IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ\_OH\_14

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**HO (aq) + CH3(CH2)5OH (aq) → products**

**Rate coefficient data**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| k/ L mol-1 s-1 | T/K | pH | I/ mol L-1 | Reference | Technique/ Comments | |
| *Relative Rate Coefficients* | | | | | | |
| 5.9 × 109 | 294 | 2.0 - 2.2 | - | Scholes and Willson, 1967 | PR/UV-Vis (a) |

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

**Comments**

1. Aerated solutions of thymine (8 × 10-5 M) were irradiated; reference reaction: HO + thymine with *k*(HO + thymine) = (4.3 ±1) × 109 M‑1 s‑1, determined relative to benzene (*k*(HO + benzene) = (4.3 ±0.9) × 109 M‑1 s‑1; the rate coefficient was recalculated using the selected rate coefficient for the reference reaction (5.38 × 109 M‑1s‑1); an error of about ± 25% for absolute rate coefficients is given by the authors; as no exact temperature is given, T = 294 K is assumed for room temperature.

**Preferred Values**

|  |  |  |
| --- | --- | --- |
| **Parameter** | **Value** | ***T*/K** |
|  |  |  |
| *k* / L mol-1 s-1 | 5.9 × 109 | 294 |
|  |  |  |

*Reliability*

|  |  |  |
| --- | --- | --- |
| Δ log *k* | ± 0.15 | 294 |
|  |  |  |

*Comments on Preferred Values*

The only available kinetic data are those of Scholes and Willson (1967). In 1988, Buxton et al. recommended a rate coefficient of 7.0 × 109 M‑1s‑1. Referring to the evaluation of the rate coefficients of reference reactions, the recalculation leads to a lower value than recommended before. As the deviation is still around 10%, both values are within the estimated uncertainty of ±33% or Δlog *k* = ±0.15. The uncertainty is chosen as a standard value for single determinations. It should be noted that this rate constant refers to room temperature, which we estimate as T = 294 K.

**References**

Buxton, G. V., Greenstock, C. L., Helman, W. P. and Ross, A. B.: J. Phys. Chem. Ref. Data, 12(2), 513 – 886, 1988.

Scholes, G. and Willson, R.L.: Trans. Faraday Soc., 63, 2983-2993, 1967.