IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx21

This data sheet last evaluated: June 2015; last change in preferred values: December 2007.

$Cl + CHF_2Cl$ (HCFC-22) $\rightarrow HCl + CF_2Cl$

$\Delta H° = -9.0$ kJ mol^{-1}

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(1.4 \pm 0.2) \times 10^{-15}$	298	Jourdain et al., 1977	DF-MS
$(1.7 \pm 0.2) \times 10^{-15}$	297	Sawerysyn et al., 1992	DF-MS
$5.3 \times 10^{-12} \exp[-(2430 \pm 90)/T]$	298-430	Talhaoui et al., 1996	DF-MS
$(1.4 \pm 0.3) \times 10^{-15}$	296		
Relative Rate Coefficients			
$(2.0 \pm 0.4) \times 10^{-15}$	298	Tuazon, et al., 1992	RR (a)
$(1.7 \pm 0.1) \times 10^{-15}$	296	Sokolov et al., 1998	RR (b)

Comments

(a) Cl atoms were generated by 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 using a rate coefficient of $k(Cl + CH_4) = 1.0 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} (Atkinson et al. 2006).

(b) Photolysis of Cl_2 in presence of CHF_2Cl and CD_4 in 920 mbar N_2 bath gas. The rate constant ratio obtained, $k(CHF_2Cl)/k(CD_4) = 0.28 \pm 0.02$ was placed on an absolute value using $k(CD_4) = 6.1 \times 10^{-15}$ cm^3 molecule^{-1} s^{-1}.

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	1.6×10^{-15}	298
k /cm^3 molecule^{-1} s^{-1}	$4.2 \times 10^{-12} \exp(-2345/T)$	290-430
Reliability		
$\Delta \log k$	± 0.15	298
Δ E/R	± 400	

Comments on Preferred Values

The rate constants reported at room temperature from the absolute rate studies by Jourdain et al. (1977), Sawerysyn et al. (1992), and Talhaoui et al. (1996) and the relative rate studies by

Tuazon et al. (1992) and Sokolov et al. (1998) are in good agreement. The recommended Arrhenius expression was derived from a fit to the combined data set from all studies.

References

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