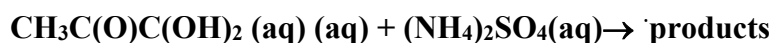


## IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

### – Data Sheet AQ\_TH1\_MGLY\_1

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



#### 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> / mol kg <sup>-1</sup>	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>					
8.3 × 10 <sup>-8</sup>	295	2.0	9.3	Sareen et al., 2010	UV-Vis (a)
6.8 × 10 <sup>-4</sup>	298	3.24	1.5	Sedehi et al., 2013	NMR (b)
5.5 × 10 <sup>-4</sup>	298	3.24	1.5	Sedehi et al., 2013	NMR (b)
4.7 × 10 <sup>-4</sup>	280	3.30	1.5	Sedehi et al., 2013	NMR (b)
2.4 × 10 <sup>-3</sup>	298	3.94	1.5	Sedehi et al., 2013	NMR (b)

#### Comments

- (a) The rate of this reaction was measured by following the appearance of a product peak at 282 nm using UV-Vis. The reaction mixtures used for the kinetic analysis initially consisted of 0-0.05 M methylglyoxal and 3.1 M AS in H<sub>2</sub>O. Products identified using Aerosol Chemical Ionization Mass Spectrometry (Aerosol-CIMS) include aldol condensation products and oligomeric species.
- (b) The rate of this reaction was measured directly using NMR. The rate constants reported here were derived based on the disappearance of methylglyoxal. The reaction mixture initially consisted of 0.50 M methylglyoxal and 0.50 M AS in D<sub>2</sub>O. pH was monitored during the reaction and average pH is reported.

#### Preferred Values

Parameter	Value	<i>T</i> /K
<i>k</i> / l mol <sup>-1</sup> s <sup>-1</sup>	10 <sup>^(2.5×pH-12)</sup>	280-298
Δ log <i>k</i>	± 0.3	

#### Comments on Preferred Values

Recommendation is based on a curve fit to the data of Sareen et al. (2010) and Sedehi et al. (2013). No clear dependence of the second order rate constant on ionic strength of the solution is apparent from the aggregate data, consistent with the observed first order dependence of the reaction rate on ammonium sulfate concentration (Sareen et al. (2010), Sedehi et al. (2013)). We note that methylglyoxal exhibits “salting-out” with ammonium sulfate in aqueous solutions (decreasing methylglyoxal solubility with increasing

ammonium sulfate concentration); Waxman et al. (2015) reported  $K_s = 0.16 \text{ l mol}^{-1}$ . Parameterization is valid for  $2.0 \leq \text{pH} \leq 3.94$ .

## References

Sareen, N., Schwier, A.N., Shapiro, E.L., Mitroo, D., and McNeill, V.F.: Atmos. Chem. Phys. 10 (3), 997, 2010.

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

Waxman, E., Elm, J., Kurtén, T., Mikkelsen, K. V., Ziemann, P.J., and Volkamer, R.: Environ. Sci. Technol., 49 (19), 11500, 2015.

