

## IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

### – Data Sheet AQ\_TH1\_GLYX\_4

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



#### 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> /	<i>Reference</i>	<i>Technique/</i> <i>Comments</i>
<i>Absolute Rate Coefficients</i>					
3.0 × 10 <sup>-5</sup>	294	3.95	0	Sedehi et al., 2013	NMR (a)
3.4 × 10 <sup>-4</sup>	298	4.92	0	Sedehi et al., 2013	NMR (a)
2.8 × 10 <sup>-5</sup>	294	5.95	0	Sedehi et al., 2013	NMR (a)
4.1 × 10 <sup>-3</sup>	298	6.14	0	Sedehi et al., 2013	NMR (a)

#### Comments

- (a) The rate constants reported here were derived based on the disappearance of glyoxal as measured using NMR (except for the point taken at 5.95, which is based on the appearance of formic acid). The reaction mixture initially consisted of 0.5 M glyoxal and 0.5 M methylamine in D<sub>2</sub>O. pH was monitored during the reaction and average pH is reported. Products include imidazoles and formic acid.

#### Preferred Values

<b>Parameter</b>	<b>Value</b>	<b><i>T</i>/K</b>
<i>k</i> / l mol <sup>-1</sup> s <sup>-1</sup>	1.1 × 10 <sup>-3</sup>	294-298

#### Reliability

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

#### Comments on Preferred Values

Preferred value is based on an average of the data of Sedehi et al. (2013) as summarized in the table above, excluding the point at pH = 6.14. No clear dependence on pH or temperature is apparent from the data. Recommendation is valid for 3.95 ≤ pH ≤ 5.95.

#### Reference

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