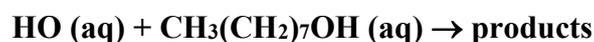


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ_OH_16

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



Rate coefficient data

$k / \text{l mol}^{-1} \text{s}^{-1}$	T/K	pH	$I / \text{mol l}^{-1}$	Reference	Technique/ Comments
<i>Relative Rate Coefficients</i>					
6.5×10^9	294	2.0 - 2.2	-	Scholes and Willson, 1967	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) Aerated solutions of thymine ($8 \times 10^{-5} \text{ M}$) were irradiated. Reference reaction: HO + thymine with $k(\text{HO} + \text{thymine}) = (4.3 \pm 1) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$, determined relative to benzene ($k(\text{HO} + \text{benzene}) = (4.3 \pm 0.9) \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$); the rate coefficient was recalculated using the selected rate coefficient for the reference reaction ($5.38 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$); an error of about $\pm 25\%$ for absolute rate coefficients is given by the authors; as no exact temperature is given, $T = 294 \text{ K}$ is assumed for room temperature.

Preferred Values

Parameter	Value	T/K
$k / \text{l mol}^{-1} \text{s}^{-1}$	6.5×10^9	294
<i>Reliability</i>		
$\Delta \log k$	± 0.15	294

Comments on Preferred Values

The only available kinetic data are those of Scholes and Willson (1967). In 1988, Buxton et al. recommended a rate coefficient of $7.7 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$. After the evaluation of the rate coefficients of reference reactions, the rate coefficient measured by Scholes and Willson was recalculated. A slightly lower rate constant than recommended before was obtained. Its uncertainty is estimated

as $\pm 33\%$ or $\Delta \log k = \pm 0.15$ as the standard value for single determinations. It should be noted that this rate coefficient refers to room temperature, which we estimate as $T = 294 \text{ K}$.

References

Buxton, G. V., Greenstock, C. L., Helman, W. P., and Ross, A. B: J. Phys. Chem. Ref. Data, 17(2), 513-886, 1988.

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