IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet SOx67

This data sheet updated: 20th November 2001.

$CH_3SCH_2 + O_2 \rightarrow CH_3SCH_2O_2$

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	**Reference**	Technique/ Comments
Absolute Rate Coefficients			
$(5.7 \pm 0.4) \times 10^{-12}$ (1 bar)	298	Wallington et al., 1993	(a)
2.3×10^{-13} (1 Torr He)	298	Butkovskaya and Le Bras, 1994	(b)
1.9×10^{-13} (1 Torr He)	298		

Comments

(a) Pulsed radiolysis of SF_6-CH_3SCH_3-O_2 mixtures. CH_3SCH_2 radicals were generated by reaction of F atoms with CH_3SCH_3, and monitored in absorption at 290 nm. The total pressure was approximately 1 bar.

(b) Discharge flow study of the NO_3-CH_3SCH_3-Br_2-O_2 system at 1.3 mbar (1 Torr) He. NO_3 radicals were produced by F + HNO_3 reaction added to CH_3SCH_3 to give CH_3SCH_2. Subsequent addition of Br_2-O_2 mixtures allowed monitoring of competition between O_2 and Br_2 for CH_3SCH_2. Competition followed by mass spectrometric measurement of [CH_3SCH_2Br] profile. Modeling of profile gives $k = 2.3 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1}. Similar study of Cl-Cl_2-CH_3SCH_3-O_2 system in which CH_3SCH_2 was produced by Cl + CH_3SCH_3 reaction gave $k = 1.9 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1}.

Preferred Values

$k = 5.7 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K and 1 bar.

Reliability

$\Delta \log k = \pm 0.4$ at 298 K and 1 bar.

Comments on Preferred Values

The preferred value of k is taken from the study of Wallington et al. (1993). Until confirmatory studies are made we confine our recommendations to 1 bar and assign substantial error limits.

References

Butkovskaya, N. I. and Le Bras, G.: J. Phys. Chem. 98, 2582, 1994.
Wallington, T. J., Ellermann, T. and Nielsen, O. J.: J. Phys. Chem. 97, 8442, 1993.