IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet SOx57

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This data sheet last evaluated: November 2017; last change in preferred values: November 2001.

$CH_3SOO + M \rightarrow CH_3S + O_2 + M$

$\Delta H° = 48.9$ kJ·mol^{-1}

Rate coefficient data

k/s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
(1.99 ± 0.74) x 10^3 107 mbar (He)	216	Turnipseed et al., 1992	(a)
(3.20 ± 0.80) x 10^3 107 mbar (He)	222		
(9.1 ± 2.6) x 10^3 107 mbar (He)	233		
(1.00 ± 0.12) x 10^4 107 mbar (He)	237		
(1.28 ± 0.12) x 10^4 107 mbar (He)	242		
(2.4 ± 0.4) x 10^4 107 mbar (He)	250		
>3.5 x 10^4 107 mbar (He)	258		

Comments

(a) Pulsed laser photolysis system with LIF detection of CH_3S radicals. The formation and decay rate coefficients of CH_3SOO radicals were derived from the observed time-concentration profiles of CH_3S radicals in the presence of O_2. The measured rate coefficients for the reactions $CH_3S + O_2 \rightarrow CH_3SOO$ were observed to vary with total pressure and with the diluent gas.

(b) See Comments on Preferred Values.

Preferred Values

The preferred data are from Turnipseed et al. (1992). These data at 107 mbar He are described by k(210-250 K) =3.5x 10^{10} exp (-3560/T) s^{-1} .

Reliability

$\Delta \log k = \pm 0.3$ at 107 mbar He over the temperature range 216-250 K.

Comments on Preferred Values

The data presented by Turnipseed et al. (1992) were the first reported for the dissociation of the CH_3SOO radical (see also the data sheet in this evaluation for the reverse reaction $CH_3S + O_2 + M \rightarrow CH_3SOO + M$). In the atmosphere, ~33% of CH_3S radicals will be present as the CH_3SOO adduct at 298 K and ground level, with the $[CH_3SOO]/[CH_3S]$ ratio being strongly temperature dependent.
Measurements of the equilibrium constant for formation and dissociation of CH_3SOO from 216 to 258 K by Turnipseed et al. (1992) were consistent with results from Butkovskaya and Barnes (2002) as analysed by Chu and Lee (2010) (see the discussion in Burkholder et al., 2015).

References

Burkholder,J. B. Sander, S. P.,Abbatt, J., Barker,J. R.,Huie,R. E.,Kolb, C. E. Kurylo, M. J., Orkin, V. L.,Wilmouth, D. M., and Wine,P. H.: Chemical Kinetics and Photochemical Data for Use in Atmospheric Studies, NASA Panel for Data Evaluation, Evaluation Number 18, JPL Publication 15-10, 2015.

Butkovskaya, N. I., and Barnes, I.: NATO Science Series 16, 147, 2002.

Chu, L.-K., and Lee, Y.-P.: J. Chem. Phys. 133, 184303, 2010.

Turnipseed, A. A., Barone, S. B., and Ravishankara, A. R.: J. Phys. Chem. 96, 7502, 1992.