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

 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.

$Cl + CHF_2CF_3$ (HFC-125) $\rightarrow HCl + CF_2CF_3$

$\Delta H° = 10.7$ kJ mol^{-1}

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Relative Rate Coefficients			
$(2.4 \pm 0.5) \times 10^{-16}$	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_2. 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 $k(Cl + CH_4) = 1.0 \times 10^{-13}$ cm^3 molecule^{-1} 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 was ratio placed on an absolute basis by use of a rate coefficient of $k(Cl + CH_3CF_2Cl) = 4.1 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} (Atkinson et al., 2008).

(c) Cl atoms were generated by the photolysis of Cl_2 in the presence of CHF_2CF_3 and CH_3CF_2Cl in 933 mbar of N_2 diluent. The decays of the reactant and reference organic were measured by FTIR spectroscopy. The measured rate coefficient ratio $k(Cl + CHF_2CF_3)/k(Cl + CH_3CF_2Cl) = 0.715 \pm 0.057$ was placed on an absolute basis by use of a rate coefficient of $k(Cl + CH_3CF_2Cl) = 4.1 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} (Atkinson et al., 2008).

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	2.6×10^{-16}	298
Reliability		
$\Delta \log k$	± 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 $k(Cl + CF_3OCF_2CF_2H)/k(Cl + CHF_2CF_3) = 1.01 \pm 0.12$ and $k(Cl + CF_3OCF_2CF_2H)/k(Cl + CHF_2Cl) = 0.168 \pm 0.021$ from which a value of $k(Cl + CHF_2CF_3)/k(Cl + CHF_2Cl) = 0.166 \pm 0.029$ can be derived. Using $k(Cl + CHF_2Cl) = 1.6 \times 10^{-15}$ (Atkinson et al., 2008) gives $k(Cl + CHF_2CF_3) = (2.7 \pm 0.5) \times 10^{-16}$ cm^3 $molecule^{-1}$ 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

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

Sehested, J., Ellermann, T., Nielsen, O. J., Wallington, T. J., and Hurley, M. D.: Int. J. Chem. Kinet., 25, 701, 1993.

Sulbaek Andersen, M. P., Nielsen, O. J., Wallington, T. J., Hurley, M. D., and DeMore, W. B.: J. Phys. Chem. A, 109, 3926, 2005.

Tuazon, E. C., Atkinson, R, and Corchnoy, S. B.: Int. J. Chem. Kinet., 24, 639, 1992.

Young, C. J., Hurley, M. D. Wallington, T. J., Mabury, S. A.: Chem. Phys. Lett., 473, 251, 2009.