IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet SOx5

This data sheet updated: 19th November 2001.

$$\mathbf{O + OCS \rightarrow SO + CO} \quad \mathbf{(1)}$$
$$\mathbf{\rightarrow CO_2 + S} \quad \mathbf{(2)}$$

$\Delta H^\circ(1) = -213$ kJ·mol^{-1}
$\Delta H^\circ(2) = -224$ kJ·mol^{-1}

Rate coefficient data ($k = k_1 + k_2$)

k/cm^3 molecule^{-1} s^{-1}	Temp./K	**Reference**	Technique/ Comments
Absolute Rate Coefficients			
(9.1 ± 1.4) x 10^{-15}	298	Sullivan and Warneck, 1965[1]	DF-MS
2.0 x 10^{-10} exp(-2920/T)	290-465	Hoyermann, Wagner and	DF-EPR
1.2 x 10^{-14}	300	Wolfrum, 1967[2]	
1.08 x 10^{-10} exp(-2770/T)	300-1150	Homann, Krome and Wagner, 1968[3]	DF-MS
1.1 x 10^{-14}	300		
3.2 x 10^{-11} exp(-2280/T)	273-808	Westenberg and deHaas, 1969[4]	DF-EPR/MS
(1.4 ± 0.1) x 10^{-14}	297		
(1.19 ± 0.06) x 10^{-14}	297	Breckenridge and Miller, 1972[5]	DF-MS
1.65 x 10^{-11} exp[-(2165 ± 30)/T]	263-502	Klemm and Stief, 1974[6]	FP-RF
(1.2 ± 0.1) x 10^{-14}	298		
2.0 x 10^{-11} exp[-(2140 ± 40)/T]	239-404	Wei and Timmons, 1975[7]	DF-EPR
(1.35 ± 0.13) x 10^{-14}	295		
(1.39 ± 0.14) x 10^{-14}	296	Manning, Braun and Kurylo, 1976[8]	FP-RF
(1.17 ± 0.12) x 10^{-14}	298	Yoshida and Saito, 1978[9]	DF-A (a)

Comments

(a) SO radicals were monitored by microwave absorption at 13044 MHz.

Preferred Values

$k = 1.2 \times 10^{-14}$ cm^3 molecule^{-1} s^{-1} at 298 K.
$k = 1.6 \times 10^{-11} \exp(-2150/T)$ cm^3 molecule^{-1} s^{-1} over the temperature range 230-500 K.

Reliability

$\Delta \log k = \pm 0.2$ at 298 K.

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

Comments on Preferred Values

The values obtained for k by a variety of techniques[1-9] are in excellent agreement over a wide range of temperatures and pressures ($\leq$340 mbar). The available evidence suggests that at low temperatures the reaction proceeds by channel (1) and that channel (2) may only become significant at temperatures above 600 K.

Because of the possible enhancement of the rate by channel 2 at high temperatures, the recommended value of E/R is the mean of the values obtained in studies by Klemm and Stief [6] and Wei and Timmons[7] which were limited to temperatures below 502 K. The value of k at 298 K is the mean of the values in refs. 1-9, and the pre-exponential factor is adjusted to fit this value of k and the recommended value of E/R.

Approximate measurements of k_2/k_1 are: 10^{-3} at 298 K[10] and 10^{-2} at 500 K.[3] Studies of detailed dynamics of this reaction have been reported by Hsu *et al.*,[11] Nickolaisen *et al.*,[12] and Chen *et al*.[13]

References

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