IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation - Data Sheet oClOx57; IV.A2.131

 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: June 2014.

HO + $CHFClCFCl_2$ (HCFC-122a) → H_2O + $CFClCFCl_2$

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$1.26 \times 10^{-12} \exp[-(1298 \pm 66)/T]$	298-460	Orkin et al., 2013	DF-EPR (a)
$(1.67 \pm 0.05) \times 10^{-14}$	298		
Relative Rate Coefficients			
$8.68 \times 10^{-19}\ T^2 \exp[-(463 \pm 42)/T]$	294-362	Hsu and DeMore, 1995	RR (b)
1.63×10^{-14}	298		

Comments

(a) HO radicals were generated by the reaction of H atoms with NO_2 in 0.4 kPa (3.0 Torr) of He diluent in a discharge flow system. Decay of HO radical concentration was monitored by EPR.

(b) HO radicals were generated by the photolysis of H_2O at 185 nm, or O_3 at 254 nm in the presence of H_2O, in H_2O (or H_2O-O_3)-$CHFClCFCl_2$-CH_3CHF_2-O_2-N_2 mixtures. The concentrations of $CHFClCFCl_2$ and CH_3CHF_2 were measured by FTIR spectroscopy. The measured rate coefficient ratio of $k(HO + CHFClCFCl_2)/k(HO + CH_3CHF_2) = (0.31 \pm 0.04) \exp[(117 \pm 42)/T]$ is placed on an absolute basis using $k(HO + CH_3CHF_2) = 2.80 \times 10^{-18}\ T^2 \exp(-580/T)$ cm^3 molecule^{-1} s^{-1} (Atkinson et al., 2008).

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	1.6×10^{-14}	298
k /cm^3 molecule^{-1} s^{-1}	$7.85 \times 10^{-13} \exp(-1155/T)$	270-340
Reliability		
$\Delta \log k$	0.10	298
$\Delta(E/R)$	± 200	270-340

Comments on Preferred Values

The results from the relative rate study of Hsu and DeMore (1995) and the absolute rate study of Orkin et al. (2013) are in excellent agreement. Fitting the three parameter expression, $k = CT^2 \exp(-D/T)$ to the data from Hsu and DeMore (1995) and Orkin et al. (2013) gives $k = 1.18 \times 10^{-18}\ T^2 \exp(-555/T)$. The preferred Arrhenius expression $k = A \exp(-B/T)$ is centered at 300 K

and is derived from the three parameter expression, with $A = C\,e^2\,T^2$ and $B = D + 2T$.

References

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

Hsu, K.-J. and DeMore, W. B.: J. Phys. Chem., 99, 1235, 1995.

Orkin, V.L., Khamaganov, V.G., Kasimovskaya, E.E. and Guschin, A.G.: J. Phys. Chem. A, 117, 5483, 2013.