IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

 – Data Sheet AQ\_TH1\_OH\_3

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This datasheet last evaluated: May 2016; last change in preferred values: May 2016

**OH·(aq) + CH(OH)2COOH(aq) → ·C(OH)2COOH + H2O (1)**

**OH·(aq) + CH(OH)2COO-(aq) → ·C(OH)2COO- + H2O (2)**

*GR*° (aq): Aqueous phase thermochemical data not available. Gas phase data for comparison also not available.

**Rate coefficient data**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| *k*/ L mol-1 s-1 | *T*/K | *pH* | *I*/ mol L-1 | Reference | Technique/ Comments |
| *Relative Rate Coefficients* |
| *k1* = (3.6 ± 0.2) × 108 | 298 | 1 |  | Ervens et al. 2003 | LP(a) |
| *k1* = 8.1 × 109  exp[- (1000 ± 400) / *T*] | 288 - 328 |
| *k2* = (2.6 ± 0.9) × 108 | 298 | 8 |  |
| *k2* = 6.0 × 1015  exp[- (4500 ± 800) / *T*] | 288 - 328 |

Glyoxylic acid is hydrated in water, as shown in the following equation:

CHOCOOH + H2O (1) → CH(OH)2COOH(aq) with K = 5.4 M-1, (Sørensen et al., 1974)

pKa value for glyoxylic acid can be found in Lide (1996) (pKa = 3.18).

**Comments**

1. Laser photolysis of H2O2 (c = 5 × 10-4 M, λ = 248 nm); pH adjusted to pH = 1 by HClO4.  Analysis light at λ = 436 nm; 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 after Chin and Wine (1992) (at pH = 6).

**Preferred Values**

|  |  |  |
| --- | --- | --- |
| **Parameter** | **Value** | ***T*/K** |
|  |  |  |
| *k1* / l mol-1 s-1 | 3.6 × 108 | 298 |
| *k1* / l mol-1 s-1 | 8.1 × 109  exp[- (1000) / *T*] | 293-353 |
|  |  |  |
| *k2* / l mol-1 s-1 | 2.6 × 108 | 298 |
| *k2* / l mol-1 s-1 | 6.0 × 1015  exp[- (4500) / *T*] | 293-353 |
|  |  |  |

*Reliability*

|  |  |  |
| --- | --- | --- |
| Δ log *k1* | ± 0.02 | 298 |
| Δ EA1/R | ± 400 | 293-353 |
|  |  |  |
| Δ log *k2* | ± 0.16 | 298 |
| Δ EA2/R | ± 800 | 293-353 |

*Comments on Preferred Values*

These are the only available kinetic data on these reactions.

**References**

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

Ervens, B., Gligorovski, S. and Herrmann, H.: Phys. Chem. Chem. Phys., 5(9), 1811-1824, 2003.

Lide, D.R.: “CRC Handbook of Chemistry and Physics”, 76th Ed., CRC Press, Boca Raton, 1996.

Sørensen, P. E.; Bruhn, K. and Lindelov, F.: Acta Chem. Scand., 28(2), 162 ‑ 168 , 1974.



Figure 1: T-dependent rate constants for the reaction of glyoxylic acid and glyoxylate with OH in aqueous solution. Data from Ervens et al. (2003).