IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ_OH_46

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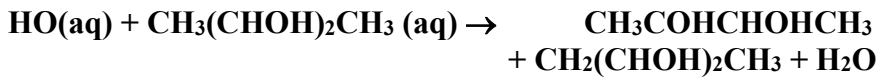

(product distribution suggested by Buxton et al., 1988)

Rate coefficient data

k/ L mol^{-1} s^{-1}	T/K	pH	I/ mol L^{-1}	Reference	Technique/ Comments
Relative Rate Coefficients					
1.35×10^9	294	-	-	Adams et al., 1965	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 + SCN$^-$ with k(HO+ SCN$^-$) = 6.6×10^9 M^{-1}s^{-1}; the selected reference rate constant $k = 1.10 \times 10^{10}$ M^{-1}s^{-1} was used for recalculation (Zhu et al., 2003); No exact value is given for the initial concentrations of the reactants; pH is given as natural; as no temperature is given in their publication, for room temperature of T = 294 K is assumed.

Preferred Values

Parameter	Value	*T*/K
k / L mol^{-1} s^{-1}	1.35×10^9	294

Reliability

$\Delta \log k$	± 0.15	294

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 recommended value of the rate constant for the reaction, given by Buxton et al. in 1988 also agrees very good with our recommendation when adjusted for the new reference rate constant. The relative error of the recommended rate constant is estimated as ±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

Adams, G.E.; Boag, J.W.; Currant, J. and Michael, B.D., Pulse Radiolysis, Ebert, M.; Keene, J.P.; Swallow, A.J. and Baxendale, J.H. (eds.): Academic Press, New York, p.131-143, 1965.

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

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