IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

 – Data Sheet AQ\_OH\_12

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OH(aq) + (CH3)2CHCH2CH2OH (aq) → products

**Rate coefficient data**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| k/ l mol-1 s-1 | T/K | pH | I/ mol l-1 | Reference | Technique/ Comments |
| *Relative Rate Coefficients* |
| 3.8 × 109 | 294 | - | - | Reuvers et al., 1973 | PR / UV-vis (a1) |
| 3.8 × 109 | 294 | - | - |  | PR / UV-vis (a2) |

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

**Comments**

1. Reference systems: [HO](http://webbook.nist.gov/cgi/cbook.cgi?ID=3352576&Units=SI) + [Fe(CN)6]4- with *k*(HO + [Fe(CN)6]4-) = 0.93 × 1010 M-1s-1 [1.03 × 1010 M‑1s‑1](a1); [HO](http://webbook.nist.gov/cgi/cbook.cgi?ID=3352576&Units=SI) + SCN- with *k*([HO](http://webbook.nist.gov/cgi/cbook.cgi?ID=3352576&Units=SI) + SCN-) = 1.1  × 1010 M-1s-1 [1.10 × 1010 M‑1s‑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 K is assumed for room temperature.

**Preferred Values**

|  |  |  |
| --- | --- | --- |
| **Parameter** | **Value** | ***T*/K** |
|  |  |  |
| *k* /L mol-1 s-1 | 3.8 × 109 | 294 |
|  |  |  |

*Reliability*

|  |  |  |
| --- | --- | --- |
| Δ 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 ±20% or Δ log *k* = 0.09. It should be noted that this rate coefficient refers to room temperature, which we estimate as T = 294 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.