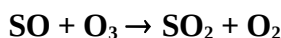


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet SOx45

Website: <http://iupac.pole-ether.fr>. See website for latest evaluated data. Data sheets can be downloaded for personal use only and must not be retransmitted or disseminated either electronically or in hardcopy without explicit written permission.

This data sheet updated: 20th November 2001.



$$\Delta H^\circ = -444.5 \text{ kJ}\cdot\text{mol}^{-1}$$

Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$2.5 \times 10^{-12} \exp[-(1057 \pm 202)/T]$	223-300	Halstead and Thrush, 1966	DF-CL
7.2×10^{-14}	298		
$(8.7 \pm 1.6) \times 10^{-14}$	296 ± 4	Robertshaw and Smith, 1980	PLP-CL
$(1.06 \pm 0.16) \times 10^{-13}$	298	Black, Sharpless and Slinger, 1982a	(a)
$4.8 \times 10^{-12} \exp[-(1170^{+80}_{-120})/T]$	230-420	Black, Sharpless and Slinger, 1982b	(a)
9.46×10^{-14}	298		

Comments

- (a) Pulsed laser photolysis of SO₂-O₃ mixtures at 193 nm with SO₂ being monitored by CL from the SO + O₃ reaction. Excess O₃ was determined by UV absorption. The total pressure = 267 mbar (200 Torr) of He.

Preferred Values

$$k = 8.9 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

$$k = 4.5 \times 10^{-12} \exp(-1170/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ over the temperature range } 230\text{-}420 \text{ K.}$$

Reliability

$$\Delta \log k = \pm 0.1 \text{ at } 298 \text{ K.}$$

$$\Delta(E/R) = \pm 150 \text{ K.}$$

Comments on Preferred Values

The studies of Halstead and Thrush (1966), Robertshaw and Smith (1980) and Black et al. (1982a,b), are in general agreement. The preferred 298 K rate coefficient is the mean of these measurements (Halstead and Thrush, 1966; Robertshaw and Smith, 1980; Black et al., 1982a,b). The temperature dependence of Black et al. (1982b) is accepted since this study covered a much larger temperature range than the earlier study of Halstead and Thrush (1966), which nevertheless gave a value of E/R within the experimental error of the later study (Black et al., 1982b).

References

- Black, G., Sharpless, R. L. and Slanger, T. G.: Chem. Phys. Lett. 90, 55, 1982a.
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Halstead, C. J. and Thrush, B. A.: Proc. R. Soc. London Ser. A 295, 380, 1966.
Robertshaw, J. S. and Smith, I. W. M.: Int. J. Chem. Kinet. 12, 729, 1980.