1970); Guthrie (1972); Cooper and Redfield (1975); Kokesh (1976); Buschmann et al. (1982); Kozlowski and Zuman (1992); Lopalco et al. (2016) and compiled in Kerber and Fernando (2010). The values for the compounds oxaloacetic acid, $\alpha$-ketopentanoic acid, dimethylpyruvic acid, trimethylpyruvic acid, $\alpha$-keto-$\beta$-methylvaleric acid, $\alpha$-ketoisocaproic acid, $\alpha$-ketoglutaric acid, $\alpha$-ketoadipinic acid and acetopyruvic acid were taken from the aforementioned references and compiled in (Table S4). Jen and Knoche (1969); Guthrie (1972); Kokesh (1976); Buschmann et al. (1982); Kozlowski and Zuman (1992) studied an even more complex system and determined the hydration and enolization equilibria.

In general, the pH dependent behaviour of the apparent hydration constant $K_{\text{app.}}$, similar to pyruvic acid, is expected because of the connected equilibria. The $\alpha$-oxocarboxylic acids were found to exist in equilibrium with the hydrate (gem-diol). The equilibrium position favours the hydrated $\alpha$-oxocarboxylic acids under acidic conditions, but at neutral pH values the dehydrated keto-form predominates, depending on the $pK_a$ values. With the exception of mesoxalic acid and acetopyruvic acid the reported values of $K_{\text{hyd.}}$ are smaller than $< 1.8$ under acidic conditions and for neutral conditions they are even smaller (cf. Table S4).

**2-imidazol-carboxaldehyde**

In addition to the compounds discussed up to here, a similar pH dependency of the hydration constant $K_{\text{hyd.}}$ was reported by Ackendorf et al. (2017) for 2-imidazol-carboxaldehyde or 2-IC (cf. Table S3). Under acidic conditions, the photochemical active side-chain aldehyde group undergoes the equilibrium reaction with water and forms the gem-diol while the imidazole ring will be fully protonated. In general, 2-IC behaves as a double-basic acid.

Regarding further studies of multifunctional carbonyl compounds, based on the findings discussed here, future studies should consider the complex equilibria which can result in complex dependencies on hydration of carbonyl compounds on acidity.

**Computational chemistry**

For simple aldehydes and ketones the comparison in Doussin and Monod (2013) of calculated towards measured hydration constants, leads to reasonable derived values for $T = 298$ K (Guthrie, 2000; Hilal et al., 2005; Gomez-Bombarelli et al., 2009; Raventos-Duran et al., 2010). Nevertheless, for molecules that are more complex the values obtained by calculation methods scatter in a broader range around the determined equilibrium constant, partly with a poor level of agreement. Apparently, there is quite some potential for improvement for numerical predictions of hydration constants, especially for more complex species.
Apparently, there is quite some potential for improvement for numerical predictions of hydration constants, especially for more complex species.
# Table S5. Compiled kinetic data ($k_{\text{OH}}(298 \text{ K})$ in M$^{-1}$ s$^{-1}$) of OH radical reactions with dissociating organic compounds.

