# IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet SOx3

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$$\mathbf{O + CS_2 \rightarrow SO + CS} \quad \mathbf{(1)}$$
$$\mathbf{\rightarrow CO + S_2} \quad \mathbf{(2)}$$
$$\mathbf{\rightarrow OCS + S} \quad \mathbf{(3)}$$

$\Delta H^\circ(1) = -83$ kJ·mol$^{-1}$
$\Delta H^\circ(2) = -348$ kJ·mol$^{-1}$
$\Delta H^\circ(3) = -231$ kJ·mol$^{-1}$

## Rate coefficient data ($k = k_1 + k_2 + k_3$)

| $k$/cm$^3$ molecule$^{-1}$ s$^{-1}$ | Temp./ K | Reference | Technique/ Comments |
|---|---|---|---|
| *Absolute Rate Coefficients* | | | |
| 1.0 x $10^{-11}$ exp[-(300 ± 150)/$T$] | 305-410 | Smith, 1968[1] | FP-UVA |
| 4.2 x $10^{-12}$ | 305 | | |
| 8.3 x $10^{-11}$ exp(-950/$T$) | 300-920 | Homann, Krome and Wagner, 1968[2] | DF-MS |
| 3.5 x $10^{-12}$ | 300 | | |
| (2.08 ± 0.08) x $10^{-12}$ | 227 | Westenberg and deHaas, 1969[3] | DF-EPR/MS |
| (3.0 ± 0.3) x $10^{-12}$ | 297 | | |
| (7.8 ± 0.3) x $10^{-12}$ | 538 | | |
| (3.7 ± 0.3) x $10^{-12}$ | 298 | Callear and Hedges, 1970[4] | FP-UVA |
| (4.0 ± 0.3) x $10^{-12}$ | 302 | Slagle, Gilbert and Gutman, 1974[5] | (a) |
| 2.8 x $10^{-11}$ exp[-(650 ± 35)/$T$] | 218-293 | Wei and Timmons, 1975[6] | DF-EPR |
| (3.1 ± 0.2) x $10^{-12}$ | 293 | | |
| (2.9 ± 0.2) x $10^{-12}$ | 249 | Graham and Gutman, 1977[7] | DF-MS |
| (3.6 ± 0.3) x $10^{-12}$ | 273 | | |
| (4.1 ± 0.2) x $10^{-12}$ | 295 | | |
| (5.1 ± 0.6) x $10^{-12}$ | 335 | | |
| (6.6 ± 0.3) x $10^{-12}$ | 376 | | |
| (8.5 ± 0.6) x $10^{-12}$ | 431 | | |
| (11.2 ± 0.8) x $10^{-12}$ | 500 | | |

## Comments

(a) Studied by using crossed molecular beams with photoionization mass spectrometric detection of products.

## Preferred Values

$k = 3.7 \times 10^{-12}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K.

$k = 3.3 \times 10^{-11} \exp(-650/T)$ cm$^3$ molecule$^{-1}$ s$^{-1}$ over the temperature range 210-500 K.

$k_1/k \geq 0.90$ over the temperature range 200-500 K.

*Reliability*

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

$\Delta(E/R) = \pm 100$ K.

*Comments on Preferred Values*

There are several determinations of $k$ at 298 K using a variety of techniques, which are in good agreement. The preferred value is an average of the values of Smith,[1] Homann *et al.*,[2] Westenberg and deHaas,[3] Callear and Hedges,[4] Slagle *et al.*,[5] Wei and Timmons,[6] and Graham and Gutman.[7] The preferred temperature coefficient is that of Wei and Timmons,[6] and that of Graham and Gutman[7] which are in good agreement.

The reported values for the branching ratios show considerable scatter. For $k_3/k$ values of 0.093,[5] 0.096,[7] 0.015,[8] 0.30[9] and 0.085[10] have been reported and for $k_2/k$ values of 0.05-0.20,[5] 0.014[11] and 0.030.[10] Channel 1 is clearly the major channel but at this stage our only recommendation is that $k_1/k \geq 0.90$.

## References


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