IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

 – Data Sheet AQ\_OH\_44

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**HO(aq) + CH3CHOH(CH2)2OH(aq) → products**

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

**Rate coefficient data**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| k/ L mol-1 s-1 | T/K | pH | I/ mol L-1 | Reference | Technique/ Comments |
| *Relative Rate Coefficients* |
| 2.17  109 | 294 | - | - | Adams et al., 1965 | PR / UV-Vis (a) |

**Comments**

(a) Referring to the reference reaction HO + SCN‑ with *k*(HO + SCN-) = 6.6  109 M-1s-1; The rate constant was recalculated with the newly recommended reference rate constant *k* = 1.10 × 1010 M‑1s‑1 after Zhu et al.. 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 | 2.17× 109 | 294 |
|  |  |  |

*Reliability*

|  |  |  |
| --- | --- | --- |
| Δ log *k* | ± 0.15 | 294 |

*Comments on Preferred Values*

The only available room temperature rate constant determined by Adams et al. (1965) has been recalculated with the newly recommended reference rate constant, its uncertainty is estimated to be ±33% or Δ 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.

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