| Reactant                  | SMILES            | $k_{298K}$ [M$^{-1}$ s$^{-1}$] | Reference                                      |
|---------------------------|-------------------|--------------------------------|------------------------------------------------|
| **Monocarboxylic acids (undissociated and dissociated)**                  |                   |                                 |                                                |
| Formic acid               | C(=O)O           | 1.30E+08                       | Buxton et al. (1988)                           |
| Formate                   | C(=O)[O-]        | 3.20E+09                       | Buxton et al. (1988); Elliott and Simons (1984) |
| Acetic acid               | CC(=O)O          | 1.70E+07                       | Chin and Wine (1994)                           |
| Acetate                   | CC(=O)[O-]       | 7.30E+07                       | Chin and Wine (1994)                           |
| Propionic acid            | CCC(=O)O         | 3.20E+08                       | Ervens et al. (2003)                           |
| Propionate                | CCC(=O)[O-]      | 7.20E+08                       | Ervens et al. (2003)                           |
| Butyric acid              | CCCC(=O)O        | 2.20E+09                       | Scholes and Willson (1967)                     |
| Butyrate                  | CCCC(=O)[O-]     | 2.00E+09                       | Anbar et al. (1966)                            |
| iso-Valeric acid          | CC(C)CC(=O)O     | 1.40E+09                       | Merz and Waters (1949)                         |
| iso-Valerate              | CC(C)CC(=O)[O-]  | 2.40E+09                       | Anbar et al. (1966)                            |
| Pivalic acid              | CC(C)(C)=CC(=O)O| 6.50E+08                       | Nauser and Bühler (1994)                       |
| Pivalate                  | CC(C)(C)=CC(=O)[O-]| 1.10E+09                     | Average of Nauser and Bühler (1994) and Anbar et al. (1966) |
| cis-Pinonic acid          | CC(=O)C1CC(C1(C)C1)=CC(=O)O | 2.70E+09 | Otto et al. (2018) |
| cis-Pinonate              | CC(=O)C1CC(C1(C)C1)=CC(=O)[O-]| 2.50E+09 | Otto et al. (2018) |
| **Unsaturated monocarboxylic acids (undissociated and dissociated)**     |                   |                                 |                                                |
| Acrylic acid              | C=CC(=O)O        | 1.50E+09                       | Walling and El-Taliawi (1973)$^a$              |
| Acrylate                  | C=CC(=O)[O-]     | 5.70E+09                       | Average of Kumar et al. (1988)$^a$ and Maruthamuthu (1980)$^a$ |
| Crotonic acid             | CC=CC(=O)O       | 2.90E+09                       | Walling and El-Taliawi (1973)$^b$              |
| Crotonate                 | CC=CC(=O)[O-]    | 5.00E+09                       | Lilie and Henglein (1970)                      |
| Methacrylic acid          | C=C(C)=CC(=O)O  | 1.20E+10                       | Schöne et al. (2014)                           |
| Methacrylate              | C=C(C)=CC(=O)[O-]| 1.20E+10 | Schöne et al. (2014) |
| Methylcrotonic acid       | CC(C)=CC(=O)O   | 9.00E+09                       | Kumar and Rao (1991)$^a$                       |
| Methylcrotonate           | CC(C)=CC(=O)[O-]| 5.90E+09                       | Average of different measurements of Kumar and Rao (1991)$^a$ |
| **Dicarboxylic acids (undissociated and dissociated)**                   |                   |                                 |                                                |
| Oxalic acid               | OC(=O)C(=O)O    | 1.40E+06                       | Sehested et al. (1971)                         |
| Oxalate monoanion         | OC(=O)C(=O)[O-] | 1.90E+08                       | Ervens et al. (2003)                           |
| Oxalate dianion           | [O-]OC(=O)C(=O)[O-]| 1.60E+08 | Ervens et al. (2003) |
| Malonic acid              | OC(=O)CC(=O)O   | 2.00E+07                       | Buxton et al. (1988)                           |
| Malonate monoanion        | OC(=O)CC(=O)[O-]| 6.00E+07                       | Ervens et al. (2003)                           |
| Malonate dianion          | [O-]OC(=O)CC(=O)[O-]| 2.70E+08 | Average of Logan (1989) and Adams et al. (1965) |
| Reactant                        | SMILES                        | $k_{298K}$ [M$^{-1}$ s$^{-1}$] | Reference                  |
|--------------------------------|-------------------------------|-------------------------------|-----------------------------|
| Succinic acid                  | OC(=O)CCC(=O)O               | 1.10E+08                      | Ervens et al. (2003)        |
