IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

 – Data Sheet AQ\_OH\_40

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**HO(aq) + HO(CH2)2OH(aq) → HOCHCH2OH + H2O**

*(product distribution suggested by Buxton et al., 1988)*

**Rate coefficient data**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| k/ L mol-1 s-1 | T/K | pH | I/ mol L-1 | Reference | Technique/ Comments |
| *Relative Rate Coefficients* |
| 1.6  109 | 294 | ~7 | - | Adams et al., 1965 | PR / UV-Vis (a1) |
| 1.4  109 | 294 | ~7 | - |  | (a2) |
| 1.5  109 | 294 | 9 | - | Anbar et al., 1966 | PR / UV-Vis (b) |
| 1.8  109 | 294 | 2.0-2.2 | - | Scholes and Willson, 1967 | PR / UV-Vis (c) |
| 1.62  109 | 294 | - | - | Willson et al., 1971 | PR / UV-Vis (d) |
| 2.30  1092.61  1092.84  1092.72  109 | 298 ±2 | - | - | Matheson et al., 1973 | PR / UV-Vis (e) |
| (1.6 ±0.03)  109 | 298 | 7 | - | Hoffmann et al., 2009 | LFP-LPA (f) |
| 3.53 × 1010 exp[-(900 ±110)/T] | 288 – 328 | 7 | - |  | (f1) |

*GR* (aq): Aqueous phase thermochemical data not available. As well, gas phase thermochemical data *R* (g) are not available.

**Comments**

(a) Reference reactions: HO + CO32- with *k*(HO + CO32-) = 2.0  108 M‑1s‑1 [3.77  108 M‑1s‑1] (a1); HO + SCN- with *k*(HO + SCN-) = 6.6  109 M-1s-1 [1.10  1010 M‑1s‑1, Zhu et al., 2003] (a2); no values given for the initial concentrations of the reactants; pH is given as natural; as no exact temperature is given, a room temperature of 294 K is assumed.

(b) Reference reaction: [HO](http://webbook.nist.gov/cgi/cbook.cgi?ID=3352576&Units=SI) + PNDA (p-nitrosodimethylaniline); reference rate constant was determined versus ethanol with *k*(HO + ethanol) = 1.10 × 109 M‑1s‑1; rate coefficients have been recalculated using the selected value for the reference reaction 1.88 × 109 M‑1s‑1; no values given for initial concentrations; air saturated solutions; all experiments were repeated at least four times and the coefficient of variation was less than ±10%; as no exact temperature is given, a room temperature of 294 K is assumed.

(c) Aerated solutions of thymine (*c*(thymine) = 8  10-5 M) were irradiated (pH range: 1.5 – 9); rate constant was determined relative to thymine reference with *k*(HO + thymine) = 4.3  109 M‑1 s‑1; rate constants have been recalculated using the selected value for the reference reaction (5.38 × 109 M‑1s‑1); as no exact temperature is given, a room temperature of 294 K is assumed.

(d) Reference reaction: HO + [Fe(CN)6]4-; *k*(HO + [Fe(CN)6]4-) = (9.3 ±0.05)  109 M‑1 s‑1; rate constants have been recalculated using the selected values for the reference reactions (1.03 × 1010 M‑1s‑1); *c*([Fe(CN)6]4-) = 2  10-3 mol/L (no information on counterions); reference values were normalized to *k*(HO + ethanol) = 1.85  109 M-1s-1; as no exact temperature is given, a room temperature of 294 K is assumed.

(e) Rate constants were determined relative to the reference reaction with *k*(HO + [Fe(CN)6]4-) = 0.93  10‑10 M‑1 s‑1; rate constants have been recalculated using the selected value for the reference reaction (1.10 × 1010 M‑1s‑1); Depending on four different concentrations of ethylene glycol (2  10‑3 M, 4  10‑3 M, 8  10‑3 M and 1  10‑2 M), rate constants were measured as listed.

(f) Radicals generated by laser flash photolysis of H2O2 (*c*(H2O2) = 1  10-4 M) at 248 nm (LP-LPA); Reference reaction: HO + SCN- with *k*(HO + SCN-) = 1.24 × 1010 M‑1 s‑1 as reported by Chin and Wine (1992); rate constants have been recalculated using the selected values for reference reactions (Zhu et al., 2003); *c*(KSCN) = 1.59  10-5 M. Arrhenius expression (f1) was calculated using the recalculated experimental data from Hoffmann et al. (2009).

**Preferred Values**

|  |  |  |
| --- | --- | --- |
| **Parameter** | **Value** | ***T*/K** |
|  |  |  |
| *k* / L mol-1 s-1 | 1.65 × 109 | 298 |
|  |  |  |
| *k* / L mol-1 s-1 | 2.82 × 1010 exp[-(850)/T] | 288 - 328 |
|  |  |  |

*Reliability*

|  |  |  |
| --- | --- | --- |
| Δ log *k* | ±0.09 | 298 |
| Δ EA/R | ±150 | 288 – 328 |
|  |  |  |

*Comments on Preferred Values*

For the Arrhenius equation regression, the temperature dependent data by Hoffmann et al. (2009), as well as the recalculated rate coefficients by Adams et al. (1965), Anbar et al. (1966), Scholes and Willson (1967) and Willson et al. (1971) have been considered. Due to the hugely different determinations by Matheson et al. (1973) to, their data is not included in the regression. The recommended rate constant is in good agreement with the temperature dependent data of Hoffmann et al. (2009). The estimated uncertainty is given as Δ log *k* = 0.09 or ±20%.

**References**

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T-dependent rate coefficients for the reaction of ethanediol with HO radical in aqueous solution. The data of Matheson et al. (1973) is excluded from the evaluation.