IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

 – Data Sheet AQ\_OH\_16

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HO (aq) + CH3(CH2)7OH (aq) → products

**Rate coefficient data**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| k/ l mol-1 s-1 | T/K | pH | I/ mol l-1 | Reference | Technique/ Comments |
| *Relative Rate Coefficients* |
| 6.5 × 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 | 6.5 × 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 7.7 × 109 M‑1s‑1. After the evaluation of the rate coefficients of reference reactions, the rate coefficient measured by Scholes and Willson was recalculated. A slightly lower rate constant than recommended before was obtained. Its uncertainty is estimated as ±33% or Δlog *k* = ±0.15 as the 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, 17(2), 513-886, 1988.

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