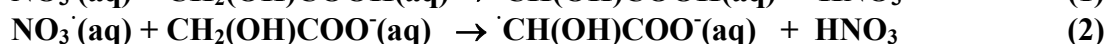


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ_TH1_NO3_2

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



ΔG_R° (aq): Aqueous phase thermochemical data not available. Gas phase data are also not available.

Rate coefficient data

$k / \text{L mol}^{-1} \text{s}^{-1}$	T/K	pH	$I / \text{mol L}^{-1}$	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>					
$k_1 = (9.1 \pm 2.3) \times 10^5$	298	0.5	0.45	de Semainville et al., 2007	LFP(a)
$k_1 = 4.5 \times 10^{11} \exp[(-3969 \pm 1680)/T]$					
$k_2 = (1.0 \pm 0.2) \times 10^7$	298	6	0.13		
$k_2 = 1.8 \times 10^{11} \exp[(-3007 \pm 1080)/T]$					

Comments

(a) NO_3 radicals were produced by laser flash photolysis of $\text{S}_2\text{O}_8^{2-}$ anions ($\lambda = 351 \text{ nm}$). The pH (0.5 and 6) was adjusted by adding HClO_4 . Analysis light at $\lambda = 632.8 \text{ nm}$; pK_a value for Glycolic acid can be found in Lide (1996) ($pK_a = 3.83$).

Preferred Values

Parameter	Value	T/K
$k_1 / \text{L mol}^{-1} \text{s}^{-1}$	9.1×10^5	298
$k_1(T) / \text{L mol}^{-1} \text{s}^{-1}$	$4.5 \times 10^{11} \exp[(-3969)/T]$	278 – 318 K
$k_2 / \text{L mol}^{-1} \text{s}^{-1}$	1.0×10^7	298
$k_2(T) / \text{L mol}^{-1} \text{s}^{-1}$	$1.8 \times 10^{11} \exp[(-3007)/T]$	278 – 318 K
<i>Reliability</i>		
$\Delta \log k_1$	± 0.13	298
$\Delta E_{A1}/R$	± 1700	278 – 318
$\Delta \log k_2$	± 0.10	298

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.

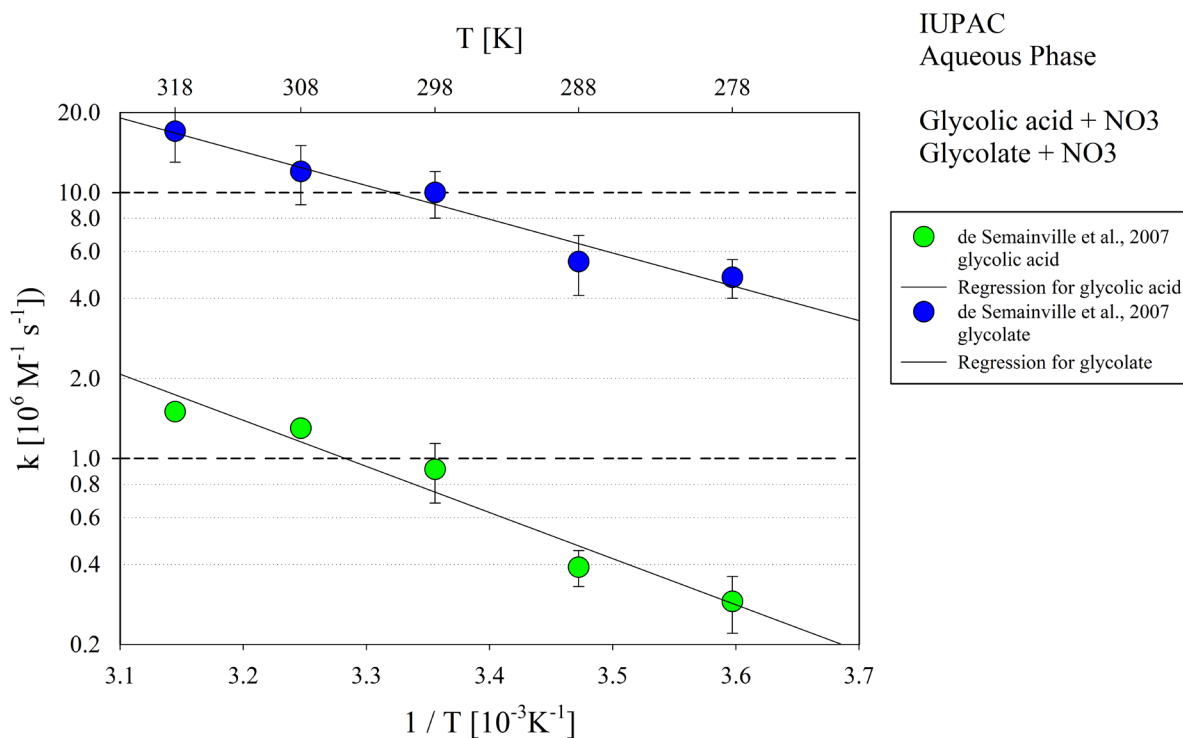


Figure 1: T-dependent rate constants for the reaction of glycolic acid and glycolate with OH in aqueous solution. Data from de Semainville et al. (2007).