IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ\_OH\_7

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

**HO(aq) + (CH3)2CHCH2OH (aq)** → **Products**

**Rate coefficient data**

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| k/ l mol-1 s-1 | T/K | pH | | I/ mol l-1 | Reference | | Technique/ Comments | |
| *Relative Rate Coefficients* | | | | | | | | |
| 3.3 × 109 | 294 | 7 | - | | | Adams et al., 1965 | PR/UV-vis abs. (a) |
| 3.59 × 109 | 294 | 9 | - | | | Anbar et al., 1966 | CW-radiolysis /UV-vis abs. (b) |
| 4.6 × 109 | 294 | 2 | - | | | Scholes and Willson, 1967 | CW-radiolysis /UV-vis abs. (c) |
| 2.9 × 109 | 294 | - | - | | | Reuvers et al., 1973 | PR/UV-vis abs. (d1) |
| 3.6 × 109 | 294 | - | - | | |  | PR/UV-vis abs. (d2) |

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

**Comments**

1. Product formation observed at 500 nm; reference reaction: [HO](http://webbook.nist.gov/cgi/cbook.cgi?ID=3352576&Units=SI) + SCN-; *k*([HO](http://webbook.nist.gov/cgi/cbook.cgi?ID=3352576&Units=SI) + SCN-) = 6.6  × 109 M-1s-1; rate constants have been recalculated using the selected value for the reference reaction (1.10 × 1010 M‑1s‑1) ; No exact value is given for the initial concentrations of the reactants (‘a few millimolar’); air or oxygen saturated solutions; as no exact temperature is given, for room temperature T = 294 K is assumed.
2. Reference reaction: [HO](http://webbook.nist.gov/cgi/cbook.cgi?ID=3352576&Units=SI) + PNDA (p-nitrosodimethylaniline); the reference rate constant was determined versus ethanol with *k*(HO + ethanol) = 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 exact temperature is given, for room temperature T = 294 K is assumed.
3. Product formation observed at 264 nm; Reference reaction: [HO](http://webbook.nist.gov/cgi/cbook.cgi?ID=3352576&Units=SI) + thymine; *k*([HO](http://webbook.nist.gov/cgi/cbook.cgi?ID=3352576&Units=SI) + thymine) = (4.3 ±1) × 109M-1s-1; rate constants have been recalculated using the selected value for reference reactions (5.38 × 109 M‑1s‑1); *c*(thymine) = 8 × 10-5 - 2 × 10-4 mol/l ; The rate constant of the reference reaction was determined relative to benzene ; aerated solutions ; The absolute rate constants in table 3 have an error of about ± 25%; as no exact temperature is given, for room temperature T = 294 K is assumed.
4. Radicals generated by pulse-radiolysis, products analysed by UV-vis-spectroscopy; reference systems: [HO](http://webbook.nist.gov/cgi/cbook.cgi?ID=3352576&Units=SI) + [Fe(CN)6]4- with *k*([HO](http://webbook.nist.gov/cgi/cbook.cgi?ID=3352576&Units=SI) + [Fe(CN)6]4-) = 0.93 × 1010 M‑1s‑1 [1.03 × 1010 M‑1s‑1](d1); HO + SCN-; *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)](d2) ; rate constants have been recalculated using the selected values for the reference reactions given in brackets; as no exact temperature is given, for room temperature T = 294 K is assumed.

**Preferred Values**

|  |  |  |
| --- | --- | --- |
| **Parameter** | **Value** | ***T*/K** |
| *k* /L mol-1 s-1 | 3.60 × 109 | 294 |
|  |  |  |

*Reliability*

|  |  |  |
| --- | --- | --- |
| Δ log *k* | ± 0.04 | 294 |
|  |  |  |

*Comments on Preferred Values*

The recalculation using current rate coefficients for the reference reactions indicated a slightly higher rate coefficient than suggested by Buxton et al. (1988). The preferred value agrees with that recommendation of 3.3 × 1010 M1s‑1 within the estimated uncertainty of 10%. It should be noted that the recommendation refers to ‘room temperature’ but was not specified in any of the studies, so T = 294 K is assumed.

**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, 131-143, 1965.

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, 17(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.

Scholes, G., and Willson, R. L.: Trans. Faraday Soc., 63, 2983-2993, 1967.

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