IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ\_OH\_15

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HO (aq) + CH3(CH2)6OH (aq) → products

**Rate coefficient data**

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| k/ l mol-1 s-1 | T/K | pH | | I/ mol l-1 | Reference | | Technique/ Comments | |
| *Relative Rate Coefficients* | | | | | | | |
| 6.1 × 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 | 6.1 × 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 7.4 × 109 M‑1s‑1. Following the evaluation of the rate coefficients of reference reactions, the recalculation of the rate coefficient measured leads to a slightly lower value than the one recommended before. Considering the uncertainty of the rate coefficient, both values still agree within error limits. The estimated uncertainty of the recommended rate constant is ±33% or Δlog *k* = 0.15. The uncertainty is chosen as a standard value for single determinations. It should be noted that this rate coefficient 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.