IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ_TH1_MGLY_5

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

$CH_3C(O)C(OH)_2$ (aq) + $HOCH_2CH(NH_2)COOH$ (aq)→ products

Rate coefficient data

k/ l mol^{-1} s^{-1}	T/K	*pH*	*I*/	*Reference*	Technique/ Comments
Absolute Rate Coefficients					
2.0×10^{-3}	294	3.49	0	Sedehi et al., 2013	NMR (a)
1.2×10^{-3}	277	3.54	0	Sedehi et al., 2013	NMR (a)
4.6×10^{-3}	298	3.73	0	Sedehi et al., 2013	NMR (a)
1.5×10^{-3}	281	3.94	0	Sedehi et al., 2013	NMR (a)
6.6×10^{-2}	298	6.47	0	Sedehi et al., 2013	NMR (a)

Comments

(a) 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 0.33-0.5M methylglyoxal and 0.25-0.33M serine in D_2O. pH was monitored during the reaction and average pH is reported. Imidazole products were reported.

Preferred Values

Parameter	Value	*T*/K
k / l mol^{-1} s^{-1}	2.3×10^{-3}	277-298

Reliability

$\Delta \log k$ ± 0.3

Comments on Preferred Values

Preferred value is based on the average of the data of Sedehi et al. (2013) as summarized in the table above, excluding the data point at pH = 6.47. No clear dependence on pH or temperature is apparent from the data. Recommendation is valid for $3.49 \leq pH \leq 3.94$.

Reference

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