

## IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

### – Data Sheet AQ\_OH\_15

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#### 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>					
$6.1 \times 10^9$	294	2.0-2.2	-	Scholes and Willson, 1967	PR/UV-Vis(a)

$\Delta G_R^\circ$  (aq): Aqueous phase thermochemical data not available. As well, gas phase thermochemical data  $H_R^\circ$  (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
$k / \text{l mol}^{-1} \text{s}^{-1}$	$6.1 \times 10^9$	294
<i>Reliability</i>		
$\Delta \log k$	$\pm 0.15$	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  $7.4 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ . Following the evaluation of the rate coefficients of reference reactions, the recalculation of the rate coefficient measured leads to a

slightly lower value than the one recommended before. Considering the uncertainty of the rate coefficient, both values still agree within error limits. The estimated uncertainty of the recommended rate constant is  $\pm 33\%$  or  $\Delta \log k = 0.15$ . The uncertainty is chosen as a 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, 12(2), 513 – 886, 1988.

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