IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet SOx52

This data sheet updated: 20th November 2001.

$CH_2SH + O_2 \rightarrow$ products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(8.5 \pm 1.0) \times 10^{-12}$	298	Anastasi et al., 1992	(a)
$(4.6 \pm 1.9) \times 10^{-12}$	298	Rahman et al., 1992	(b)

Comments

(a) Pulsed radiolysis of CH_3SH-O_2-SF_6 mixtures at 1 bar total pressure. CH_2SH and CH_3S radicals were generated by reactions of the radiolytically produced F atoms with CH_3SH. [CH_2SH], was monitored by UV absorption over range 220-380 nm.

(b) Fast flow discharge study. CH_2SH radicals were generated by reaction of F atoms with CH_3SH, and [CH_2SH] was monitored by mass spectrometry. The source reactions were simulated to check consumption of F atoms. The total pressure was 3 mbar.

Preferred Values

$k = 6.6 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K.

Reliability

$\Delta \log k = \pm 0.3$ at 298 K.

Comments on Preferred Values

The only two measurements of k differ by almost a factor of 2. The values of $k(CH_2SH + NO_2)$ measured in these two studies also differ, although the error limits are large enough to encompass the two results. Until further studies are carried out, a mean of the two values is recommended, with substantial error limits.

References

Anastasi, C., Broomfield, M., Nielsen, O. J. and Pagsberg, P.: J. Phys. Chem. 96, 696, 1992.
Rahman, M. M., Becker, E., Wille, U. and Schindler, R. N.: Ber. Bunsenges. Phys. Chem. 96, 783, 1992.