IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ_TH1_NO3_1

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

$NO_3^{\cdot}(aq) + [CH(OH)_2]_2(aq) \rightarrow {\cdot}C(OH)_2COOH + HNO_3$

$\Delta G_R°$ (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					
$(4.5 \pm 0.3) \times 10^6$	298	6		Schaefer *et al.*, 2015	LFP(a)
6.22×10^{12} exp[(-4210 ± 1200)/T]	278 -313				

Comments

(a) A modified thermostated laser flash photolysis-differentially amplified laser long path absorption setup was used; 1×10^{-3} M Glyoxal; detection of NO_3 radicals at $\lambda = 442$ nm. The reaction of glyoxal with these radicals (SO_4^-, NO_3, 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): $K_{hydr1} = 350$, respectively $K_{hydr2} = 207$.

$CHOCHO(aq) + H_2O(l) \rightarrow CHOCH(OH)_2(aq)$ with K_{hydr1}
$CHOCH(OH)_2(aq) + H_2O(l) \rightarrow [CH(OH)_2]_2(aq)$ with K_{hydr2}

Preferred Values

Parameter	Value	*T*/K
k / L mol^{-1} s^{-1}	4.5×10^6	298
$k(T)$ / L mol^{-1} s^{-1}	6.22×10^{12} exp[-(4210)/T]	278 - 313
Reliability		
$\Delta \log k$	± 0.03	298
$\Delta E_A/R$	± 1200	278 - 313

Comments on Preferred Values

This is the only available study on NO_3 + 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.

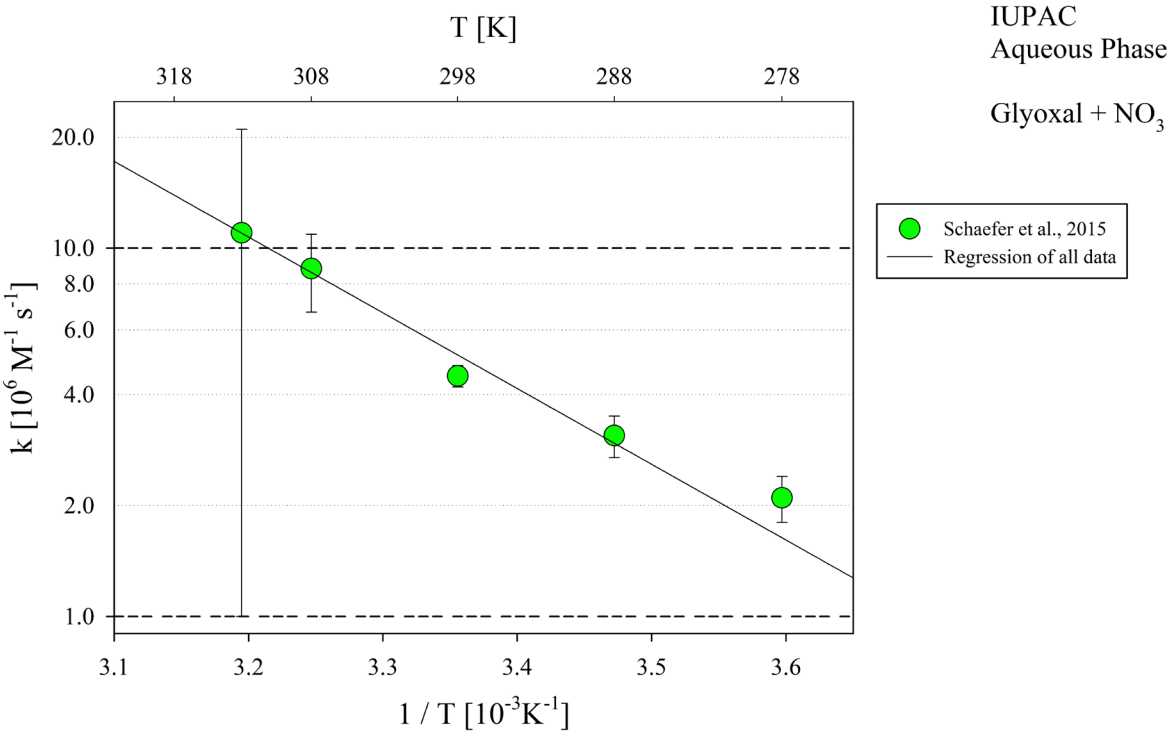

Figure 1: T-dependent rate constants for the reaction of glyoxal with OH in aqueous solution. Data from Schaefer et al. (2015).