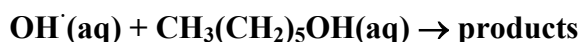


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ_OH_14

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This datasheet last evaluated: May 2017; last change in preferred values: January 2016



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

Rate coefficient data

$k / \text{L mol}^{-1} \text{s}^{-1}$	T/K	pH	$I / \text{mol L}^{-1}$	Reference	Technique/ Comments
<i>Relative Rate Coefficients</i>					
4.7×10^9		2.0 - 2.2		Scholes and Willson, 1967	PR/UV-Vis (a)
7.0×10^9	298	2.0 - 2.2		Buxton et al., 1988	Recalculated value (b)

Comments

(a) The molar extinction coefficient of thymine was determined to be $\epsilon_{264 \text{ nm}} = 7950 \pm 50$ over the pH range 1.2-5.9; Aerated solutions of thymine ($8 \times 10^{-5} \text{ M}$) were irradiated. Reference reaction: $\cdot\text{OH} + \text{thymine}$ with $k(\cdot\text{OH} + \text{thymine}) = (4.3 \pm 1) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$. The rate constant of the reference reaction was determined relative to benzene. The absolute rate constants in table 3 have an error of about $\pm 25\%$. NIST lists this value as $7.0 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$, referring to $k(\cdot\text{OH} + \text{thymine}) = 6.4 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$.
<http://kinetics.nist.gov/solution/Detail?id=1967SCH/WIL2983-2993:13>

(b) Buxton et al. recalculated the value originally determined by Scholes and Willson (1967) using the selected rate constant for reference reactions $k(\cdot\text{OH} + \text{thymine}) = 6.4 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$.

Preferred Values

Parameter	Value	T/K
$k / \text{L mol}^{-1} \text{s}^{-1}$	7.0×10^9	298
<i>Reliability</i> $\Delta \log k$	± 0.04	298

Comments on Preferred Values

The former value recommended by Buxton et al. (1988) is also recommended. There have been no newer determinations. The relative error of the rate constant is estimated as $\pm 10\%$.

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.