

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ_TH1_GLYX_2

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Rate coefficient data (*k*)

<i>k</i> / l mol ⁻¹ s ⁻¹	<i>T</i> /K	<i>pH</i>	<i>I</i> /	<i>Reference</i>	<i>Technique/</i> <i>Comments</i>
<i>Absolute Rate Coefficients</i>					
$(3.15 \pm 0.42) \times 10^{-7}$	295	6	0	De Haan et al., 2009	NMR (a)
1.9×10^{-4}	294	3.98	0	Sedehi et al., 2013	NMR (b)
1.3×10^{-3}	294	4.85	0	Sedehi et al., 2013	NMR (b)
7.2×10^{-3}	298	5.08	0	Sedehi et al., 2013	NMR (b)
7.4×10^{-4}	294	5.12	0	Sedehi et al., 2013	NMR (b)
1.3×10^{-2}	298	5.8	0	Sedehi et al., 2013	NMR (b)

Comments

- (a) The rate of this reaction was measured directly by following the disappearance of arginine using NMR. The reaction mixture initially consisted of 1 M glyoxal and 0.86 M arginine in D₂O. Glyoxal is hydrated in water, see Ervens and Volkamer (2010) for data on the involved equilibria. The reaction rate is reported based on total glyoxal concentration, although the likely reactant is glyoxal monohydrate (expected to be 7×10^{-4} of total glyoxal at the experimental conditions). Glyoxal-arginine adducts were observed using ESI-MS at 233 amu for aqueous reaction mixtures which were dried to a solid residue and redissolved.
- (b) The rate constants reported here were derived based on the disappearance of glyoxal as measured using NMR. The reaction mixture initially consisted of 0.44-1.0M glyoxal and 0.25-0.86M arginine in D₂O. pH was monitored during the reaction and average pH is reported. Products reported were imidazoles and formic acid.

Preferred Values

Parameter	Value	<i>T</i> /K
<i>k</i> / l mol ⁻¹ s ⁻¹	$10^{(0.99 \times \text{pH} - 7.7)}$	294-298

Reliability

$$\Delta \log k \quad \pm 0.3$$

Comments on Preferred Values

Preferred value is based on the data of Sedehi et al. (2013) as summarized in the table

above. The production of formic acid influences the pH of the reaction mixture, biasing the rates reported by De Haan et al. (2009). Parameterization is valid for $3.98 \leq \text{pH} \leq 5.8$. The recommended value is based on our own curve fit to the data.

References

De Haan, D. O., Corrigan, A. L., Smith, K. W., Stroik, D. R., Turley, J. J., Lee, F. E., Tolbert, M. A., Jimenez, J. L., Cordova, K. E., and Ferrell, G. R.: *Environ. Sci. Technol.*, 43 (8), 2818, 2009.

Sedehi, N., Takano, H., Blasic, V. A., Sullivan, K. A., and De Haan, D. O.: *Atmos. Environ.*, 77, 656, 2013.

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

