

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ_OH_49

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HO (aq) + HO(CH₂)₆OH(aq) → products

Rate coefficient data

$k / \text{L mol}^{-1} \text{s}^{-1}$	T/K	pH	I/ mol L ⁻¹	Reference	Technique/ Comments
<i>Relative Rate Coefficients</i>					
4.6×10^9	294	9	-	Anbar et al., 1966	PR / UV-Vis (a)

ΔG_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); reference rate constant was determined versus ethanol with $k(\text{HO} + \text{ethanol}) = 1.10 \times 10^9 \text{ M}^{-1}\text{s}^{-1}$; a recalculation of the rate coefficient was performed using the newly recommended value for the reference reaction ($1.88 \times 10^9 \text{ M}^{-1}\text{s}^{-1}$); 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 $\pm 10\%$; as no temperature is given, for room temperature $T = 294 \text{ K}$ is assumed.

Preferred Values

Parameter	Value	T/K
$k / \text{L mol}^{-1} \text{s}^{-1}$	4.6×10^9	294
<i>Reliability</i>		
$\Delta \log k$	± 0.15	294

Comments on Preferred Values

The recalculation of the only available kinetic data leads to a rate coefficient which is slightly lower than the original value. The uncertainty of the recommended rate constant is estimated as $\pm 33\%$ or $\Delta \log k = \pm 0.15$. It should be noted that this rate coefficient refers to room temperature, which is estimated as $T = 294 \text{ K}$.

References

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

Buxton, G. V., Greenstock, C. L., Helman, W. P. and Ross, A. B.: J. Phys. Chem. Ref. Data, 12(2), 513 – 886, 1988.