IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ_OH_7

This datasheet last evaluated: May 28th 2017; last change in preferred values: January 20th 2016

$OH(aq) + (CH_3)_2CHCH_2OH\ (aq) \rightarrow$ Products

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

Rate coefficient data

k/ l mol^{-1} s^{-1}	T/K	pH	I/ mol l^{-1}	*Reference*	Technique/ Comments
Relative Rate Coefficients					
2.00×10^9	-	7	-	Adams et al., 1965	PR/UV-vis abs. (a)
2.1×10^9	-	9	-	Anbar et al., 1966	CW-radiolysis /UV-vis abs. (b)
3.7×10^9	-	2	-	Scholes and Willson, 1967	CW-radiolysis /UV-vis abs. (c)
2.6×10^9	-	-	-	Reuvers et al., 1973	PR/UV-vis abs. (d1)
3.6×10^9	-	-	-		PR/UV-vis abs. (d2)
3.3×10^9	298	-	-	Buxton et al., 1988	Average value (e1)
3.3×10^9	298				Recalculated value (e2)
2.9×10^9	298				Recalculated value (e3)

Comments

(a) Radicals generated by pulse-radiolysis, products analysed by UV-vis-spectroscopy (500 nm); Carbonate, thiocyanate or selenite were used as reference systems; here: thiocyanate reference: ·OH + SCN^-; k(·OH + SCN^-) = 6.6×10^9 $M^{-1}s^{-1}$; No exact value is given for the initial concentrations of the reactants ('a few millimolar') ; air or oxygen saturated solutions. NIST lists these values as 3.3×10^9 $M^{-1}s^{-1}$, relative to k(OH + SCN^-) = 1.1×10^{10} $M^{-1}s^{-1}$
http://kinetics.nist.gov/solution/Detail?id=1965ADA/BOA131-143B:38

(b) Radicals generated by CW-irradiation, products analysed by UV-vis-spectroscopy; Reference reaction: ·OH + PNDA (p-nitrosodimethylaniline); no values given for initial concentrations; no values given for the reference rate constants; air saturated

solutions; all experiments were repeated at least four times and the coefficient of variation was less than ± 10%

(c) Radicals generated by CW-irradiation, products analysed by UV-vis-spectroscopy (264 nm); Reference reaction: ·OH + thymine; k(·OH + thymine) = (4.3 ± 1) × 10^9 $M^{-1}s^{-1}$; c(thymine) = 8 × 10^{-5} - 2 × 10^{-4} mol/l ; The rate constant of the reference reaction was determined relative to benzene ; aerated solutions ; The absolute rate constants in table 3 have an error of about ± 25%

(d) Radicals generated by pulse-radiolysis, products analysed by UV-vis-spectroscopy; ferrocyanide (d_1) and thiocyanate (d_2) were used as reference systems; ferrocyanide reference: ·OH + $[Fe(CN)_6]^{4-}$; k(·OH + $[Fe(CN)_6]^{4-}$) = 0.93 × 10^{10} $M^{-1}s^{-1}$; thiocyanate reference: ·OH + SCN^-; k(·OH + SCN^-) = 1.1 × 10^{10} $M^{-1}s^{-1}$. NIST lists these values as (d1) 2.9 × 10^9 $M^{-1}s^{-1}$, relative to k(OH + $Fe(CN)_6^{-4}$) = 1.0 × 10^{10} $M^{-1}s^{-1}$ and (d2) 3.6 × 10^9 $M^{-1}s^{-1}$, relative to k(OH + SCN^-) = 1.1 × 10^{10} $M^{-1}s^{-1}$.
http://kinetics.nist.gov/solution/Detail?id=1973REU/GRE533-536:8
http://kinetics.nist.gov/solution/Detail?id=1973REU/GRE533-536:9

(e) Buxton et al. calculated the average value of three rate constants (e1), determined by the original authors that were recalculated, using the selected rate constants for reference reactions; Adams et al. (1965)[3.3 × 10^9 $M^{-1}s^{-1}$, relative to k(OH + SCN^-) = 1.1 × 10^{10} $M^{-1}s^{-1}$ (e2)] and Reuvers et al. (1973)[2.9 × 10^9 $M^{-1}s^{-1}$, relative to k(OH + $Fe(CN)_6^{-4}$) = 1.0 × 10^{10} $M^{-1}s^{-1}$ (e3) and 3.6 × 10^9 $M^{-1}s^{-1}$, relative to k(OH + SCN^-) = 1.1 × 10^{10} $M^{-1}s^{-1}$].

Preferred Values

Parameter	Value	*T*/K
k /L mol^{-1} s^{-1}	3.3 × 10^9	298
Reliability		
Δ log k	± 0.04	298

Comments on Preferred Values

The recommended value is the same as recommended by Buxton et al. (1988) as there have been no new kinetic studies of this system since then which warrant a new recommendation. The uncertainty of the recommendation is estimated as ± 10 %.

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.

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Reuvers, A. P., Greenstock, C. L., Borsa, J., and Chapman, J. D.: Int. J. Rad. Biol., 24(5), 533-536, 1973.

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