IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ_OH_62

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$H_2O + CH_3CH_2CHO$ (aq) → $CH_3CH_2CH(OH)_2$ (aq) **(1)**

HO (aq) + CH_3CH_2CHO (aq) → **products** **(2)**

HO (aq) + $CH_3CH_2CH(OH)_2$ (aq) → **products** **(3)**

Rate coefficient data

k/ L mol^{-1} s^{-1}	T/K	pH	I/ mol L^{-1}	Reference	Technique/ Comments
Absolute Rate Coefficients					
$(2.8 \pm 0.3) \times 10^9$	298	6.1	-	Hesper, 2003	LP-LPA (a)
2.6×10^{11} exp[-(1300 ± 300)/T]	283 - 313	6.1	-		
Relative Rate Coefficients					
$(2.33 \pm 0.06) \times 10^9$	298	5.2	-	Mezyk, 1994	PR / UV-Vis (b)
8.01×10^{13} exp[-(3100 ± 100)/T]	275 - 310	5.2	-		PR / UV-Vis (b)
$(3.65 \pm 0.5) \times 10^9$	298	2	-	Monod et al., 2005	Fenton reaction (c)

The equilibrium constant for the hydration (1) is recommended as $K_{298\,K} = 0.85$ by Doussin and Monod (2013).

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

Comments

(a) Direct observation of the peroxyl-radicals at 248 nm, formed by the reaction between HO, propanal and O_2. Reviewed by Herrmann (2003).

(b) Reference reaction: HO + SCN^- with k(HO + SCN^-) = 1.22×10^{10} $M^{-1}s^{-1}$ according to Chin and Wine (1992); recalculation has been performed using the selected T dependence for the reference reaction by Zhu et al. (2003); experiments were performed in deoxygenated N_2O / N_2 saturated solutions.

(c) Radicals generated by dark Fenton reaction; Global rate constant for the reaction of HO radicals with propanal (2) and its hydrate (3) has been determined; $K_{298\,K}$ was considered to be 0.71 (Bell and Evans, 1966); no specific information given on the reference reactions

used for the determination; in general, multiple references were used: HO + methanol; $k(T) = 9.7 \times 10^8 \exp[-4800/R(1/T-1/298)]$ (Elliot and Simsons, 1984); HO + 2-propanol; $k(T) = 1.6 \times 10^9 \exp[-5000/R(1/T-1/298)]$ (Elliot and Simsons, 1984); HO + formaldehyde; $k(T) = \exp[-1020\pm90\ (1/T)]$ (Chin and Wine, 1994).

Preferred Values

Parameter	Value	*T*/K
k / L mol^{-1} s^{-1}	2.53×10^9	298
k / L mol^{-1} s^{-1}	$8.25 \times 10^{12} \exp[-(2400)/T]$	275 - 313

Reliability

$\Delta \log k$	±0.24	298
$\Delta E_A/R$	±400	275 – 313

Comments on Preferred Values

Data from Mezyk (1994) and Hesper (2003) were used for regression. The rate coefficient determined by Monod et al. (2005) could not be used for further evaluation, as the publication does not identify the specific reference reactions. It is assumed that the value given results from a mean of determinations versus several reference systems. It is therefore not included in the regression for the determination of the preferred value. The estimated uncertainty of the recommended rate coefficient is given as $\Delta \log k = \pm0.24$ or ±50%

References

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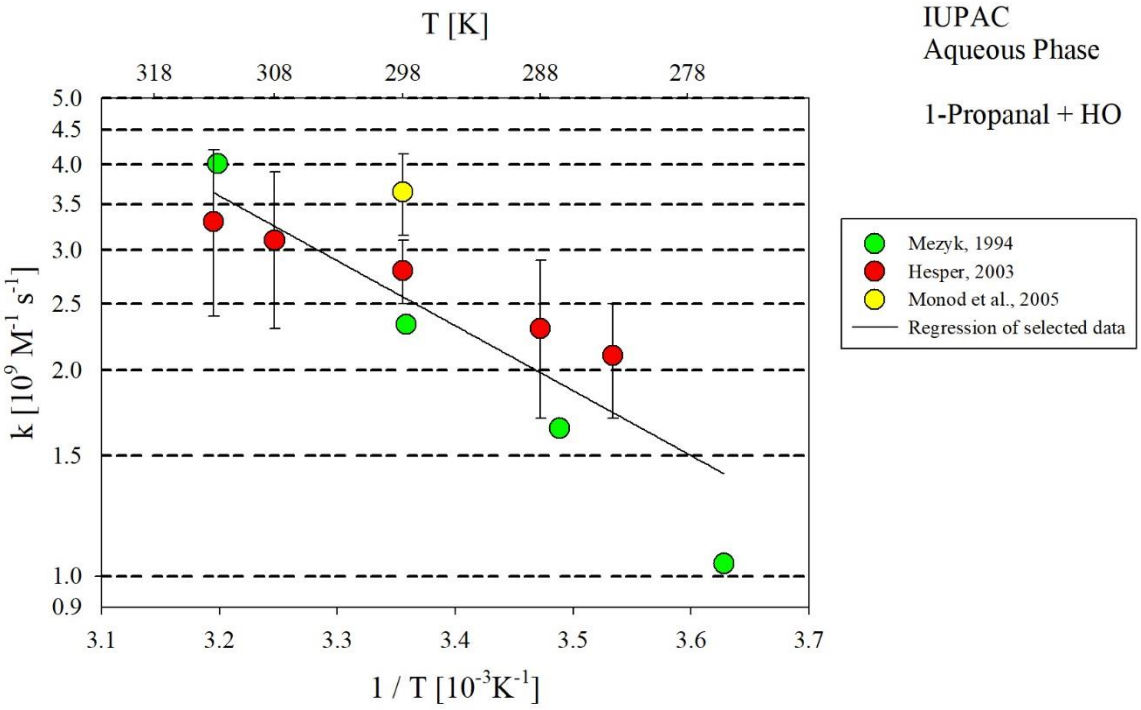

T-dependent rate coefficients for the reaction of 1-propanal with HO in aqueous solution. Data from Mezyk (1994) and Hesper (2003) have been used for regression.