IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ_OH_9

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

HO (aq) + $CH_3(CH_2)_4OH$ (aq) → products

Rate coefficient data

k/ l mol^{-1} s^{-1}	T/K	pH	I/ mol l^{-1}	Reference	Technique/ Comments
Relative Rate Coefficients					
4.8×10^9	294	9	-	Anbar et al., 1966	CW-radiolysis /UV-vis (a)
5.1×10^9	294	2	-	Scholes and Willson, 1967	CW-radiolysis /UV-vis (b)
5.5×10^9	294	5	-		
3.9×10^9	294	-	-	Reuvers et al., 1973	PR/UV-vis (c1)
3.7×10^9	294	-	-		PR/UV-vis (c2)
$(5.1 \pm 0.2) \times 10^9$	298	-	-	Stemmler and von Gunten, 2000	CW-radiolysis /GC-FID (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) Reference reaction: HO + PNDA (p-nitrosodimethylaniline); the reference rate coefficient 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, T = 294 K is assumed for room temperature.

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

(c) Reference reactions: HO + $[Fe(CN)_6]^{4-}$ with k(HO + $[Fe(CN)_6]^{4-}$) = 0.93×10^{10} $M^{-1}s^{-1}$ [1.03×10^{10} $M^{-1}s^{-1}$](c1); HO + SCN^- with k(HO + SCN^-) = 1.1×10^{10} $M^{-1}s^{-1}$

[1.10 × 10^{10} $M^{-1}s^{-1}$, Zhu et al., 2003](c2); the recalculation of the rate coefficients has been done, using the selected values for the reference systems given in brackets; as no exact temperature is given, T = 294 K is assumed for room temperature.

(d) Reference reaction: HO + n-butanol with k(HO + n-butanol) = 4.2 × 10^9 $M^{-1}s^{-1}$ (Buxton et al., 1988; the rate coefficient has been recalculated using the recommened value for the reference reaction of 4.3 × 10^9 $M^{-1}s^{-1}$.

Preferred Values

Parameter	Value	*T*/K
k /L mol^{-1} s^{-1}	4.7 × 10^9	294
Reliability		
Δ log k	± 0.06	294

Comments on Preferred Values

The one most recent re-determination indicates that the rate coefficient might be somewhat higher than the value of 3.9 × 10^9 $M^{-1}s^{-1}$, recommended by Buxton et al. (1988). Hence, the average of all available recalculated rate coefficients is recommended. The recommended value is in agreement with both Buxton et al. (1988) as well as Stemmler and von Gunten (2000) within its error limits. The uncercainty is estimated to be ±15% or Δ log k = ±0.06. It should be noted that this rate coefficient refers to room temperature, which is estimated as T = 294 K.

References

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

Stemmler, K. and von Gunten, U.: Atmos. Environ., 34(25), 4241-4252, 2000.

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