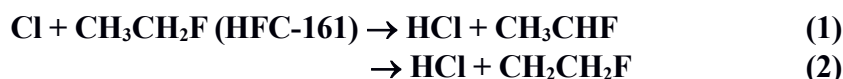


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx24

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: December 2007.



$$\Delta H^\circ(1) = -9.6 \text{ kJ mol}^{-1}$$

$$\Delta H^\circ(2) = 5.3 \text{ kJ mol}^{-1}$$

Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$6.8 \pm 0.5 \times 10^{-12}$	298	Hitsuda et al., 2001	PLP-LIF (a)
<i>Relative Rate Coefficients</i>			
$k_1 = 1.0 \times 10^{-11} \exp(-130/T)$	281-368	Tschuikow-Roux et al., 1985	RR (b)
$k_1 = 6.5 \times 10^{-12}$	298		
$k_2 = 8.3 \times 10^{-12} \exp(-720/T)$	281-368		
$k_2 = 7.4 \times 10^{-13}$	298		

Comments

- (a) Laser photolysis of HCl at 193 nm as Cl atom source. Both $\text{Cl}(^2\text{P}_{3/2})$ and $\text{Cl}(^2\text{P}_{1/2})$ detected by VUV-LIF.
- (b) Cl atoms were generated by the photolysis of Cl_2 . Product yield ratios were determined by GC and the measured rate coefficient ratios of $k_1/k(\text{Cl} + \text{CH}_4) = 1.60 \exp(1113/T)$ and $k_2/k(\text{Cl} + \text{CH}_4) = 1.26 \exp(515/T)$ were placed on an absolute basis using $k(\text{Cl} + \text{CH}_4) = 6.6 \times 10^{-12} \exp(-1240/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson et al., 2006).

Preferred Values

Parameter	Value	T/K
$k_1 / \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	6.5×10^{-12}	298
$k_1 / \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$1.0 \times 10^{-11} \exp(-130/T)$	280-370
$k_2 / \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	7.4×10^{-13}	298
$k_2 / \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$8.3 \times 10^{-12} \exp(-720/T)$	280-370
<i>Reliability</i>		
$\Delta \log k_1 = \Delta \log k_2$	± 0.3	298
$\Delta(E_1/R) = \Delta(E_2/R)$	± 500	

Comments on Preferred Values

The recommended values are based on the results of the relative rate study of Tschuikow-Roux et al. (1985). The overall rate constant k at room temperature, ($k = k_1 + k_2$) of Hitsuda et al. (2001) is consistent with this recommendation.

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>
- Hitsuda, K., Takahashi, K., Matsumi, Y., and Wallington, T. J.: *J. Phys. Chem. A*, 105, 5131, 2001.
- Tschuikow-Roux, E., Yano, T., and Niedzielski, J.: *J. Chem. Phys.*, 82, 65, 1985.

