IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet SOx44

$$SO + O_2 \rightarrow SO_2 + O$$
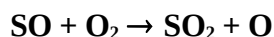
ΔH° = -52.6 kJ·mol^{-1}

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(1.07 \pm 0.16) \times 10^{-16}$	298	Black, Sharpless and Slanger, 1982a	(a)
$2.4 \times 10^{-13} \exp[-(2370^{+200}_{-250})/T]$	230-420	Black, Sharpless and Slanger, 1982b	(a)
8.4×10^{-17}	298		
$1.00 \times 10^{-13} \exp[-(2180 \pm 117)/T]$	262-363	Goede and Schurath, 1983	(b)
6.7×10^{-17}	298		
$(2.2 \pm 0.5) \times 10^{-13} \exp[-(2340 \pm 90)/T]$	250-585	Garland, 1998	(c)
8.6×10^{-17}	298		

Comments

(a) Pulsed laser photolysis of SO$_2$ at 193 nm, with SO radicals being detected by chemiluminescence from the SO + O$_3$ reaction. Pseudo-first-order decays of SO were monitored in the presence of excess O$_2$. Total pressure = 133-667 mbar (100-500 Torr) of O$_2$ + He.

(b) SO produced from the O + OCS reaction in a flow system. Controlled admission of SO radicals to a static volume where the pseudo-first-order decay of SO in excess O$_2$ was followed by SO + O$_3$ chemiluminescence. Total pressure = 0.0013-0.27 mbar (1-200 mTorr) O$_2$. Only an Arrhenius expression was given with no individual rate coefficients at the temperatures studied.

(c) PLP of DMSO at 222 nm coupled with LIF detection of SO at 236.35 nm at 2×10^{-3} mbar of DMSO, up to 13.3 mbar of O$_2$ and 27 mbar total pressure of Ar in a flowing gas experiment. The measurements were performed under pseudo-first order conditions in the range 450–585K and resulted in the Arrhenius expression displayed in the table when combined with the data of Black et al. (1982b).

Preferred Values

$k = 7.6 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1} at 298 K.
$k = 1.6 \times 10^{-13} \exp(-2280/T)$ over the temperature range 230-420 K.

Reliability

    $\Delta\log k = \pm\ 0.15$ at 298 K.

    $\Delta(E/R) = \pm\ 500$ K.

Comments on Preferred Values

    This reaction is very slow and measurement of the rate coefficient k is subject to errors due to impurities. For this reason, Black et al. (1982a,b) favor their lower value of k at 298 K obtained in the temperature dependence study (1982b). The Goede and Schurath (1983) values are systematically about 35% lower than those from Black et al. (1982b), but appear to have less experimental uncertainty at temperatures <300 K. The preferred value for the rate coefficient k at 298 K and for the temperature dependence are from Black et al. (1982b) and Goede and Schurath (1983). The *A*-factor has been adjusted to give the preferred 298 K rate coefficient.

References

Black, G., Sharpless, R. L. and Slanger, T. G.: Chem. Phys. Lett. 90, 55, 1982a.
Black, G., Sharpless, R. L. and Slanger, T. G.: Chem. Phys. Lett. 93, 598, 1982b.
Garland, N. L.: Chem. Phys. Lett. 290, 385, 1998.
Goede, H.-J. and Schurath, U.: Bull. Soc. Chim. Belg. 92, 661, 1983.