

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

$k / \text{L mol}^{-1} \text{s}^{-1}$	T/K	pH	I/ mol L ⁻¹	Reference	Technique/ Comments
<i>Relative Rate Coefficients</i>					
5.9×10^9	294	2.0 - 2.2	-	Scholes and Willson, 1967	PR/UV-Vis (a)

ΔG_R° (aq): Aqueous phase thermochemical data not available. As well, gas phase thermochemical data H_R° (g) are not available.

Comments

- (a) Aerated solutions of thymine ($8 \times 10^{-5} \text{ M}$) were irradiated; reference reaction: HO + thymine with $k(\text{HO} + \text{thymine}) = (4.3 \pm 1) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$, determined relative to benzene ($k(\text{HO} + \text{benzene}) = (4.3 \pm 0.9) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$); the rate coefficient was recalculated using the selected rate coefficient for the reference reaction ($5.38 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$); an error of about $\pm 25\%$ 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
$k / \text{L mol}^{-1} \text{ s}^{-1}$	5.9×10^9	294
<i>Reliability</i>		
$\Delta \log k$	± 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 $7.0 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$. 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 $\pm 33\%$ or $\Delta \log k = \pm 0.15$. 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 $T = 294 \text{ K}$.

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.