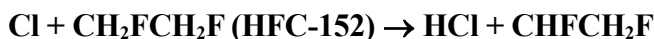


# IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx26

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. The citation for this data sheet is: Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., Troe, J., and Wallington, T. J.: Atmos. Chem. Phys., 9, 4141, 2008; IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation, <http://iupac.pole-ether.fr>. This data sheet last evaluated: June 2015; last change in preferred values: November 2003



$$\Delta H^\circ = -4.6 \text{ kJ mol}^{-1}$$

## Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Relative Rate Coefficients</i>			
$2.8 \times 10^{-11} \exp(-1065/T)$	280-360	Yano and Tschuikow-Roux, 1986	RR (a)
$7.8 \times 10^{-13}$	298		
$(6.6 \pm 0.2) \times 10^{-13}$	296	Wallington et al., 1994	RR (b)
$(6.5 \pm 0.4) \times 10^{-13}$	296		RR (c)

## Comments

- (a) Cl atoms were generated by the photolysis of  $\text{Cl}_2$ . Product yield ratios were measured by GC and the measured rate coefficient ratio  $k(\text{Cl} + \text{CH}_2\text{FCH}_2\text{F})/k(\text{Cl} + \text{C}_2\text{H}_6) = 0.333 \exp(-965/T)$  was placed on an absolute basis using  $k(\text{Cl} + \text{C}_2\text{H}_6) = 8.1 \times 10^{-11} \exp(-100/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (Atkinson et al., 2006).
- (b) Cl atoms were generated by the photolysis of  $\text{Cl}_2$  in presence of  $\text{CH}_2\text{FCH}_2\text{F}-\text{CH}_4$  in air at 930 mbar total pressure. Loss of reactants was monitored by FTIR. The measured rate coefficient ratio  $k(\text{Cl} + \text{CH}_2\text{FCH}_2\text{F})/k(\text{Cl} + \text{CH}_4) = (6.60 \pm 0.16)$  was placed on an absolute basis using  $k(\text{Cl} + \text{CH}_4) = 1.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (Atkinson et al., 2006).
- (c) Cl atoms were generated by the photolysis of  $\text{Cl}_2$  in presence of  $\text{CH}_2\text{FCH}_2\text{F}-\text{CH}_3\text{Cl}$  mixtures in air at 930 mbar total pressure. Loss of reactants was monitored by FTIR. The measured rate coefficient ratio  $k(\text{Cl} + \text{CH}_2\text{FCH}_2\text{F})/k(\text{Cl} + \text{CH}_3\text{Cl}) = (1.36 \pm 0.07)$  was placed on an absolute basis using  $k(\text{Cl} + \text{CH}_3\text{Cl}) = 4.8 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (Atkinson et al., 2006).

## Preferred Values

Parameter	Value	T/K
$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$7.0 \times 10^{-13}$	298
$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$2.5 \times 10^{-11} \exp(-1065/T)$	280-360
<i>Reliability</i>		
$\Delta \log k$	$\pm 0.2$	298
$\Delta(E/R)$	$\pm 400$	

### Comments on Preferred Values

The recommended value at 298 K is an average of the rate constants obtained by the relative rate studies of Yano and Tschuikow-Roux, (1986) and Wallington et al. (1994). The expression for the temperature dependence is taken from Yano and Tschuikow-Roux, (1986), modified to reproduce the recommended value at 298 K.

### References

Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., and Troe, J.: *Atmos. Chem. Phys.*, 6, 3625, 2006; IUPAC Subcommittee for Gas Kinetic Data Evaluation, <http://iupac.pole-ether.fr>.

Wallington, T. J., Hurley, M. D., Ball, J. C., Ellermann, T., Nielsen, O. J. and Sehested, J.: *J. Phys. Chem.*, 98, 5435, 1994.

Yano, T. and Tschuikow-Roux, E.: *J. Photochem.*, 32, 25, 1986.

