IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ_OH_43

This datasheet last evaluated: June 2019; last change in preferred values: June 2019

HO(aq) + HO(CH$_2$)$_4$OH(aq) → products

Rate coefficient data

k/ L mol^{-1} s^{-1}	T/K	pH	I/ mol L^{-1}	Reference	Technique/ Comments
Relative Rate Coefficients					
3.23×10^9	294	-	-	Adams et al., 1965	PR / UV-Vis(a)
$(3.4 \pm 0.1) \times 10^9$	298	7	-	Hoffmann et al., 2009	LFP-LPA (b)
9.7×10^{10} exp[-(1000 ± 80)/T]	288 - 328	7	-		LFP-LPA (b1)

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

Comments

(a) Reference reaction: HO + SCN$^-$ with k(HO + SCN$^-$) = 6.6×10^9 M^{-1}s^{-1}; the selected reference rate coefficient $k = 1.10 \times 10^{10}$ M^{-1}s^{-1} was used for recalculation; No exact value is given for the initial concentrations of the reactants; pH is given as natural; as no exact temperature is given, T = 294 K is assumed for room temperature.

(b) Radicals generated by laser flash photolysis (LFP) of H_2O_2 ($c(H_2O_2) = 1 \times 10^{-4}$ M) at 248 nm; reference reaction: HO + SCN$^-$ with k(HO + SCN$^-$) = 1.24×10^{10} M^{-1} s^{-1}; the selected reference rate constant $k = 1.19 \times 10^{10}$ M^{-1}s^{-1} was used for recalculation; c(KSCN) = 1.59×10^{-5} M. Arrhenius expression (b1) was calculated using the recalculated experimental data from Hoffmann et al. (2009), based on the recommended Arrhenius expression $k(T) = 3.45209 \times 10^{12} \times \exp(-14050 / RT)$ (Zhu et al., 2003).

Preferred Values

Parameter	Value	*T*/K
k / L mol^{-1} s^{-1}	3.33×10^9	298
k / L mol^{-1} s^{-1}	9.04×10^{10} exp[-(1000)/T]	288 – 328
Reliability		
$\Delta \log k$	±0.09	298

$\Delta E_A/R$	±70	288 – 328

Comments on Preferred Values

For the recommended rate constant, data determined by Adams et al. (1965) and Hoffmann et al. (2009) have been used for regression. The available data agree well with each other as well as with the former recommendation by Buxton et al. of 1988 when the latter is recalculated to 3.2×10^{10} M^{-1} s^{-1}. The uncertainty is estimated as ±20% or $\Delta \log k = \pm 0.09$.

References

Adams, G. E., Boag, J. W. and Michael, B. D.: Trans. Faraday Soc., 61, 1417-1424, 1965.

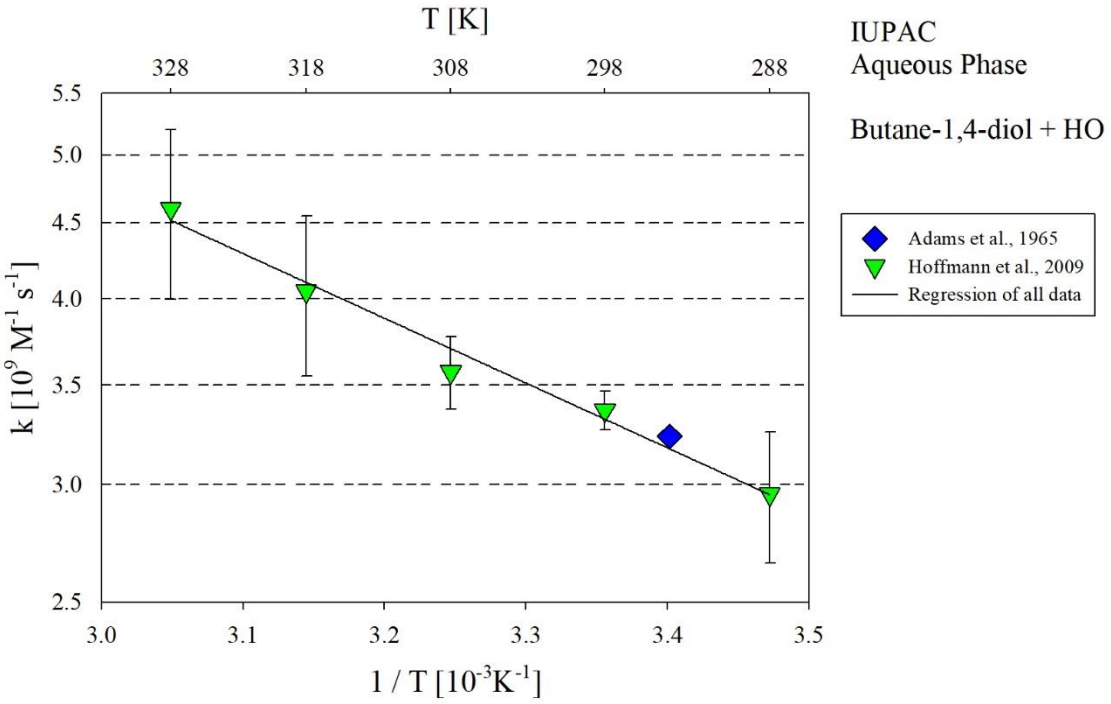
Buxton, G. V., Greenstock, C. L., Helman, W. P. and Ross, A. B.: J. Phys. Chem. Ref. Data, 12(2), 513 – 886, 1988.

Chin, M., and Wine, P. H: J. Photochem. Photobiol., A, 69(1), 17-25, 1992.

Hoffmann, D., Weigert, B., Barzaghi, P. and Herrmann, H.: Phys. Chem. Chem. Phys., 11, 9351-9363, 2009.

Monod, A. and Doussin, J. F.: Atmos. Environ., 42, 7611–7622, 2008.

Zhu, L., Nicovich, J. M. and Wine, P. H.: Aquat. Sci., 65(4), 425-435, 2003.



T-dependent rate constants for the reaction of butane-1,4-diol with HO in aqueous solution. All data shown in the figure has been used for regression.