| Succinate dianion              | [O-]C(=O)CCC(=O)[O-]         | 5.00E+08                      | Ervens et al. (2003)        |
| Glutaric acid                  | OC(=O)CCCCC(=O)O             | 2.00E+08                      | Herrmann (2003)             |
| Glutarate dianion              | [O-]C(=O)CCCCC(=O)[O-]       | 1.00E+09                      | Herrmann (2003)             |
| Adipic acid                    | OC(=O)CCCCCCC(=O)O           | 1.70E+09                      | Herrmann (2003)             |
| Adipate dianion                | [O-]C(=O)CCCCCCC(=O)[O-]     | 2.40E+09                      | Herrmann (2003)             |
| Pimelic acid                   | OC(=O)CCCCCCC(=O)O           | 2.40E+09                      | Herrmann (2003)             |
| Pimelate dianion               | [O-]C(=O)CCCCCCC(=O)[O-]     | 2.90E+09                      | Herrmann (2003)             |
| Suberic acid                   | OC(=O)CCCCCCCCC(=O)O         | 5.00E+09                      | Hesper (2003)               |
| Suberate dianion               | [O-]C(=O)CCCCCCCCC(=O)[O-]   | 5.80E+09                      | Hesper (2003)               |
| (+)-Camphoric acid             | CC1(C(CCC1(C)C(=O)O)C(=O)O)C | 2.00E+09                      | Otto et al. (2018)          |
| (+)-Camphoriate monoanion      | CC1(C(CCC1(C)C(=O)O)C(=O)[O-])C | 2.60E+09              | Otto et al. (2018)          |
| (+)-Camphoriate monoanion      | CC1(C(CCC1(C)C(=O)[O-])C(=O)[O-])C | 2.60E+09              | Otto et al. (2018)          |
| Glycolic acid                  | OCC(=O)O                     | 6.00E+08                      | Buxton et al. (1988)        |
| Glycolate                      | OCC(=O)[O-]                  | 1.20E+09                      | Logan (1989)$^a$            |
| Hydrated glyoxylic acid        | OC(O)C(=O)O                  | 3.60E+08                      | Ervens et al. (2003)        |
| Hydrated glyoxylate            | OC(O)C(=O)[O-]               | 2.60E+09                      | Ervens et al. (2003)        |
| Lactic acid                    | CC(O)C(=O)O                  | 5.24E+08                      | Martin et al. (2009)        |
| Lactate                        | CC(O)C(=O)[O-]               | 7.77E+08                      | Martin et al. (2009)        |
| Pyruvic acid                   | CC(=O)C(=O)O                 | 1.20E+08                      | Ervens et al. (2003)        |
| Pyruvate                       | CC(=O)C(=O)[O-]              | 7.00E+08                      | Ervens et al. (2003)        |
| Tartronic acid                 | OC(=O)C(O)C(O)C(=O)O         | 1.70E+08                      | Schuchmann et al. (1995)    |
| Tartronate monoanion           | OC(=O)C(O)C(O)[O-]           | 3.60E+08                      | Schuchmann et al. (1995)    |
| Tartronate dianion             | [O-]C(=O)C(O)C(O)[O-]        | 4.40E+08                      | Schuchmann et al. (1995)    |
| Mesoxalic acid                 | OC(=O)C(O)C(O)C(=O)O         | 1.80E+08                      | Gligorovski et al. (2009)   |
| Mesoxalate monoanion           | OC(=O)C(O)C(O)[O-]           | 5.70E+07                      | Schuchmann et al. (1991)    |
| Mesoxalate dianion             | [O-]C(=O)C(O)C(O)[O-]        | 1.00E+08                      | Schuchmann et al. (1991)    |
| Malic acid                     | OC(=O)CC(O)C(O)C(=O)O        | 3.60E+08                      | Gligorovski et al. (2009)   |
| Malate monoanion               | OC(=O)CC(O)C(O)[O-]          | 9.70E+08                      | Gligorovski et al. (2009)   |
| Malate dianion                 | [O-]C(=O)CC(O)C(O)[O-]       | 8.50E+08                      | Gligorovski et al. (2009)   |
| Tartaric acid                  | OC(=O)C(O)C(O)C(O)O          | 1.10E+09                      | Average of Scholes and Willson (1967)$^b$ and Moore et al. (1979)$^a$ |
| Tartrate dianion               | [O-]C(=O)C(O)C(O)C(O)[O-]    | 1.00E+08                      | Average of Kraljic (1967)$^{ab}$ and Logan (1989) |
| Citric acid                    | OC(=O)CC(O)C(=O)OCC(=O)O     | 5.00E+07                      | Adams et al. (1965)$^b$     |
| Reactant                  | SMILES                                      | $k_{298K}$ [M$^{-1}$ s$^{-1}$] | Reference                          |
|--------------------------|---------------------------------------------|---------------------------------|------------------------------------|
| Citrate                  | [O-]C(=O)CC(O)(C(=O)[O-])CC(=O)[O-]         | 1.50E+08                        | Zepp et al. (1992)                 |

