IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ_OH_12

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

$OH(aq) + (CH_3)_2CHCH_2CH_2OH\ (aq) \rightarrow$ 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					
3.4×10^9				Reuvers et al., 1973	PR / UV-vis (a1)
3.8×10^9					PR / UV-vis (a2)
3.8×10^9	298			Buxton et al., 1988	Average value (b)

Comments

(a) Radicals generated by pulse-radiolysis, products analysed by UV-vis-spectroscopy; ferrocyanide (a1) and thiocyanate (a2) were used as reference systems; ferrocyanide reference: $\cdot OH + [Fe(CN)_6]^{4-}$; $k(\cdot OH + [Fe(CN)_6]^{4-}) = 0.93 \times 10^{10}$ M^{-1}s^{-1}; thiocyanate reference: $\cdot OH + SCN^-$; $k(\cdot OH + SCN^-) = 1.1 \times 10^{10}$ M^{-1}s^{-1}. NIST lists the value (a1) as 3.8×10^9 M^{-1}s^{-1}, referring to $k(\cdot OH + [Fe(CN)_6]^{4-}) = 1.0 \times 10^{10}$ M^{-1}s^{-1}. http://kinetics.nist.gov/solution/Detail?id=1973REU/GRE533-536:6

(b) Buxton et al. suggest the average of two recalculated values, originally determined by Reuvers et al. (1973); the selected rate constants for reference reactions have been used for the recalculation of the original data: 3.8×10^9 M^{-1}s^{-1} relative to $k(\cdot OH + [Fe(CN)_6]^{4-}) = 1.05 \times 10^{10}$ M^{-1}s^{-1} and 3.7×10^9 M^{-1}s^{-1} relative to $k(\cdot OH + SCN^-) = 1.1 \times 10^{10}$ M^{-1}s^{-1}.

Preferred Values

Parameter	Value	T/K
k /L mol^{-1} s^{-1}	3.8×10^9	298
Reliability		
$\Delta \log k$	± 0.05	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.

Reuvers, A. P., Greenstock, C. L., Borsa, J. and Chapman, J. D.: Int. J. Rad. Biol., 24(5), 533-536, 1973.