IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ_TH1_MGLY_2

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

$CH_3C(O)C(OH)_2$ (aq) + H2NC(=NH)NH(CH2)3CH(NH2)CO2H (aq)→ products

Rate coefficient data (*k*)

k/ l mol^{-1} s^{-1}	*T*/K	*pH*	*I*/	*Reference*	Technique/ Comments
Absolute Rate Coefficients					
2.0×10^{-3}	298	3.61	0	Sedehi et al., 2013	NMR (a)
2.3×10^{-2}	294	5.31	0	Sedehi et al., 2013	NMR (a)
1.6×10^{-1}	298	8.00	0	Sedehi et al., 2013	NMR (a)
3.0×10^{-4}	294	8.00	0	Sedehi et al., 2013	NMR (a)
7.7×10^{-5}	277	8.00	0	Sedehi et al., 2013	NMR (a)

Comments

(a) The rate constants reported here were derived based on the disappearance of methylglyoxal as measured using NMR. Two imidazole products were reported. The reaction mixture initially consisted of 0.20-0.50 M methylglyoxal and 0.20-0.43M arginine in D_2O. pH was monitored during the reaction and average pH is reported.

Preferred Values

Parameter	Value	*T*/K
k / l mol^{-1} s^{-1}	0.05	294-298

Reliability

$\Delta \log k$ ± 0.3

Comments on Preferred Values

The recommended value is based on an average of the kinetic data of Sedehi et al. (2013) as summarized in the table above. Only the data taken at 294-298K were considered. No clear dependence of the rate constant on pH or temperature is apparent from the data. Recommendation is valid for $3.61 \leq pH \leq 8.00$.

References

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