IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

 – Data Sheet AQ\_TH1\_NO3\_1

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This datasheet last evaluated: May 2017; last change in preferred values: June 2016

**NO3·(aq) + [CH(OH)2]2(aq) → ·C(OH)2COOH + HNO3**

*GR*° (aq): Aqueous phase thermochemical data not available

Gas phase data are also not available because of the hydration of glyoxal.

**Rate coefficient data**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| *k*/ L mol-1 s-1 | *T*/K | *pH* | *I*/ mol L-1 | Reference | Technique/ Comments |
| *Absolute Rate Coefficients* |
| (4.5 ± 0.3) × 106 | 298 | 6 |  | Schaefer *et al.*, 2015 | LFP(a) |
| 6.22 × 1012 exp[(-4210 ± 1200)/T] | 278 -313 |  |

**Comments**

1. A modified thermostated laser flash photolysis-differentially amplified laser long path absorption setup was used; 1 × 10−3 M Glyoxal; detection of NO3 radicals at λ = 442 nm. The reaction of glyoxal with these radicals (SO4-, NO3, OH) appear to be pH independent.

The rate constants obtained here are comparable with those of other mono- and polyfunctional alcohols (with reference to Hoffmann et al., 2009).

General:

Glyoxal is completely hydrated in aqueous solution. Equilibrium constants for the first and the second hydration of Glyoxal can be found in Ervens et al. (2010): Khydr1 = 350, respectively Khydr2 = 207.

CHOCHO(aq) + H2O(l) → CHOCH(OH)2(aq) with Khydr1

CHOCH(OH)2(aq) + H2O(l) → [CH(OH)2]2(aq) with Khydr2

**Preferred Values**

|  |  |  |
| --- | --- | --- |
| Parameter | Value | *T*/K |
|  |  |  |
| *k* / L mol-1 s-1 | 4.5 × 106 | 298 |
| *k(T)* / L mol-1 s-1 | 6.22 × 1012 exp[-(4210)/T] | 278 - 313 |
|  |  |  |

*Reliability*

|  |  |  |
| --- | --- | --- |
| Δ log *k* | ± 0.03 | 298 |
| Δ EA/R | ± 1200 | 278 - 313 |

*Comments on Preferred Values*

This is the only available study on NO3 + glyoxal in aqueous solution.

**References**

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

Hoffmann, D., Weigert, B., Barzaghi, P. and Herrmann, H.: Phys. Chem. Chem. Phys., 11, 9351 – 9363, 2009.

Schaefer, T., van Pinxteren, D. and Herrmann, H.: Environ. Sci. Technol., 49 (1), 343 – 350, 2015.



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