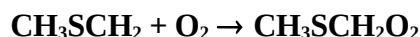


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet SOx67

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This data sheet updated: 20th November 2001.



Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$(5.7 \pm 0.4) \times 10^{-12}$ (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 SF₆-CH₃SCH₃-O₂ mixtures. CH₃SCH₂ radicals were generated by reaction of F atoms with CH₃SCH₃, and monitored in absorption at 290 nm. The total pressure was approximately 1 bar.
- (b) Discharge flow study of the NO₃-CH₃SCH₃-Br₂-O₂ system at 1.3 mbar (1 Torr) He. NO₃ radicals were produced by F + HNO₃ reaction added to CH₃SCH₃ to give CH₃SCH₂. Subsequent addition of Br₂-O₂ mixtures allowed monitoring of competition between O₂ and Br₂ for CH₃SCH₂. Competition followed by mass spectrometric measurement of [CH₃SCH₂Br] profile. Modeling of profile gives $k = 2.3 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$. Similar study of Cl-Cl₂-CH₃SCH₃-O₂ system in which CH₃SCH₂ was produced by Cl + CH₃SCH₃ reaction gave $k = 1.9 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$.

Preferred Values

$k = 5.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ 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.