IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx29

This data sheet last evaluated: June 2015; last change in preferred values: November 2003.

$Cl + CH_3CF_2Cl$ (HCFC-142b) $\rightarrow HCl + CH_2CF_2Cl$

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(5.3 \pm 1.1) \times 10^{-16}$	297	Jourdain et al., 1977	DF-MS
$(5.6 \pm 2.0) \times 10^{-16}$	297	Sawerysyn et al., 1992	DF-MS
$< 4.4 \times 10^{-15}$	298	Warren and Ravishankara, 1993	PLP-RF
$1.5 \times 10^{-12} \exp[-(2420 \pm 400)/T]$	296-438	Talhaoui et al., 1996	DF-MS
$(4.7 \pm 1.3) \times 10^{-16}$	296		
Relative Rate Coefficients			
$(3.90 \pm 0.52) \times 10^{-16}$	295	Wallington and Hurley, 1992	RR (a)
$(3.7 \pm 0.8) \times 10^{-16}$	298	Tuazon et al., 1992	RR (b)

Comments

(a) Cl atoms were generated by the photolysis of Cl_2. The decays of the reactant and reference organic were measured by FTIR spectroscopy. The measured rate coefficient ratio is placed on an absolute basis by use of a rate coefficient of $k(Cl + CH_4) = 1.0 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} (Atkinson et al., 2006).

(b) Cl atoms were generated by the photolysis of Cl_2. The decays of the reactant and reference organic were measured by FTIR spectroscopy. The measured rate coefficient is placed on an absolute basis by use of a rate coefficient of $k(Cl + CH_4) = 1.0 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} (Atkinson et al., 2006).

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	4.1×10^{-16}	298
k /cm^3 molecule^{-1} s^{-1}	$1.4 \times 10^{-12} \exp(-2420/T)$	296-440
Reliability		
$\Delta \log k$	± 0.15	298
$\Delta(E/R)$	± 500	

Comments on Preferred Values

The preferred value of the rate constant at 298 K is based on the results reported by Wallington and Hurley (1992), Tuazon et al. (1992) and Talhaoui et al. (1996). The latter study supersedes

the work of Sawerysyn et al. (1992). The single temperature dependent study of Talhaoui et al. (1996) forms the basis for the recommendation of k(T), with the A-factor adjusted to reproduce the recommended value of k at 298 K.

References

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