IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

 – Data Sheet AQ\_OH\_42

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**HO (aq) + CH3CHOHCH2OH(aq) → products**

**Rate coefficient data**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| k/ L mol-1 s-1 | T/K | pH | I/ mol L-1 | Reference | Technique/ Comments |
| *Relative Rate Coefficients* |
| 1.68  109 | 294 | 7 | - | Adams et al., 1965 | PR / UV-Vis (a) |
| 1.7  109 | 294 | 9 | - | Anbar et al., 1966 | PR / UV-Vis (b) |
| (1.6 ±0.3) × 109 | 298 | 7 | - | Hoffmann et al., 2009 | LFP-LPA (c) |
| 9.37 × 1010 exp[-(1200 ± 340)/T] | 288 - 328 | 7 | - |  | LFP-LPA (c1) |

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

**Comments**

(a) Reference reaction: HO + SCN- with *k*(HO + SCN-) = 6.6  109 M‑1s‑1; rate constnats have been recalculated using the selected values for the reference reactions (1.10 × 1010  M‑1s‑1); No exact value is given for the initial concentrations of the reactants; pH is given as natural; as no exact temperature is given, T = 294 K is assumed for room temperature.

(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; recalculation of the rate coefficient was performed 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, T = 294 K is assumed for room temperature.

(c) Radicals generated by laser flash photolysis of H2O2 (*c*(H2O2) = 1  10-4 M) at 248 nm (LF-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 the temperature dependent reference reaction by Zhu et al., 2003; *c*(KSCN) = 1.59  10‑5 M. Arrhenius expression (c1) was calculated using the recalculated experimental data from Hoffmann et al. (2009).

**Preferred Values**

|  |  |  |
| --- | --- | --- |
| **Parameter** | **Value** | ***T*/K** |
|  |  |  |
| *k* / L mol-1 s-1 | 1.75 × 109 | 298 |
|  |  |  |
| *k* / L mol-1 s-1 | 8.32× 1010 exp[-(1200)/T] | 288 – 328 |
|  |  |  |
|  |  |  |

*Reliability*

|  |  |  |
| --- | --- | --- |
| Δ log *k* | ±0.15 | 298 |
| Δ EA/R | ±240 | 288 - 328 |
|  |  |  |

*Comments on Preferred Values*

The room temperature rate coefficients determined by Adams et al. (1965), Anbar et al. (1966) and the T-dependent data by Hoffmann et al. (2009) have been used for regression. As the room temperature rate coefficients contribute perfectly to the Arrhenius expression of Hoffmann et al., the result is the mean of them, with an estimated uncertainty of Δ log *k*= ±0.15 or ±33%.

**References**

Adams, G.E.; Boag, J.W.; Currant, J. and Michael, B.D., Pulse Radiolysis, Ebert, M.; Keene, J.P.; Swallow, A.J. and Baxendale, J.H. (eds.): Academic Press, New York, p.131-143, 1965.

Anbar, M., Meyerstein, D. and Neta, P.: J. Chem. Soc. B, 742-747, 1966.

Hoffmann, D., Weigert, B., Barzaghi, P. and Herrmann, H.: Phys. Chem. Chem. Phys., 11, 9351-9363, 2009

Kraljić, I. and Trumbore, C. N.: J. Am. Chem. Soc. 87(12), 2547-2550, 1965.

Monod, A. and Doussin, J. F.: Atmos. Environ., 42, 7611-7622, 2008.

Zhu, L., Nicovich, J. M. and Wine, P. H.: Aquat. Sci., 65(4), 425-435, 2003.



T-dependent rate constants for the reaction of propane-1,2-diol with HO in aqueous solution. All available data has been used for regression.