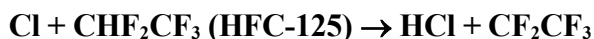


# IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx34

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., 8, 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: June 2011.



$$\Delta H^\circ = 10.7 \text{ kJ mol}^{-1}$$

## Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Relative Rate Coefficients</i>			
$(2.4 \pm 0.5) \times 10^{-16}$	298	Tuazon et al., 1992	RR (a)
$(2.6 \pm 0.6) \times 10^{-16}$	295	Sehested et al., 1993	RR (b)
$(2.93 \pm 0.23) \times 10^{-16}$	296	Young et al., 2009	RR (c)

## Comments

- (a) Cl atoms were generated by the photolysis of Cl<sub>2</sub>. The decays of the reactant and reference organic were measured by FTIR spectroscopy. The measured rate coefficient was placed on an absolute basis by use of a rate coefficient of  $k(\text{Cl} + \text{CH}_4) = 1.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (Atkinson et al., 2006).
- (b) Cl atoms were generated by the photolysis of Cl<sub>2</sub>. The decays of the reactant and reference organic were measured by FTIR spectroscopy. The measured rate coefficient was ratio placed on an absolute basis by use of a rate coefficient of  $k(\text{Cl} + \text{CH}_3\text{CF}_2\text{Cl}) = 4.1 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (Atkinson et al., 2008).
- (c) Cl atoms were generated by the photolysis of Cl<sub>2</sub> in the presence of CHF<sub>2</sub>CF<sub>3</sub> and CH<sub>3</sub>CF<sub>2</sub>Cl in 933 mbar of N<sub>2</sub> diluent. The decays of the reactant and reference organic were measured by FTIR spectroscopy. The measured rate coefficient ratio  $k(\text{Cl} + \text{CHF}_2\text{CF}_3)/k(\text{Cl} + \text{CH}_3\text{CF}_2\text{Cl}) = 0.715 \pm 0.057$  was placed on an absolute basis by use of a rate coefficient of  $k(\text{Cl} + \text{CH}_3\text{CF}_2\text{Cl}) = 4.1 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (Atkinson et al., 2008).

## Preferred Values

Parameter	Value	T/K
$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$2.6 \times 10^{-16}$	298
<i>Reliability</i>		
$\Delta \log k$	$\pm 0.1$	298

*Comments on Preferred Values*

The preferred value at 298 K is based on the results of the relative rate studies of Tuazon et al. (1992) and Sehested et al. (1993), which are in good agreement. Since studies have only been carried out at room temperature, no temperature dependence is recommended. In a relative rate study Sulbaek Andersen et al. (2005) measured  $k(\text{Cl} + \text{CF}_3\text{OCF}_2\text{CF}_2\text{H})/k(\text{Cl} + \text{CHF}_2\text{CF}_3) = 1.01 \pm 0.12$  and  $k(\text{Cl} + \text{CF}_3\text{OCF}_2\text{CF}_2\text{H})/k(\text{Cl} + \text{CHF}_2\text{Cl}) = 0.168 \pm 0.021$  from which a value of  $k(\text{Cl} + \text{CHF}_2\text{CF}_3)/k(\text{Cl} + \text{CHF}_2\text{Cl}) = 0.166 \pm 0.029$  can be derived. Using  $k(\text{Cl} + \text{CHF}_2\text{Cl}) = 1.6 \times 10^{-15}$  (Atkinson et al., 2008) gives  $k(\text{Cl} + \text{CHF}_2\text{CF}_3) = (2.7 \pm 0.5) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  consistent with the recommended value above.

### 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>
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