IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

 – Data Sheet AQ\_TH1\_OH\_1

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OH·(aq) + [CH(OH)2]2(aq) → ·C(OH)2CH(OH)2 + H2O (l)

Aqueous phase thermochemical data not available. Thermochemical gas phase data for comparison also not available because of the hydration of glyoxal in aqueous solution.

**Rate coefficient data**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| *k*/ L mol-1 s-1 | *T*/K | *pH* | *I*/ mol L-1 | Reference | Technique/ Comments |
|  |
| *Relative Rate Coefficients* |
| 6.6 × 107 | 298 | 1.3 |  | Buxton et al., 1988 | (a) |
| (1.10 ± 0.04) × 109 | 293 | 2.0 – 6.0 |  | Buxton et al., 1997 | PR-UV/Vis (b1) |
| (1.10 ± 0.1) × 109 | 293 | 4 |  | PR-UV/Vis (b2) |
| 1.9 × 1011 exp[(-1516 ± 30)/T] | 279 - 319 | 4 |  |
| (9.4 ± 0.4) × 108 | 298 | 2.0 |  | Schaefer et al., 2015 | LFP (c) |
| (9.2 ± 0.5) × 108 | 298 | 6.0 |  |
| (1.1 ± 0.1) × 109 | 298 | 9.0 |  |
| 5.8 × 1010 exp[(‑1200 ± 120)/T] | 278 - 318 | 6.0 |  |

**Comments**

1. Buxton et al. refers to a value determined by Draganic and Marcovic (1968, unpublished work) in their review, relative to [·OH](http://webbook.nist.gov/cgi/cbook.cgi?ID=3352576&Units=SI) + oxalic acid; for the rate constant of oxalic acid, Buxton et al. recommends *k*([·OH](http://webbook.nist.gov/cgi/cbook.cgi?ID=3352576&Units=SI) + oxalic acid) = 1.4 × 109 M‑1 s‑1; these values are also given in the NIST database.

<http://kinetics.nist.gov/solution/Detail?id=1968DRA/MARB:1>

1. Measured in N2O-saturated solution; competition kinetics; reference reaction: [·OH](http://webbook.nist.gov/cgi/cbook.cgi?ID=3352576&Units=SI) + Fe(CN)64- with *k*([·OH](http://webbook.nist.gov/cgi/cbook.cgi?ID=3352576&Units=SI) + Fe(CN)64-) = 1.0 × 1010  M-1 s-1 (Buxton et al., 1988); measured at λ = 420 nm; the rate constant has been confirmed by direct observation; temperature dependent data was gathered via direct observation with no specific values for *k*(T) given; activation energy is given as EA = (12.6 ± 0.9) kJ mol-1; Arrhenius expression was calculated using the given data; reviewed by Schaefer et al. (2015).
2. Reference reaction (RR): [·OH](http://webbook.nist.gov/cgi/cbook.cgi?ID=3352576&Units=SI) + SCN-; rate constant is given by *k*(T) = 7.26 × 1012 exp[(-1900 ± 190) / T] M-1s-1 according to Chin and Wine (1992) (at pH = 6). An activation energy EA of (12.6 ± 0.9) kJ mol-1 was obtained from direct measurements of *k*.

**Preferred Values**

|  |  |  |
| --- | --- | --- |
| **Parameter** | **Value** | ***T*/K** |
|  |  |  |
| *k* / l mol-1 s-1 | 9.2 × 108 | 298 |
| *k* / l mol-1 s-1 | 5.8 × 1010 · exp[- (1200)/T] | 278 - 318 |
|  |  |  |

*Reliability*

|  |  |  |
| --- | --- | --- |
| Δ log *k* | ± 0.390 | 298 |
| Δ EA/R | ± 120 | 278 - 318 |

*Comments on Preferred Values*

The recent T-dependent determination by Schaefer at al. (2015) leads to a slightly lower rate constant than suggested by Buxton et al. in the first determination of this rate constant when the data for pH 6 are compared. The value previously recommended by Buxton et al. (1988) as determined by Draganic and Marcovic (1968, unpublished) is not confirmed by the later determinations.

**References**

Adams, G. E., and R. L. Willson: Trans. Faraday Soc., 65, 2981-2987, 1969.

Buxton, George V., Malone, T. N. and Salmon, G. Arthur: J. Chem. Soc., Faraday Trans., **93**, 2889-2891, 1997.

Chin, M., and Wine, P. H: J. Photochem. Photobiol., A, 69(1), 17-25, 1992.

Ervens, B., and Volkamer, R.: Atmos. Chem. Phys., 10 (17), 8219 – 8244, 2010.

Schaefer, T., van Pinxteren, D., and Herrmann, H.: Environ. Sci. Technol., 49, 343 – 350, 2015.



Figure 1: T-dependent rate constants for the reaction of glyoxal with OH in aqueous solution.
Data from Buxton et al. (1997) and Schaefer et al. (2015).