IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx52

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HO + CH_2ClCF_2Cl (HCFC-132b) → H_2O + $CHClCF_2Cl$

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$1.87 \times 10^{-12} \exp[-(1351 \pm 78)/T]$	250-350	Watson et al., 1979	FP-RF (a)
$(1.9 \pm 0.2) \times 10^{-14}$	298		
$5.54 \times 10^{-26}\ T^{4.58} \exp[(252 \pm 377)/T]$	249-473	Jeong et al., 1984	DF-RF
$(2.42 \pm 0.16) \times 10^{-14}$	297		
$8.53 \times 10^{-19}\ T^{2.28} \exp[-(937 \pm 296)/T]$	295-788	Fang et al., 1999	PLP-LIF
$(1.84 \pm 0.07) \times 10^{-14}$	295		

Comments

(a) The sample of CH_2ClCF_2Cl used was shown by GC to contain ~0.045% of C_2 halogenated alkenes. After correction for possible contributions to the observed OH radical decays from these measured impurities, assuming a rate coefficient for reaction of the C_2 halogenated alkene impurities with HO radicals of 5×10^{-12} cm^3 molecule^{-1} s^{-1} independent of temperature, then the rate coefficient was estimated to be $3 \times 10^{-12} \exp(-1578/T)$ cm^3 molecule^{-1} s^{-1} over the temperature range of 250-350 K, with a rate coefficient at 298 K of 1.67×10^{-14} cm^3 molecule^{-1} s^{-1}.

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	1.7×10^{-14}	298
k /cm^3 molecule^{-1} s^{-1}	$3.5 \times 10^{-12} \exp(-1585/T)$	250-350
Reliability		
$\Delta \log k$	± 0.15	298
$\Delta(E/R)$	± 300	250-350

Comments on Preferred Values

The rate coefficients of Jeong et al. (1984) are higher than those of Watson et al. (1979) and Fang et al. (1999), especially at <300 K, suggesting the presence of reactive impurities in the CH_2ClCF_2Cl sample used. The rate coefficients of Jeong et al. (1984) are therefore not used in

the evaluation. The rate coefficients of Fang et al. (1999) at 295 K and 347 K are in good agreement with the corrected data of Watson et al. (1979) at 298 K and 350 K (see Comment (a) above). Accordingly, the absolute rate coefficients of Watson et al. (1979) [corrected for the impurity observed; see Comment (a)] and Fang et al. (1999) have been fitted to the three parameter equation $k = CT^2 \exp(-D/T)$, resulting in $k = 5.72 \times 10^{-18} T^2 \exp(-1006/T)$ cm^3 molecule^{-1} s^{-1} over the temperature range 250-788 K. The preferred Arrhenius expression, $k = A \exp(-B/T)$, is centered at 290 K and is obtained from the three parameter equation with $A = C e^2 T^2$ and $B = D + 2T$.

References

Fang, T. D., Taylor, P. H. and Berry, R. J.: J. Phys. Chem. A, 103, 2700, 1999.
Jeong, K.-M. Hsu, K.-J., Jeffries, J. B. and Kaufman, F.: J. Phys. Chem., 88, 1222, 1984.
Watson, R. T., Ravishankara, A. R., Machado, G., Wagner, S. and Davis, D. D.: Int. J. Chem. Kinet., 11, 187, 1979.