**Phenols and other aromatic compounds with alcohol functionalities**

| Phenol                        | c1cccccc1O                                   | 1.01E+10                        | Chen and Schuler (1993); partial $k$ @ ortho-/meta-/para-position: $2.37 \cdot 10^9/1.3 \cdot 10^8/3.56 \cdot 10^9$ M$^{-1}$ s$^{-1}$ |
| Phenolate                    | c1cccccc1[O-]                                | 9.60E+09                        | Bonin et al. (2007)                |
| 2-Nitrophenol               | Oc1cccccc1N(=O)=O                            | 9.20E+09                        | Savel'eva et al. (1972)$^d$        |
| 2-Nitrophenolate            | [O-]c1cccccc1N(=O)=O                         | 9.20E+09                        | Savel'eva et al. (1972)$^b$        |
| 3-Nitrophenol               | c1ccc(O)cc1N(=O)=O                           | 4.10E+09                        | Biswal et al. (2013)               |
| 3-Nitrophenolate            | c1ccc([O-])cc1N(=O)=O                        | 8.70E+09                        | Biswal et al. (2013)               |
| 2,4-Nitrophenol             | c1cc(O)cccc1N(=O)=O                          | 1.76E+09                        | Albinet et al. (2010)              |
| 2,4-Nitrophenolate          | c1cc([O-])ccccc1N(=O)=O                      | 2.33E+09                        | Albinet et al. (2010)              |
| 2-Hydroxybenzaldehyde       | c1(O)ccccc1C=O                               | 5.20E+09                        | Geeta et al. (2001)                |
| 2-Hydroxybenzaldehyde, conjugated base | c1([O-])cccccc1C=O                  | 5.20E+09                        | Savel'eva et al. (1972)$^b$        |
| 4-Hydroxybenzaldehyde       | c1cc(O)cccc1C=O                              | 1.21E+10                        | Geeta et al. (2001)                |
| 4-Hydroxybenzaldehyde, conjugated base | c1cc([O-])cccc1C=O                  | 1.00E+10                        | Savel'eva et al. (1972)$^2$        |

**Aromatic mono-/dicarboxylic acids (undissociated and dissociated)**

| Benzoic acid                | c1cccccc1C(=O)O                              | 3.10E+09                        | Average of Wander et al. (1968)$^b$ and Ashton et al. (1995)$^a$ |
| Benzoate                    | c1cccccc1C(=O)[O-]                           | 5.90E+09                        | Buxton et al. (1988)               |
| 2-Hydroxybenzoic acid       | c1(O)ccccc1C(=O)O                            | 2.20E+10                        | Buxton et al. (1988)               |
| 2-Hydroxybenzoate           | c1(O)cccccc1C(=O)[O-]                        | 1.60E+10                        | Buxton et al. (1988)               |
| 4-Hydroxybenzoic acid       | c1cc(O)cccc1C(=O)O                           | 7.70E+09                        | Average of Neta and Dorfman (1968)$^a$; Anderson et al. (1987)$^a$; and Shetiya et al. (1976)$^a$ |
| 4-Hydroxybenzoate           | c1cc(O)cccc1C(=O)[O-]                        | 8.50E+09                        | Buxton et al. (1988)               |
| Gallic acid                 | c1=c(c=cc(=c10)O)OC(=O)O                    | 6.40E+09                        | Dwibedy et al. (1999)              |
| Gallate                     | c1=c(c=cc(=c10)O)OC(=O)[O-]                 | 1.10E+10                        | Dwibedy et al. (1999)              |
| Salicylic acid              | c1=cc=c(c(=c1)C(=O)O)O                     | 2.20E+10                        | Buxton et al. (1988)               |
| Salicylate anion            | c1=cc=c(c(=c1)C(=O)[O-])O                   | 1.60E+10                        | Buxton et al. (1988)               |

