IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ\_OH\_49

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This datasheet last evaluated: November 2019; last change in preferred values: June 2019

**HO (aq) + HO(CH2)6OH(aq) → products**

**Rate coefficient data**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| k/ L mol-1 s-1 | T/K | pH | I/ mol L-1 | Reference | Technique/ Comments | |
| *Relative Rate Coefficients* | | | | | | |
| 4.6  109 | 294 | 9 | - | Anbar et al., 1966 | 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](http://webbook.nist.gov/cgi/cbook.cgi?ID=3352576&Units=SI) + PNDA (p-nitrosodimethylaniline); reference rate constant was determined versus ethanol with *k*(HO + ethanol) = 1.10 × 109 M‑1s‑1; a recalculation of the rate coefficient was performed using the newly recommended value for the reference reaction (1.88 × 109 M‑1s‑1); no values given for initial concentrations; air saturated solutions; all experiments were repeated at least four times and the coefficient of variation was less than ± 10%; as no temperature is given, for room temperature T = 294 K is assumed.

**Preferred Values**

|  |  |  |
| --- | --- | --- |
| **Parameter** | **Value** | ***T*/K** |
|  |  |  |
| *k* / L mol-1 s-1 | 4.6 × 109 | 294 |
|  |  |  |

*Reliability*

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

*Comments on Preferred Values*

The recalculation of the only available kinetic data leads to a rate coefficient which is slightly lower than the original value. The uncertainty of the recommended rate constant is estimated as ±33 % or Δ log *k* = ±0.15. It should be noted that this rate coefficient refers to room temperature, which is estimated as T = 294 K.

**References**

Anbar, M., Meyerstein, D. and Neta, P.: J. Chem. Soc. B, 742-747, 1966.

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