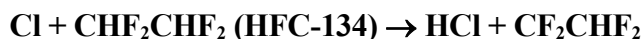


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx33

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.



$$\Delta H^\circ = 6.5 \text{ kJ mol}^{-1}$$

Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Relative Rate Coefficients</i>			
$8.9 \times 10^{-12} \exp(-2444/T)$	280-360	Yano and Tschuikow-Roux, 1986	RR (a)
2.4×10^{-15}	298		
1.9×10^{-15}	298	Nielsen et al., 1992	RR (b)

Comments

- (a) Cl atoms were generated by the photolysis of Cl_2 . Product yield ratios were measured by GC. The measured rate coefficient ratio of $k(\text{Cl} + \text{CHF}_2\text{CHF}_2)/k(\text{Cl} + \text{C}_2\text{H}_6) = 0.107 \exp(-2343/T)$ was placed on an absolute basis using $k(\text{Cl} + \text{C}_2\text{H}_6) = 8.3 \times 10^{-11} \exp(-100/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson et al., 2006).
- (b) Cl atoms were generated by the photolysis of Cl_2 . The decays of the reactant and reference organic were measured by FTIR spectroscopy. The measured rate coefficient ratio 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).

Preferred Values

Parameter	Value	T/K
$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	2.2×10^{-15}	298
$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$7.9 \times 10^{-12} \exp(-2440/T)$	280-360
<i>Reliability</i>		
$\Delta \log k$	± 0.2	298
$\Delta(E/R)$	± 500	

Comments on Preferred Values

The recommended value at 298 K is an average of the results of Nielsen et al. (1992) and Yano and Tschuikow-Roux (1986). The expression for the temperature dependence is that of Yano and Tschuikow-Roux (1986), with the A-factor modified to reproduce the recommended value of k 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 Task Group on Atmospheric Chemical Kinetic Data Evaluation, <http://iupac.pole-ether.fr>
- Nielsen, O. J., Ellermann, T., Sehested, J. and Wallington, T. J.: J. Phys. Chem., 96, 10875, 1992.
- Yano, T. and Tschuikow-Roux, E.: J. Photochem., 32, 25, 1986.