**Imidazoles**

| Imidazole-2-carboxaldehyde (pH=0) | C1=C[NH+]C(N1)C(=O)O | 1.80E+09 | Felber et al. (2019) |
| Imidazole-2-carboxaldehyde (pH=9.1) | C1=CN=C(N1)C=O | 4.40E+09 | Felber et al. (2019) |
| 1-Methylimidazole (pH=2) | CN1C=C[NH+]C1 | 2.30E+09 | Felber et al. (2019) |
| Reactant                        | SMILES                  | k\textsubscript{298K} [M\textsuperscript{-1} s\textsuperscript{-1}] | Reference               |
|--------------------------------|-------------------------|-------------------------------------------------|-------------------------|
| 1-Methylimidazole (pH=9.1)     | CN1C=CN=C1              | 6.10E+09                                        | Felber et al. (2019)    |
| 2-Methylimidazole (pH=2)       | CC1=[NH+]C=CN1          | 3.90E+09                                        | Felber et al. (2019)    |
| 2-Methylimidazole (pH=9.2)     | CC1=NC=CN1              | 5.70E+09                                        | Felber et al. (2019)    |
| 4-Methylimidazole (pH=2)       | CC1=C[NH]+=CN1          | 3.20E+09                                        | Felber et al. (2019)    |
| 4-Methylimidazole (pH=9.1)     | CC1=CN=CN1              | 6.90E+09                                        | Felber et al. (2019)    |
| 1-Ethylimidazole (pH=2)        | CCN1C=C[NH]+=C1         | 2.60E+09                                        | Felber et al. (2019)    |
| 1-Ethylimidazole (pH=9.1)      | CCN1C=CN=C1             | 5.70E+09                                        | Felber et al. (2019)    |
| 2-Ethylimidazole (pH=2)        | CCC1=[NH+]C=CN1         | 3.90E+09                                        | Felber et al. (2019)    |
| 2-Ethylimidazole (pH=9.2)      | CCC1=NC=CN1             | 6.40E+09                                        | Felber et al. (2019)    |

**Remarks:** References taken from: aNIST database: Ross et al. (1998); bBuxton et al. (1988); cWarneck (2005); dBarzaghi and Herrmann (2004)
Figure S3. Schematic of second-order OH reaction rate constants ($k_{OH}(298 \text{ K})$ in M$^{-1}$ s$^{-1}$) of protonated organic compounds included in Table S5.
Figure S4. Schematic of the second-order OH reaction rate constants ($k_{\text{OH}}(298 \text{ K})$ in M$^{-1}$ s$^{-1}$) of deprotonated organic compounds included in Table S5.
Table S6. Compiled kinetic data ($k_{\text{NO}_3}(298 \text{ K})$ in M$^{-1}$ s$^{-1}$) of NO$_3$ radical reactions with dissociating organic compounds.

