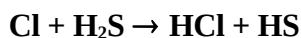


## IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet SOx9

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: 19<sup>th</sup> November 2001.



$$\Delta H^\circ = -50.0 \text{ kJ}\cdot\text{mol}^{-1}$$

### Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K		Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$(7.3 \pm 0.9) \times 10^{-11}$	298	Nesbitt and Leone, 1980 <sup>1</sup>	PLP-CL
$(4.00 \pm 0.08) \times 10^{-11}$	296	Clyne and Ono, 1983 <sup>2</sup>	DF-RF
$(5.1 \pm 0.7) \times 10^{-11}$	296	Clyne <i>et al.</i> , 1984 <sup>3</sup>	DF-MS
$(6.29 \pm 0.46) \times 10^{-11}$	211-353	Nava, Brobst and Stief, 1985 <sup>4</sup>	FP-RF
$3.69 \times 10^{-11} \exp[(208 \pm 24)/T]$	202-430	Nicovich, Wang and Wine, 1995 <sup>5</sup>	PLP-RF
$(7.4 \pm 1.1) \times 10^{-11}$	298		

### Preferred Values

$k = 7.4 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K.

$k = 3.7 \times 10^{-11} \exp(208/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  over the temperature range 200-430 K.

#### Reliability

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

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

#### Comments on Preferred Values

The preferred value accepts the results of the recent study of Nicovich *et al.*<sup>5</sup> which was an extensive study conducted over a wide range of experimental conditions. In that study the value of  $k$  at room temperature was found to be independent of pressure over the range studied [33-800 mbar (25-600 Torr)]. The room temperature value of  $k$  reported by Nesbitt and Leone<sup>1</sup> is in excellent agreement with the preferred value, that of Nava *et al.*<sup>4</sup> is 15% lower, and those of Clyne and Ono<sup>2</sup> and Clyne *et al.*<sup>3</sup> are significantly lower. In the study of Nicovich *et al.*,<sup>5</sup> experimental conditions were adjusted to minimize interferences from radical-radical secondary reactions. An ab initio study of reactions of chlorine atoms with several reduced sulfur compounds has been reported by Wilson and Hirst.<sup>6</sup> For this reaction these

results indicate that adduct formation is the dominant reaction pathway but that hydrogen atom abstraction could be significant.

### References

- <sup>1</sup> D. J. Nesbitt and S. R. Leone, *J. Chem. Phys.* **72**, 1722 (1980).
- <sup>2</sup> M. A. A. Clyne and Y. Ono, *Chem. Phys. Lett.* **94**, 597 (1983).
- <sup>3</sup> M. A. A. Clyne, A. J. MacRobert, T. P. Murrells, and L. J. Stief, *J. Chem. Soc. Faraday Trans. 2*, **80**, 877 (1984).
- <sup>4</sup> D. F. Nava, W. D. Brobst, and L. J. Stief, *J. Phys. Chem.* **89**, 4703 (1985).
- <sup>5</sup> J. M. Nicovich, S. Wang, and P. H. Wine, *Int. J. Chem. Kinet.* **27**, 359 (1995).
- <sup>6</sup> C. Wilson and D. M. Hirst, *J. Chem. Soc. Faraday Trans.* **93**, 2831 (1997).