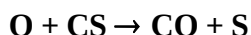


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet SOx1

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: 19th November 2001.



$$\Delta H^\circ = -361 \text{ kJ}\cdot\text{mol}^{-1}$$

Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$(2.06 \pm 0.14) \times 10^{-11}$	305	Slagle <i>et al.</i> , 1975 ¹	DF-MS
$(2.24 \pm 0.36) \times 10^{-11}$	300	Bida, Breckenridge and Kolln, 1976 ²	DF-UVA
$2.6 \times 10^{-10} \exp[-(760 \pm 140)/T]$ 2.0×10^{-11}	156-294 298*	Lilenfeld and Richardson, 1977 ³	DF-EPR/MS
<i>Relative Rate Coefficients</i>			
2.2×10^{-11}	298	Hancock and Smith, 1971 ⁴	RR (a)

Comments

- (a) Discharge flow system. O(³P) was added to CS₂, and the infrared chemiluminescence from the O + CS reaction monitored. NO₂ was added to compete for O atoms. A rate coefficient ratio of $k/k(\text{O} + \text{NO}_2) = 2.3$ was obtained, and placed on an absolute basis by use of $k(\text{O} + \text{NO}_2) = 9.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (this evaluation).

Preferred Values

$$k = 2.1 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

$$k = 2.7 \times 10^{-10} \exp(-760/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ over the temperature range } 150\text{-}300 \text{ K.}$$

Reliability

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

$$\Delta(E/R) = \pm 250 \text{ K.}$$

Comments on Preferred Values

Because of its significance in the CO chemical laser, this reaction has been the subject of a number of studies.¹⁻⁴ The values of k obtained at 298 K fall within a range of about 20%. The preferred value is the mean of these measurements,¹⁻⁴ all of which seem reliable. To obtain the preferred expression for k , the only available value of E/R is accepted³ and the pre-exponential factor is adjusted to fit the preferred 298 K rate coefficient.

References

- ¹ I. R. Slagle, R. E. Graham, J. R. Gilbert, and D. Gutman, *Chem. Phys. Lett.* **32**, 184 (1975).
- ² G. T. Bida, W. H. Breckenridge, and W. S. Kolln, *J. Chem. Phys.* **64**, 3296 (1976).
- ³ H. V. Lilenfeld and R. J. Richardson, *J. Chem. Phys.* **67**, 3991 (1977).
- ⁴ G. Hancock and I. W. M. Smith, *Trans. Faraday Soc.* **67**, 2586 (1971).