| Reactant                        | SMILES                              | $k_{298\text{K}}$ [M$^{-1}$ s$^{-1}$] | Reference                                      |
|---------------------------------|--------------------------------------|---------------------------------------|------------------------------------------------|
| **Monocarboxylic acids (undissociated and dissociated)** |                                      |                                       |                                                 |
| Formic acid                     | C(=O)O                               | 3.80E+05                              | Exner et al. (1994)                            |
| Formate                         | C(=O)[O-]                            | 5.10E+07                              | Exner et al. (1994)                            |
| Acetic acid                     | CC(=O)O                              | 1.30E+04                              | Exner et al. (1994)                            |
| Acetate                         | CC(=O)[O-]                           | 2.90E+06                              | Exner et al. (1994)                            |
| cis-Pinonic acid                | CC(=O)C1CC(C1(C)C)CC(=O)O            | 1.51E+06                              | Otto et al. (2018)                             |
| cis-Pinonate                    | CC(=O)C1CC(C1(C)CC(=O)[O-]           | 1.58E+07                              | Otto et al. (2018)                             |
| **Unsaturated monocarboxylic acids (undissociated and dissociated)** |                                      |                                       |                                                 |
| Acrylic acid                    | C=CC(=O)O                           | 6.90E+06                              | Schöne et al. (2014)                           |
| Acrylate                        | C=CC(=O)[O-]                         | 4.40E+07                              | Schöne et al. (2014)                           |
| Methacrylic acid                | C=C(C(C)C(=O)O                      | 9.20E+07                              | Schöne et al. (2014)                           |
| Methacrylate                    | C=C(C(C)C(=O)[O-]                   | 1.70E+08                              | Schöne et al. (2014)                           |
| **Dicarboxylic acids (undissociated and dissociated)**       |                                      |                                       |                                                 |
| Oxalic acid                     | OC(=O)C(=O)O                        | 2.40E+04                              | Yang et al. (2004)                             |
| Oxalate monoanion               | OC(=O)C(=O)[O-]                     | 6.10E+07                              | Avg. of Yang et al. (2004) and de Sémainville et al. (2010) with $E_a/R$ of Raabe (1996) |
| Oxalate dianion                 | [O-]C(=O)C(=O)[O-]                  | 2.20E+08                              | Average of Yang et al. (2004) and de Sémainville et al. (2010) with $E_a/R$ of de Sémainville et al. (2010) |
| Malonic acid                    | OC(=O)CC(=O)O                       | 5.10E+04                              | de Sémainville et al. (2010)                   |
| Malonate monoanion              | OC(=O)CC(=O)[O-]                    | 5.60E+06                              | de Sémainville et al. (2010)                   |
| Malonate dianion                | [O-]C(=O)CC(=O)[O-]                 | 2.30E+07                              | de Sémainville et al. (2010)                   |
| Succinic acid                   | OC(=O)CCC(=O)O                      | 5.00E+03                              | de Sémainville et al. (2010)                   |
| Succinate monoanion             | OC(=O)CCC(=O)[O-]                   | 1.10E+07                              | de Sémainville et al. (2010)                   |
| Succinate dianion               | [O-]C(=O)CCC(=O)[O-]                | 1.80E+07                              | de Sémainville et al. (2010)                   |
| (+)-Camphoric acid              | CC1(CCCCCCC1(C)(=O)O)C(=O)OCC1(CCCCCCC1(C)(=O)O)C(=O)[O-]C | 8.80E+05                              | Otto et al. (2018)                             |
| (+)-Camphoriate monoanion       | CC1(CCCCCCC1(C)(=O)O)C(=O)[O-]C      | 4.31E+07                              | Otto et al. (2018)                             |
| (+)-Camphoriate dianion         | CC1(CCCCCCC1(C)(=O)[O-])C(=O)[O-]C  | 5.93E+07                              | Otto et al. (2018)                             |
| **Substituted mono-/dicarboxylic acids (undissociated and dissociated)** |                                      |                                       |                                                 |
| Glycolic acid                   | OCC(=O)O                            | 9.10E+05                              | de Semainville et al. (2007)                   |
| Glycolate                       | OCC(=O)[O-]                         | 1.00E+07                              | de Semainville et al. (2007)                   |
| Lactic acid                     | CC(O)C(=O)O                         | 2.10E+06                              | de Semainville et al. (2007)                   |
| Lactate                         | CC(O)C(=O)[O-]                      | 1.00E+07                              | de Semainville et al. (2007)                   |
| Pyruvic acid                    | CC(=O)C(=O)O                       | 2.40E+06                              | de Semainville et al. (2007)                   |
| Reactant                      | SMILES                              | $k_{298K}$ [M$^{-1}$ s$^{-1}$] | Reference                  |
|------------------------------|-------------------------------------|-------------------------------|----------------------------|
| Pyruvate                     | CC(=O)C(=O)[O-]                      | 1.90E+07                      | de Semainville et al. (2007)|
| Mesoxalic acid               | OC(=O)C(=O)C(=O)O                   | 1.70E+06                      | de Semainville et al. (2007)|
| Mesoxalate monoanion         | OC(=O)C(=O)C(=O)[O-]                | 2.30E+07                      | de Semainville et al. (2007)|
| Mesoxalate dianion           | [O-]C(=O)C(=O)C(=O)[O-]             | 4.90E+07                      | de Semainville et al. (2007)|
| Aromatic acids (undissociated and dissociated) | | | |
| 4-Hydroxybenzoic acid        | c1cc(O)ccc1C(=O)O                   | 1.60E+09                      | Weller et al. (2010)        |
| 4-Hydroxybenzoate            | c1cc(O)ccc1C(=O)[O-]                | 6.00E+09                      | Anderson et al. (1987)      |
| 4-Methoxybenzoic acid        | c1cc(OC)ccc1C(=O)O                  | 6.90E+08                      | Umschlag et al. (2002)      |
| 4-Methoxybenzoate            | c1cc(OC)ccc1C(=O)[O-]               | 8.00E+09                      | O’Neill et al. (1977)       |
Figure S5. Schematic of second-order NO₃ reaction rate constants ($k_{NO3}(298 \text{ K})$ in M⁻¹ s⁻¹) of deprotonated and protonated organic compounds included in Table S6.
Table S7. Compiled kinetic data ($k_{O3}(298 \text{ K})$ in M$^{-1}$ s$^{-1}$) of O$_3$ reactions with dissociating organic compounds.

