IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet I.A4.109 SOx37

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This data sheet last evaluated: November 2017; last change in preferred values: November 2001.

HS + NO + M → HSNO + M

$\Delta H° = -139$ kJ·mol^{-1}

Low-pressure rate coefficients
Rate coefficient data

k_0/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$2.7 \times 10^{-31} (T/300)^{-2.48}$ [N_2]	250-445	Black et al., 1984	PLP-LIF (a)
$(1.4 \pm 0.13) \times 10^{-30}$ [Ar]	293	Bulatov et al., 1985	PLP (b)

Comments

(a) HS formed by photolysis of H_2S at 193 nm and detected at 354.5 nm. The pressure dependence was studied over the range 40-1013 mbar (50–750 Torr). The falloff curve was represented with $F_c = 0.6$ and $k_\infty = 2.7 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}. Theoretical modeling with the given ΔH°.

(b) Intracavity laser spectroscopic detection of HSO radicals at 583 nm in photolyzed H_2S-NO-NO_2-Ar mixtures, with HSO radicals being formed from the reaction HS + NO_2. Measurements were carried out at 16 mbar (12 Torr) total pressure.

Preferred Values

$k_0 = 2.4 \times 10^{-31} (T/300)^{-2.5}$ [N_2] cm^3 molecule^{-1} s^{-1} over the temperature range 250-300 K.

Reliability

$\Delta \log k_0 = \pm 0.3$ at 298 K.

$\Delta n = \pm 1$.

Comments on Preferred Values

The temperature-dependent measurements from Black et al. (1984) give a consistent picture for the association reaction. Earlier work from Tiee et al. (1981) at low pressures did not identify the termolecular nature of the reaction and yielded significantly higher rate coefficients (5.6 x 10^{-13} cm^3 $molecules^{-1}$ s^{-1} at 10 Torr Ar and 298 K).

High-pressure rate coefficients
Rate coefficient data

k_∞/cm^3 $molecule^{-1}$ s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients (2.7 ± 0.5) x 10^{-11}	250-300	Black et al. 1984	PLP-LIF (a)

Comments

(a) See comment (a) for k_0.

Preferred Values

k_∞ = 2.7 x 10^{-11} cm^3 $molecule^{-1}$ s^{-1}, independent of temperature over the range 250-300 K.

Reliability

$\Delta \log k_\infty = 0.5$ over the temperature range 250-300 K.

Comments on Preferred Values

The falloff extrapolation with $F_c = 0.6$ towards k_∞ appears less certain than to k_0. The preferred values are based on the data of Black et al. (1984).

The following text-line combines the preferred values for the high and low pressure limiting rate coefficients to generate a single, cut-and-paste expression for calculation of k:

=((2.4e-31*(*T*/300)^-2.5)*M*(2.7e-11))/((2.4e-31*(*T*/300)^-2.5)*M+(2.7e-11))*10^(log10(0.6)/(1+(log10((2.4e-31*(*T*/300)^-2.5)*M/(2.7e-11))/(0.75-1.27*log10(0.6)))^2))

The molecular density, M = 7.243×10^{21}P(bar)/T(K)

References

Black, G., Patrick, R., Jusinski, L. E., and Slanger, T. G.: J. Chem. Phys. 80, 4065, 1984.

Bulatov, V. P., Kozliner, M. Z., and Sarkisov, O. M.: Khim Fiz. 4, 1353, 1985.

Tiee, J. J.,Wampler, J. B., Oldenburg, R. C., and Rice, W.,W.: Chem. Phys. Lett. 82, 80, 1981.