IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ_OH_42

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HO (aq) + $CH_3CHOHCH_2OH$(aq) → products

Rate coefficient data

k/ L mol^{-1} s^{-1}	T/K	pH	I/ mol L^{-1}	Reference	Technique/ Comments
Relative Rate Coefficients					
1.68×10^9	294	7	-	Adams et al., 1965	PR / UV-Vis (a)
1.7×10^9	294	9	-	Anbar et al., 1966	PR / UV-Vis (b)
$(1.6 \pm 0.3) \times 10^9$	298	7	-	Hoffmann et al., 2009	LFP-LPA (c)
9.37×10^{10} exp[-(1200 ± 340)/T]	288 - 328	7	-		LFP-LPA (c1)

$\Delta G_R°$ (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 $M^{-1}s^{-1}$; rate constnats have been recalculated using the selected values for the reference reactions (1.10×10^{10} $M^{-1}s^{-1}$); 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) Reference reaction: HO + PNDA (p-nitrosodimethylaniline); reference rate constant was determined versus ethanol with k(HO + ethanol) = 1.10×10^9 $M^{-1}s^{-1}$; recalculation of the rate coefficient was performed using the selected value for the reference reaction (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.

(c) Radicals generated by laser flash photolysis of H_2O_2 ($c(H_2O_2) = 1 \times 10^{-4}$ M) at 248 nm (LF-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 the temperature dependent reference reaction by Zhu et al., 2003; c(KSCN) = 1.59×10^{-5} M. Arrhenius expression (c1) was calculated using the recalculated experimental data from Hoffmann et al. (2009).

Preferred Values

Parameter	Value	*T*/K
k / L mol^{-1} s^{-1}	1.75×10^{9}	298
k / L mol^{-1} s^{-1}	8.32×10^{10} exp[-(1200)/T]	288 – 328

Reliability

$\Delta \log k$	±0.15	298
$\Delta E_A/R$	±240	288 - 328

Comments on Preferred Values

The room temperature rate coefficients determined by Adams et al. (1965), Anbar et al. (1966) and the T-dependent data by Hoffmann et al. (2009) have been used for regression. As the room temperature rate coefficients contribute perfectly to the Arrhenius expression of Hoffmann et al., the result is the mean of them, with an estimated uncertainty of $\Delta \log k = \pm 0.15$ or ±33%.

References

Adams, G.E.; Boag, J.W.; Currant, J. and Michael, B.D., Pulse Radiolysis, Ebert, M.; Keene, J.P.; Swallow, A.J. and Baxendale, J.H. (eds.): Academic Press, New York, p.131-143, 1965.

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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.

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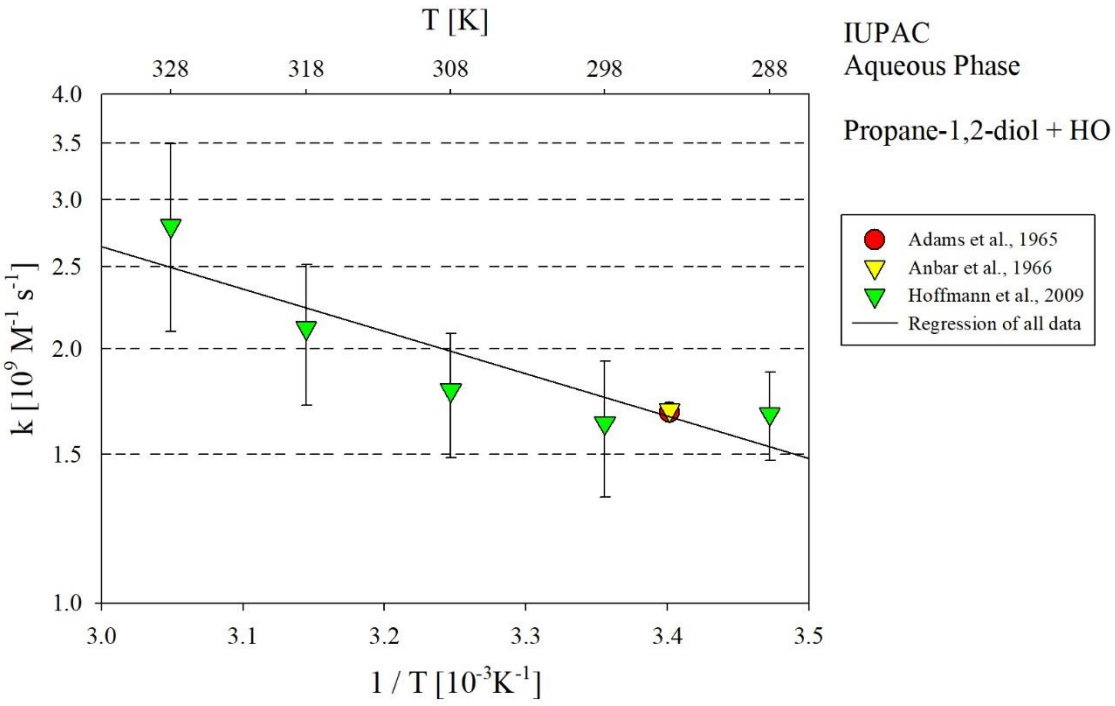

T-dependent rate constants for the reaction of propane-1,2-diol with HO in aqueous solution. All available data has been used for regression.