

## IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

### – Data Sheet AQ\_TH1\_GLYX\_5

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#### Rate coefficient data (*k*)

<i>k</i> / l mol <sup>-1</sup> s <sup>-1</sup>	<i>T</i> /K	<i>pH</i>	<i>I</i> /	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>					
$(4.5 \pm 0.5) \times 10^{-8}$	295	6	0	De Haan et al., 2009	NMR (a)
$5.5 \times 10^{-6}$	298	2.45	0	Sedehi et al., 2013	NMR (b)
$8.4 \times 10^{-4}$	294	4.15	0	Sedehi et al., 2013	NMR (b)
$4.4 \times 10^{-3}$	296	5.34	0	Sedehi et al., 2013	NMR (b)
$2.3 \times 10^{-2}$	280	6.40	0	Sedehi et al., 2013	NMR (b)

#### Comments

- (a) The rate of this reaction was measured directly by following the disappearance of serine using NMR. The reaction mixture initially consisted of 1 M glyoxal and 0.48 M serine in D<sub>2</sub>O. 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 and total serine concentration, although the likely reactants are glyoxal monohydrate (expected to be  $7 \times 10^{-4}$  of total glyoxal at the experimental conditions) and serine with a deprotonated amine group ( $7.1 \times 10^{-4}$  of the total serine at pH 6). A 1,3-disubstituted imidazole product was observed using ESI-MS at 245.13 amu for aqueous reaction mixtures which were dried to a solid residue and redissolved. Browning of the reaction mixture suggests the additional presence of melanoidin products which were not identified with ESI-MS or H<sup>1</sup>-NMR.
- (b) The rate constants reported here were derived based on the disappearance of glyoxal as measured using NMR (except for the point at pH 2.22, which is based on the appearance of formic acid). The reaction mixture initially consisted of 0.33-1.0M glyoxal and 0.33-0.5M serine in D<sub>2</sub>O. pH was monitored during the reaction and average pH is reported. Reported products include imidazoles and formic acid.

#### Preferred Values

Parameter	Value	<i>T</i> /K
<i>k</i> / l mol <sup>-1</sup> s <sup>-1</sup>	$10^{(0.9 \times \text{pH} - 7.2)}$	280-298

#### 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 reported reaction rates of De Haan et al. (2009). The recommended value is based on our own curve fit to the data. Parameterization is valid for  $2.45 \leq \text{pH} \leq 6.4$ .

### 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.

