IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ\_TH1\_NO3\_2

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

**NO3·(aq) + CH2(OH)COOH(aq) → ·CH(OH)COOH(aq) + HNO3 (1)**

**NO3·(aq) + CH2(OH)COO-(aq) → ·CH(OH)COO-(aq) + HNO3 (2)**

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

**Rate coefficient data**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| *k*/ L mol-1 s-1 | *T*/K | *pH* | *I*/ mol L-1 | Reference | Technique/ Comments | | |
| *Absolute Rate Coefficients* | | | | | | | |
| *k*1 = (9.1 ± 2.3) × 105 | 298 | 0.5 | 0.45 | de Semainville et al., 2007 | | LFP(a) |
| *k*1 = 4.5 × 1011 exp[(-3969 ± 1680)/T] |  |  |
| *k*2 =  (1.0 ± 0.2) × 107 | 298 | 6 | 0.13 |
| *k*2 = 1.8 × 1011 exp[(-3007 ± 1080)/T] |  |  |

**Comments**

1. NO3 radicals were produced by laser flash photolysis of S2O82- anions (λ = 351 nm). The pH (0.5 and 6) was adjusted by adding HClO4. Analysis light at λ = 632.8 nm; pKa value for Glycolic acid can be found in Lide (1996) (pKa = 3.83).

**Preferred Values**

|  |  |  |
| --- | --- | --- |
| **Parameter** | **Value** | ***T*/K** |
|  |  |  |
| *k1* / L mol-1 s-1 | 9.1 × 105 | 298 |
| *k*1(T) / L mol-1 s-1 | 4.5 × 1011 exp[(-3969)/T] | 278 – 318 K |
|  |  |  |
| *k2* / L mol-1 s-1 | 1.0 × 107 | 298 |
| *k*2(T) / L mol-1 s-1 | 1.8 × 1011 exp[(-3007)/T] | 278 – 318 K |

*Reliability*

|  |  |  |
| --- | --- | --- |
| Δ log *k1* | ± 0.13 | 298 |
| Δ EA1/R | ± 1700 | 278 – 318 |
|  |  |  |
| Δ log *k2* | ± 0.10 | 298 |
| Δ EA2/R | ± 1100 | 278 - 318 |

*Comments on Preferred Values*

The recommended values are from the currently only available study on these reactions. The activation energies carry considerable error.

**References**

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

Gaillard de Semainville, Ph., Hoffmann, D., George, Ch. and Herrmann, H.: Phys. Chem. Chem. Phys., 9, 958 - 968, 2007.



Figure 1: T-dependent rate constants for the reaction of glycolic acid and glycolate with OH in aqueous solution. Data from de Semainville et al. (2007).