IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ\_OH\_46

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**HO(aq) + CH3(CHOH)2CH3 (aq) → CH3COHCHOHCH3**

**+ CH2(CHOH)2CH3 + H2O**

*(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  109 | 294 | - | - | Adams et al., 1965 | PR / UV-Vis (a) |

*GR* (aq): Aqueous phase thermochemical data not available. As well, gas phase thermochemical data *R* (g) are not available.

**Comments**

(a) Reference reaction HO + SCN‑ with *k*(HO+ SCN-) = 6.6  109 M-1s-1; the selected reference rate constant *k* = 1.10 × 1010 M‑1s‑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 × 109 | 294 |

*Reliability*

|  |  |  |
| --- | --- | --- |
| Δ 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 Δlog *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.