IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ_OH_41

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

HO (aq) + $HO(CH_2)_3OH$(aq) → products

Rate coefficient data

k/ L mol^{-1} s^{-1}	T/K	pH	I/ mol L^{-1}	Reference	Technique/ Comments
Relative Rate Coefficients					
2.4×10^9	294	9	-	Anbar et al., 1966	PR / UV-Vis (a)
$(2.6 \pm 02) \times 10^9$	298	7	-	Hoffmann et al., 2009	LFP-LPA (b)
1.31×10^{11} exp[-(1200 ±250)/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 + PNDA (p-nitrosodimethylaniline); the reference rate constant was determined versus ethanol with k(HO + ethanol) = 1.10×10^9 $M^{-1}s^{-1}$; recalculation was performed using the selected value for the reference rate coefficient (1.88×10^9 $M^{-1}s^{-1}$); no values given for initial concentrations; air saturated solutions; all experiments were repeated at least four times and the coefficient of variation was less than ±10%; as no exact temperature is given, T = 294 K is assumed for room temperature.

(b) Radicals generated by laser flash photolysis of H_2O_2 ($c(H_2O_2) = 1 \times 10^{-4}$ M) at 248 nm (LP-LPA); Reference reaction: HO + SCN^- with k(HO + SCN^-) = 1.24×10^{10} M^{-1} s^{-1} as reported by Chin and Wine (1992); rate constants have been recalculated using the selected values for temperature dependent reference reaction by Zhu et al., 2003; c(KSCN) = 1.59×10^{-5} M. Arrhenius expression (b1) was calculated using the recalculated experimental data from Hoffmann et al. (2009).

Preferred Values

Parameter	Value	*T*/K
k / L mol^{-1} s^{-1}	2.50×10^9	298
k / L mol^{-1} s^{-1}	1.26×10^{11} exp[-(1200)/T]	288 - 328

Reliability

$\Delta \log k$	±0.15	298
$\Delta E_A/R$	±200	288 - 328

Comments on Preferred Values

For the evaluation, the recalculated temperature-dependent data by Hoffmann et al. (2009) and the room temperature rate coefficient by Anbar et al. (1966) have been used for regression. As these data are in general agreement, the result is the mean of them, with an estimated uncertainty of $\Delta \log k$ = ±0.15 or ±33%.

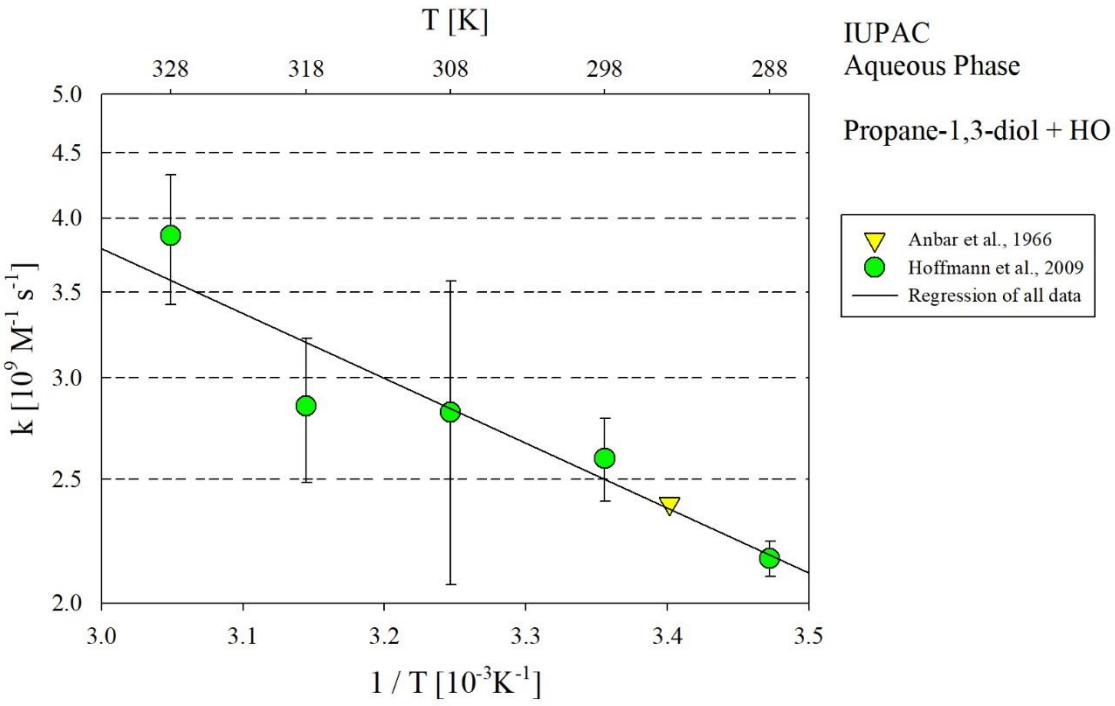
References

Anbar, M., Meyerstein, D. and Neta, P.: J. Chem. Soc. B, 742-747, 1966.

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

Kraljić, I. and Trumbore, C. N.: J. Am. Chem. Soc. 87(12), 2547-2550, 1965.

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



T-dependent rate constants for the reaction of propane-1,3-diol with HO in aqueous solution. Data from Anbar et al. (1966) and Hoffmann et al. (2009).