IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ_OH_7

This datasheet last evaluated: November 2019; last change in preferred values: November 2019

HO(aq) + $(CH_3)_2CHCH_2OH$ (aq) → Products

Rate coefficient data

k/ l mol^{-1} s^{-1}	T/K	pH	I/ mol l^{-1}	Reference	Technique/ Comments
Relative Rate Coefficients					
3.3×10^9	294	7	-	Adams et al., 1965	PR/UV-vis abs. (a)
3.59×10^9	294	9	-	Anbar et al., 1966	CW-radiolysis /UV-vis abs. (b)
4.6×10^9	294	2	-	Scholes and Willson, 1967	CW-radiolysis /UV-vis abs. (c)
2.9×10^9	294	-	-	Reuvers et al., 1973	PR/UV-vis abs. (d1)
3.6×10^9	294	-	-		PR/UV-vis abs. (d2)

$\Delta G_R°$ (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 500 nm; reference reaction: HO + SCN^-; k(HO + SCN^-) = 6.6×10^9 $M^{-1}s^{-1}$; rate constants have been recalculated using the selected value for the reference reaction (1.10×10^{10} $M^{-1}s^{-1}$) ; 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.

(b) Reference reaction: HO + PNDA (p-nitrosodimethylaniline); the reference rate constant 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.

(c) 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 constants have been recalculated using the selected value for reference reactions (5.38×10^9 $M^{-1}s^{-1}$); 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%; as no exact temperature is given, for room temperature T = 294 K is assumed.

(d) Radicals generated by pulse-radiolysis, products analysed by UV-vis-spectroscopy; reference systems: HO + $[Fe(CN)_6]^{4-}$ with k(HO + $[Fe(CN)_6]^{4-}$) = 0.93×10^{10} $M^{-1}s^{-1}$ [1.03×10^{10} $M^{-1}s^{-1}$](d1); HO + SCN^-; k(HO + SCN^-) = 1.1×10^{10} $M^{-1}s^{-1}$ [1.10×10^{10} $M^{-1}s^{-1}$ (Zhu et al., 2003)](d2) ; rate constants have been recalculated using the selected values for the reference reactions given in brackets; 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}	3.60×10^9	294
Reliability		
$\Delta \log k$	± 0.04	294

Comments on Preferred Values

The recalculation using current rate coefficients for the reference reactions indicated a slightly higher rate coefficient than suggested by Buxton et al. (1988). The preferred value agrees with that recommendation of 3.3×10^{10} $M^{1}s^{-1}$ within the estimated uncertainty of 10%. It should be noted that the recommendation refers to ‘room temperature’ but was not specified in any of the studies, so T = 294 K is assumed.

References

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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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