| Reactant                          | $k_{298K}$ M$^{-1}$ s$^{-1}$ | Formula                                      | Remark          | Reference              |
|-----------------------------------|------------------------------|----------------------------------------------|-----------------|------------------------|
| **Saturated aliphatic mono-carboxylic acids (undissociated and dissociated)** |                              |                                              |                 |                        |
| Glycolic acid                     | 0.055                        | C(O)(=O)O                                    | pH = 1.0        | Schöne and Herrmann (2014) |
| Glycolate                         | 0.71                         | C(O)(=O)[O-]                                  | pH = 7.0        | Schöne and Herrmann (2014) |
| Glyoxylic acid                    | 0.14                         | O=CC(=O)O                                    | pH = 1.0        | Schöne and Herrmann (2014) |
| Glyoxylate                        | 2.3                          | O=C(C(=O))[O-]                                | pH = 7.0        | Schöne and Herrmann (2014) |
| Pyruvic acid                      | 0.13                         | CC(=O)C(=O)O                                 | pH = 1.0        | Schöne and Herrmann (2014) |
| Pyruvate                          | 0.98                         | CC(=O)C(=O)[O-]                               | pH = 7.0        | Schöne and Herrmann (2014) |
| **Unsaturated aliphatic mono/di-carboxylic acids (undissociated and dissociated)** |                              |                                              |                 |                        |
| Acrylic acid                      | 2.80E+04                     | C=CC(=O)O                                    | pH = 2.0        | Leitzke and von Sonntag (2009) |
| Acrylate                          | 1.60E+05                     | C=CC(=O)[O-]                                  | pH = 7.0        | Leitzke and von Sonntag (2009) |
| Methacrylic acid                  | 1.50E+05                     | C=CC(C)(=O)O                                 | pH = 2.0        | Leitzke and von Sonntag (2009) |
| Methacrylate                      | 3.70E+06                     | C=CC(C)(=O)[O-]                               | pH = 7.0        | Leitzke and von Sonntag (2009) |
| Maleic acid                       | 1.40E+03                     | O=C(O)C=CC(=O)O                              |                 | Leitzke and von Sonntag (2009) |
| Maleic acid monoanion             | 4.20E+03                     | O=C(O)C=CC(=O)[O-]                           |                 | Leitzke and von Sonntag (2009) |
| Maleic acid dianion               | ≈ 7.0E+03                    | OC([O-])C=CC(=O)[O-]                         |                 | Leitzke and von Sonntag (2009) |
| Fumaric acid                      | 8.50E+03                     | O=C(O)C=CC(=O)O                              | pH = 10         | Average of Leitzke and von Sonntag (2009) and King et al. (2008) |
| Fumaric acid dianion              | 1.68E+05                     | OC([O-])C=CC(=O)[O-]                         | pH = 3.1        | Mvula and Sonntag (2003) |
| cis-cis-Muconic acid monoanion    | 4.00E+04                     | O=C(O)C=CC=CC(=O)[O-]                        | pH = 6.0        | Leitzke and von Sonntag (2009) |
| cis-trans-Muconic acid            | 1.40E+04                     | O=C(O)C=CC=CC(=O)[O-]                        | pH = 3.0        | Ramseier and Gunten (2009) |
| trans-trans-Muconic acid monoanion| 1.60E+04                    | O=C(O)C=CC=CC(=O)[O-]                        | pH = 7.0        | Ramseier and Gunten (2009) |
| trans-trans-Muconic acid dianion  | 1.40E+05                     | OC([O-])C=CC=CC(=O)[O-]                      | pH = 7.0        | Beltran et al. (2006) |
| Limononic acid                    | 2.60E+04                     | CC(=C)C(CCC(=O)CC(=O)O                     | pH = 2          | Witkowski et al. (2018a); Witkowski et al. (2018b) |
| Limononic acid mono-anion         | 5.70E+04                     | CC(=C)C(CCC(=O)CC(=O)[O-]                   | pH = 7          | Witkowski et al. (2018b); Witkowski et al. (2018b) |
| β-Caryophyllonic acid             | 4.80E+05                     | CC(=O)CCC1CC1(C)C(=C) C(=O)O     | pH = 2          | Witkowski et al. (2019) |
| β-Caryophyllonic acid mono-anion  | 6.00E+05                     | CC(=O)CCC1CC1(C)C(=C)C(=O)[O-]              | pH = 8          | Witkowski et al. (2019) |
| Limononic acid                    | 2.30E+04                     | OC(=O)CCC(CC(=O)OC(=C)C | pH = 2          | Witkowski et al. (2018a) |
| Compound                          | pK_a (pH = 7) | Chemical Structure | pH     | Reference                          |
|----------------------------------|---------------|-------------------|--------|------------------------------------|
| Limonic acid mono-anion          | 4.60E+04      | [O-]C(=O)CCC(CC(=O)O)C(=C)C | pH = 7 | Witkowski et al. (2018a)           |
| 7-Hydroxylimonic acid            | 2.90E+04      | O=CCC(CC(=O)O)C(=C)CCO | pH = 2 | Witkowski et al. (2018a)           |
| 7-Hydroxylimonic acid mono-anion | 5.30E+04      | [O-]C(CCC(CC(=O)O)C(=C)C)CO | pH = 7 | Witkowski et al. (2018a)           |

