IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ_OH_50

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

HO (aq) + $HOC(CH_3)_2C(CH_3)_2OH$ (aq) → products

Rate coefficient data

k/ L mol^{-1} s^{-1}	T/K	pH	I/ mol L^{-1}	Reference	Technique/ Comments
Relative Rate Coefficients					
5.5×10^8	294	9	-	Anbar et al., 1966	PR / UV-Vis (a)

$\Delta G_R°$ (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 constant was determined versus ethanol with k(HO + ethanol) = 1.10×10^9 $M^{-1}s^{-1}$; the recalculation of the rate coefficient was performed using the selected value for the reference reaction (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 temperature is given, for room temperature T = 294 K is assumed.

Preferred Values

Parameter	Value	*T*/K
k / L mol^{-1} s^{-1}	5.47×10^8	298
Reliability		
$\Delta \log k$	±0.15	298

Comments on Preferred Values

The only available rate constant determined by Adams et al. (1965), has been recalculated using the recommended rate constant for the reference reaction. The uncertainty of the recommended value is estimated to ±33 % or $\Delta \log k = 0.15$. It should be noted that this rate coefficient refers to room temperature, which we estimate as T = 294 K.

References

Anbar, M., D. Meyerstein, and P. Neta: Journal of the Chemical Society B: Physical Organic, 742-747, 1966.