

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet SOx55

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CH₂SH + NO₂ → products

Rate coefficient data

<i>k</i> /cm ³ molecule ⁻¹ s ⁻¹	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
(3.8 ± 1.0) × 10 ⁻¹¹	298	Anastasi et al., 1992	(a)
(6.9 ± 4) × 10 ⁻¹¹	298	Rahman et al., 1992	(b)

Comments

- (a) Pulsed radiolysis of CH₃SH-O₂-SF₆ mixtures at 1 bar total pressure. CH₂SH and CH₃S radicals were generated by reactions of the radiolytically produced F atoms with CH₃SH, and [CH₂SH] was monitored by UV absorption over the wavelength range 220-380 nm.
- (b) Fast flow discharge study. CH₂SH radicals were generated by the reaction of F atoms with CH₃SH and were monitored by MS. Source reactions were simulated to check consumption of F atoms. The total pressure was 3 mbar.

Preferred Values

$$k = 4.4 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

Reliability

$$\Delta \log k = \pm 0.5 \text{ at } 298 \text{ K.}$$

Comments on Preferred Values

The only two measurements (Anastasi et al., 1992; Rahman et al., 1992) of *k* differ substantially but because the error limits are large enough to encompass the two results it is difficult to know whether the difference is significant. In the same two studies the values obtained for *k*(CH₂SH + O₂) differed to the same degree with much smaller error limits.

Until further studies are carried out, we recommend a weighted mean of the two values and 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.