**Aromatic organic compounds (undissociated and dissociated)**

| Compound                          | pK_a (pH = 2.0) | Chemical Structure | pH     | Reference                          |
|----------------------------------|-----------------|--------------------|--------|------------------------------------|
| Phenol                           | 8.67E+02        | c1cccccc1O        | pH = 2.0 | Poznyak and Vivero (2005)          |
| Phenolate                        | 1.17E+03        |                    | pH = 7.0 | Poznyak and Vivero (2005)          |
| Tyrosol                          | 3.00E+03        | c1=cc(=cc=c1CCCO)O | pH = 2.0 | Beltrán et al. (2000)              |
| 4-α-Nonylphenol                  | 3.80E+04        | CCCCCCCCc1=cc=c(c=c1)O | pH = 2.0 | Deborde et al. (2005)              |
| 4-α-Nonylphenol anion            | 3.90E+04        |                    | pH = 6.3 | Ning et al. (2007)                 |
|                                 | 6.80E+09        | CCCCCCCCc1=cc=c(c=c1)[O-] |         | Deborde et al. (2005)              |

**Aromatic acids (undissociated and dissociated)**

| Compound                          | pK_a (pH = 2.0) | Chemical Structure | pH     | Reference                          |
|----------------------------------|-----------------|--------------------|--------|------------------------------------|
| p-Hydroxybenzoic acid            | 2.0E+02         | c1=cc(=cc=c1C(=O)O)O | pH = 2.0 | Beltrán et al. (2000)              |
| Gallic acid                      | 9.7E+04         | c1=c(c=c(c1O)O)O(C(=O)O | pH = 2.0 | Beltrán et al. (2000)              |
|                                 | 4.7E+05         |                     | pH = 6.3 | Beltrán et al. (2000)              |
| Cinnamic acid                    | 1.0E+05         | c1=cc=c(c=c1)C=CC(=O)O |         | Jans (1996)                        |
| Cinnamic acid monoanion          | 1.2E+06         | c1=cc=c(c=c1)C=CC(=O)[O-] |         | Jans (1996)                        |
|                                 | 3.8E+05         |                     |         | Leitzke et al. (2001)              |
| 4-methoxy Cinnamic acid          | 1.3E+05         | COc1=cc=c(c=c1)C=CC(=O)O |         | Leitzke et al. (2001)              |
| 4-methoxy Cinnamic acid monoanion| 6.8E+05         | COc1=cc=c(c=c1)C=CC(=O)[O-] |         | Leitzke et al. (2001)              |
| 3-methoxy-4-hydroxy Cinnamic acid| 1.1E+06         | COc1=cc=c(c=c1)C=CC(=O)O |         | Jans (1996)                        |
| 3-methoxy-4-hydroxy Cinnamic acid monoanion | 7.9E+06 | COc1=cc=c(c=c1)C=CC(=O)([O-]) |         | Jans (1996)                        |
| 3,4-dihydroxy Cinnamic acid      | 2.0E+06         | c1=cc(=cc1C=CC(=O)O)O |         | Jans (1996)                        |
| 3,4-dihydroxy Cinnamic acid monoanion | 1.2E+07       | c1=cc(=cc1C=CC(=O)([O-])O) |         | Jans (1996)                        |
Figure S6. Schematic of second-order O₃ reaction rate constants (kₒ₃(298 K) in M⁻¹ s⁻¹) of deprotonated and protonated organic compounds included in Table S7.
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