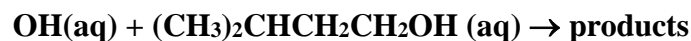


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ_OH_12

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This datasheet last evaluated: November 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>					
3.8×10^9	294	-	-	Reuvers et al., 1973	PR / UV-vis (a1)
3.8×10^9	294	-	-		PR / UV-vis (a2)

ΔG_R° (aq): Aqueous phase thermochemical data not available. As well, gas phase thermochemical data H_R° (g) are not available.

Comments

- (a) Reference systems: $\text{HO} + [\text{Fe}(\text{CN})_6]^{4-}$ with $k(\text{HO} + [\text{Fe}(\text{CN})_6]^{4-}) = 0.93 \times 10^{10} \text{ M}^{-1}\text{s}^{-1}$ [$1.03 \times 10^{10} \text{ M}^{-1}\text{s}^{-1}$](a1); $\text{HO} + \text{SCN}^-$ with $k(\text{HO} + \text{SCN}^-) = 1.1 \times 10^{10} \text{ M}^{-1}\text{s}^{-1}$ [$1.10 \times 10^{10} \text{ M}^{-1}\text{s}^{-1}$, Zhu et al., 2003](a2); rate coefficients were re-calculated, using the selected rate coefficients for reference reactions given in brackets; as no exact temperature is given, $T = 294 \text{ K}$ is assumed for room temperature.

Preferred Values

Parameter	Value	T/K
$k / \text{L mol}^{-1} \text{s}^{-1}$	3.8×10^9	294
<i>Reliability</i> $\Delta \log k$	± 0.09	294

Comments on Preferred Values

The only available kinetic data are those of Reuvers et al. (1973). Their determination was confirmed by using two different reference systems. The change of the reference rate coefficient leads to a rate constant slightly larger than the former recommendation by Buxton et al. in 1988.

The uncertainty is estimated to be $\pm 20\%$ or $\Delta \log k = 0.09$. 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.

Reuvers, A. P., Greenstock, C. L., Borsa, J. and Chapman, J. D.: *Int. J. Rad. Biol.*, 24(5), 533-536, 1973.

Zhu, L., Nicovich, J. M. and Wine, P. H.: *Aquat. Sci.*, 65(4), 425-435, 2003.