IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation - Data Sheet oFOx87; VII.A2.2

This datasheet last evaluated: June 2014; last change in preferred values: June 2009.

$HO + CH_2ClCH_2Cl \rightarrow CHClCH_2Cl + H_2O$

Rate coefficient data (k)

k/cm^3 molecule^{-1} s^{-1}	T/K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(2.2\pm0.5) \times 10^{-13}$	296	Howard and Evenson (1976)	DF-LMR (a)
$4.08\times10^{-12}(T/300)^{1.0}$ exp[-(825±88/T)]	292-775	Taylor et al. (1991)	PLP-LIF (b)
$(2.48\pm0.38) \times 10^{-13}$	292		
1.05×10^{-11} exp[-(1141±107)/T]	292-363	Qiu et al (1992)	DF-RF (c)
2.14×10^{-13}	295		
Relative Rate Coefficients			
$(2.50\pm0.54) \times 10^{-13}$	297	Arnts et al. (1989)	RR (d)

Comments

(a) HO radicals were generated by the reaction of H atoms with NO_2 in 0.1-1.0 kPa (0.7-7 Torr) of helium diluent.

(b) HO radicals were produced by the 193 nm (ArF eximer laser) photolysis of N_2O to produce $O(^1D)$ atoms in the presence of H_2O in 730-750 Torr (973-1000 mbar) of helium diluent.

(c) HO radicals were produced by the reaction of F atoms with H_2O in 2-3 Torr (2.7-4.0 mbar) of argon diluent gas.

(d) The rate coefficient ratio $k(HO+CH_2ClCH_2Cl)/k(HO+C_2H_6) = 1.02 \pm 0.22$ was placed on an absolute basis using $k(HO+C_2H_6) = 1.49 \times 10^{-17}\ T^2 \exp(-499/T)$ cm^3 molecule^{-1} s^{-1} (Atkinson et al., 2006).

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	2.4×10^{-13}	298
k /cm^3 molecule^{-1} s^{-1}	8.69×10^{-12} exp(-1070/T)	290-360
Reliability		
Δ log k	0.08	298
Δ E/R	± 200	

Comments on Preferred Values

The rate coefficients of Howard and Evenson (1976), Arnts et al. (1989), Taylor et al. (1991), and Qiu et al. (1992) are in good agreement. Fitting the three parameter equation $k = CT^2 \exp(-D/T)$ to the data from Howard and Evenson (1976), Arnts et al. (1989), Taylor et al. (1991), and Qiu et al. (1992) gives $k = 1.08 \times 10^{-17}\ T^2 \exp(-410/T)$ cm^3 molecule^{-1} s^{-1}. Centering this expression at 330 K with $A = C\ e^2\ T^2$ and $B = D + 2T$ gives $k = 8.69 \times 10^{-12} \exp(-1070/T)$ cm^3 molecule^{-1} s^{-1}.

References

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