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

This data sheet updated: 19th November 2001.

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

$\Delta H^\circ = 48.9$ 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, Barone and Ravishankara, 1992[1]	(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

Data of Turnipseed *et al.*,[1] given in above table. 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*.[1] 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,[1] with the $[CH_3SOO]/[CH_3S]$ ratio being strongly temperature dependent.[1]

References

[1] A. A. Turnipseed, S. B. Barone, and A. R. Ravishankara, J. Phys. Chem. **96**, 7502 (1992).