IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ_TH1_GLYX_3

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

$[CH(OH)_2]_2(aq) + NH_2CH_2COOH\ (aq) \rightarrow$ products

Rate coefficient data (k)

k/ l mol^{-1} s^{-1}	T/K	pH	I/	Reference	Technique/ Comments
Absolute Rate Coefficients					
$(1.4 \pm 0.5) \times 10^{-8}$	295	6	0	De Haan et al., 2009	NMR (a)
5.0×10^{-6}	298	2.22	0	Sedehi et al., 2013	NMR (b)
7.4×10^{-5}	294	3.79	0	Sedehi et al., 2013	NMR (b)
3.8×10^{-4}	298	4.08	0	Sedehi et al., 2013	NMR (b)
3.0×10^{-4}	298	4.52	0	Sedehi et al., 2013	NMR (b)
3.3×10^{-4}	298	4.54	0	Sedehi et al., 2013	NMR (b)
1.8×10^{-3}	298	5.7	0	Sedehi et al., 2013	NMR (b)

Comments

(a) The rate of this reaction was measured directly by following the disappearance of glycine using NMR. The reaction mixture initially consisted of 1 M glyoxal and 1 M glycine in D_2O. Glyoxal is hydrated in water, see Ervens and Volkamer (2010) for data on the involved equlibria. The reaction rate is reported based on total glyoxal concentration and total glycine concentration, although the likely reactants are glyoxal monohydrate (expected to be 7×10^{-4} of total glyoxal at the experimental conditions) and glycine with a deprotonated amine group (1.7×10^{-4} of the total glycine at pH 6). A 1,3-disubstituted imidazole product was observed using ESI-MS at 185.07 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^1-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 0.46-1.5M glyoxal and 0.46-1M glycine in D_2O. pH was monitored during the reaction and average pH is reported. Products reported were imidazoles and formic acid.

Preferred Values

Parameter	Value	*T*/K
k / l mol^{-1} s^{-1}	10^(0.74×pH – 6.8)	294-298

Reliability

$\Delta \log k$ ± 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 2.22 ≤ pH ≤ 5.7.

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.