IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx56

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HO + $CHCl_2CF_2Cl$ (HCFC-122) → H_2O + CCl_2CF_2Cl

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$1.13 \times 10^{-12} \exp[-(918 \pm 52)/T]$	298-460	Orkin and Khamaganov, 1993	DF-EPR
$(5.30 \pm 0.41) \times 10^{-14}$	298		
Relative Rate Coefficients			
$9.0 \times 10^{-13} \exp(-(868 \pm 32)/T]$	303-363	DeMore, 1996	RR (a,b)
4.87×10^{-14}	298*		
$1.36 \times 10^{-18} T^2 \exp(-(256 \pm 98)/T]$	313-371	DeMore, 1996	RR (a,c)
5.12×10^{-14}	298*		

Comments

(a) 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)-$CHCl_2CF_2Cl$-CH_2Cl_2 (or $CHCl_2CF_3$)-O_2-N_2 mixtures. The concentrations of $CHCl_2CF_2Cl$ and CH_2Cl_2 (or $CHCl_2CF_3$) were measured by FTIR spectroscopy. The measured rate coefficient ratios of $k(HO + CHCl_2CF_2Cl)/k(HO + CH_2Cl_2) = (0.50 \pm 0.05) \exp[-(8 \pm 32)/T]$ and $k(HO + CHCl_2CF_2Cl)/k(HO + CHCl_2CF_3) = (0.96 \pm 0.28) \exp[(114 \pm 98)/T]$ are placed on an absolute basis using $k(HO + CH_2Cl_2) = 1.8 \times 10^{-12} \exp(-860/T)$ cm^3 molecule^{-1} s^{-1} (Atkinson et al., 2008) and $k(HO + CHCl_2CF_3) = 1.42 \times 10^{-18} T^2 \exp(-370/T)$ cm^3 molecule^{-1} s^{-1} (Atkinson et al., 2008).

(b) Relative to $k(HO + CH_2Cl_2)$.

(c) Relative to $k(HO + CHCl_2CF_3)$.

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	5.1×10^{-14}	298
k /cm^3 molecule^{-1} s^{-1}	$8.1 \times 10^{-13} \exp(-825/T)$	270-340
Reliability		
$\Delta \log k$	± 0.20	298
$\Delta(E/R)$	± 200	270-340

Comments on Preferred Values

Over the temperature range 298-371 K, the absolute rate coefficients of Orkin and Khamaganov (1993) and the relative rate coefficients of DeMore (1996), using both CH_2Cl_2 and

$CHCl_2CF_3$ as reference compounds, are in good agreement. Accordingly, the three parameter equation $k = CT^2 \exp(-D/T)$ was fitted to the rate coefficients of Orkin and Khamaganov (1993) and DeMore (1996) resulting in $k = 1.23 \times 10^{-18} T^2 \exp(-227/T)$ cm^3 molecule^{-1} s^{-1} over the temperature range 298-460 K. The preferred Arrhenius expression, $k = A \exp(-B/T)$, is centered at 300 K and is obtained from the three parameter equation with $A = C\,e^2\,T^2$ and $B = D + 2T$.

References

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DeMore, W. B.: J. Phys. Chem., 100, 5813, 1996.

Orkin, V. L. and Khamaganov, V. G.: J. Atmos. Chem., 16, 157, 1993.