IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ_OH_15

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

$OH^{\cdot}$ (aq) + $CH_3(CH_2)_6OH$ (aq) → products

$\Delta G_R°$ (aq): Aqueous phase thermochemical data not available. As well, gas phase thermochemical data $H_R°$ (g) are not available.

Rate coefficient data

k/ l mol^{-1} s^{-1}	T/K	pH	I/ mol l^{-1}	*Reference*	Technique/ Comments
Relative Rate Coefficients					
4.9×10^9		2.0-2.2		Scholes and Willson, 1967	PR/UV-Vis(a)
7.4×10^9	298	2.0-2.2		Buxton et al., 1988	Recalculated value (b)

Comments

(a) The molar extinction coefficient of thymine was determined to be $\varepsilon_{264\ nm} = 7950 \pm 50$ over the pH range 1.2 - 5.9; Aerated solutions of thymine (8×10^{-5} M) were irradiated. Reference reaction: ·OH + thymine with k(·OH + thymine) = $(4.3 \pm 1) \times 10^9$ M^{-1} 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 ± 25%. NIST lists this value as 7.4×10^9 M^{-1} s^{-1}, referring to k(·OH + thymine) = 6.4×10^9 M^{-1} s^{-1}.
http:/kinetics.nist.gov/solution/Detail?id=1967SCH/WIL2983-2993:12

(b) Buxton et al. recalculated the value originally determined by Scholes and Wilson (1967) using the selected rate constant for reference reactions k(·OH + thymine) = 6.4×10^9 M^{-1} s^{-1}.

Preferred Values

Parameter	Value	T/K
k / l mol^{-1} s^{-1}	7.4×10^9	298
Reliability		
$\Delta \log k$	± 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 ± 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.