IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ_OH_6

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

HO (aq) + $CH_3CH_2CH(OH)CH_3$ (aq) → Products

Rate coefficient data

k/ l mol^{-1} s^{-1}	T/K	pH	I/ mol l^{-1}	Reference	Technique/ Comments
Absolute Rate Coefficients					
$3.5 \pm 0.4 \times 10^9$ $4.7 \pm 0.8 \times 10^9$ $6.3 \pm 0.5 \times 10^9$ $6.8 \pm 1.4 \times 10^9$ $6.3 \pm 1.2 \times 10^9$ $7.3 \pm 2.5 \times 10^9$ $5.4 \pm 3.0 \times 10^9$	298	5.8	0 0.5 (0.46) 1.0 (0.85) 1.5 (1.21) 2.0 (1.53) 2.5 (1.83) 3.0 (2.11)	Hesper, 2003	LP/LPA (a1)
7.4×10^{10} exp[-(910 ± 330)K/T]	288-328	-	-		LP/LPA (a2)
Relative Rate Coefficients					
3.1×10^9	294	7	-	Adams et al., 1965	PR/UV-vis (b)
2.4×10^9	294	9	-	Anbar and Neta, 1966	CW-radiolysis /UV-vis (c)
2.8×10^9	294	2	-	Scholes and Willson, 1967	CW-radiolysis /UV-vis (d)

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

Comments

(a) Product formation observed at 260 nm; direct observation of optical absorption of the peroxyl-radicals formed by the reaction between HO, 2-Butanol and O_2; oxygen saturated solutions (a1): determination of ion strength influence; $NaClO_4$ was used to adjust the ion strength; the numbers given in parenthesis refer to the calculated effective ion strength; (a2): determination of the temperature influence from 288-328 K; the Arrhenius expression was calculated using these values. Reviewed by Herrmann (2003).

(b) Product formation observed at 500 nm; reference reaction: HO + SCN^-; k(HO + SCN^-) = 6.6×10^9 $M^{-1}s^{-1}$; the rate coefficient has been recalculated using the selected value for the reference reaction (1.10×10^{10} $M^{-1}s^{-1}$, Zhu et al., 2003); No exact value is given for the initial

concentrations of the reactants ('a few millimolar'); air or oxygen saturated solutions; as no exact temperature is given, for room temperature T = 294 K is assumed.

(c) Reference reaction: HO + PNDA (p-nitrosodimethylaniline); rate coefficient for the reference reaction was determined versus ethanol with k(HO + ethanol) = 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, for room temperature T = 294 K is assumed.

(d) Product formation observed at 264 nm; Reference reaction: HO + thymine; k(HO + thymine) = $(4.3 \pm 1) \times 10^9$ $M^{-1}s^{-1}$; the rate coefficient has been recalculated using the selected value for the reference reaction (5.38×10^9 $M^{-1}s^{-1}$); c(thymine) = 8×10^{-5} - 2×10^{-4} mol/l ; The rate coefficient of the reference reaction was determined relative to benzene ; aerated solutions ; The absolute rate coefficients in table 3 have an error of about ±25%; as no exact temperature is given, for room temperature T = 294 K is assumed.

Preferred Values

Parameter	Value	T/K
k / l mol^{-1} s^{-1}	3.19×10^9	298
k / l mol^{-1} s^{-1}	2.53×10^{11} exp[-(1300) / T]	288 – 328

Reliability

$\Delta \log k$	± 0.04	298
$\Delta E_A/R$	± 330	288 – 328

Comments on Preferred Values

The recommended value is a combination of the more recent determination by Hesper et al. (2003) and the three room temperature rate coefficients of Adams et al. (1965), Anbar and Neta (1966) and Scholes and Willson (1967). The error of the room temperature rate coefficient is estimated to be $\Delta \log k = \pm 0.04$ or ±10%. The data by Hesper essentially confirm the older value by an independent measurement.

References

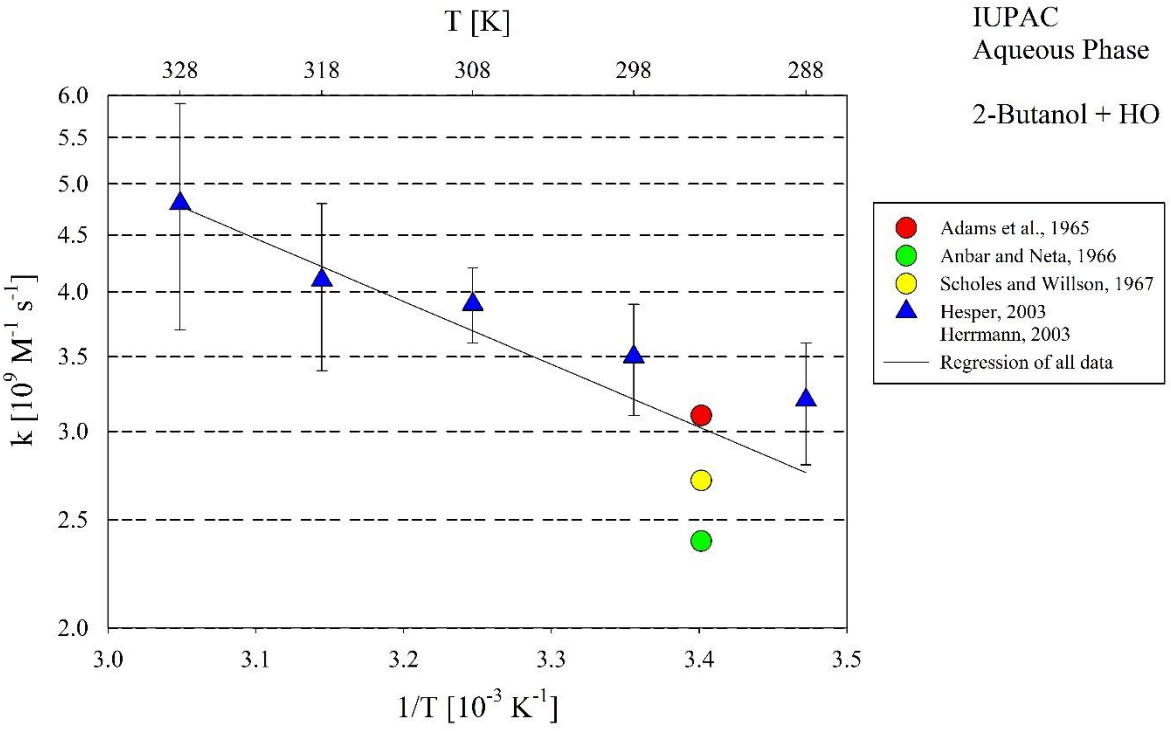
Adams, G.E., Boag, J.W., Currant, J. and Michael, B.D., Pulse Radiolysis, Ebert, M., Keene, J.P., Swallow, A.J. and Baxendale, J.H. (eds.): Academic Press, New York, 131-143, 1965.

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

Herrmann, H.: Chem. Rev., 103(12), 4691-4716, 2003.

Hesper, J.: Ph.D. Dissertation, University of Leipzig, Leipzig, Germany, 2003.

Scholes, G. and Willson, R. L.: Trans. Faraday Soc., 63, 2983-2993, 1967.



T-dependent rate coefficients for the reaction of 2-Butanol with HO radicals in aqueous solution. All data has been used for regression.