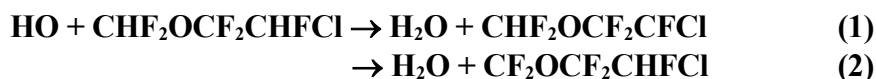


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx72

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



Rate coefficient data ($k = k_1 + k_2$)

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$(1.7 \pm 0.5) \times 10^{-14}$	302	Brown et al., 1989, 1990	DF-RF
$(4.7 \pm 0.7) \times 10^{-14}$	422		
$7.46 \times 10^{-13} \exp[-(1230 \pm 80)/T]$	250-430	Tokuhashi et al., 1999	PLP/FP/DF-LIF
$(1.19 \pm 0.06) \times 10^{-14}$	298		
$(1.2 \pm 0.2) \times 10^{-14}$	298	Langbein et al., 1999	PLP-UVA
<i>Relative Rate Coefficients</i>			
$<3 \times 10^{-13}$	300 ± 3	McLoughlin et al., 1993	RR (a)

Comments

- (a) HO radicals were generated by the photolysis of $\text{CH}_3\text{ONO-NO-CHF}_2\text{OCF}_2\text{CHFCl}$ -diethyl ether air mixtures at ~1 bar pressure. The concentrations of $\text{CHF}_2\text{OCF}_2\text{CHFCl}$ and diethyl ether were measured by GC. The measured upper limit to the rate coefficient ratio $k(\text{HO} + \text{CHF}_2\text{OCF}_2\text{CHFCl})/k(\text{HO} + \text{diethyl ether})$ is placed on an absolute basis by using a rate coefficient of $k(\text{HO} + \text{diethyl ether}) = 1.31 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 300 K (Atkinson, 1994).

Preferred Values

Parameter	Value	T/K
$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	1.2×10^{-14}	298
$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$7.5 \times 10^{-13} \exp(-1230/T)$	250-430
<i>Reliability</i>		
$\Delta \log k$	± 0.10	298
$\Delta(E/R)$	± 150	250-430

Comments on Preferred Values

The study of Tokuhashi et al. (1999) used samples of $\text{CHF}_2\text{OCF}_2\text{CHFCl}$ purified by GC (99.999% purity as analyzed by GC), and the 298 K rate coefficients obtained using three independent techniques (PLP-LIF, FP-LIF and DF-LIF) were identical within the experimental errors. The earlier measurements of Brown et al. (1989, 1990) at 302 K and 422 K are higher than the data of Tokuhashi et al. (1999), probably in part because of the presence of reactive impurities in the $\text{CHF}_2\text{OCF}_2\text{CHFCl}$ sample used by Brown et al. (1989, 1990) [see Tokuhashi et

al. (1999)]. The 298 K rate coefficients from the absolute rate studies of Tokuhashi et al. (1999) and Langbein et al. (1999) are in excellent agreement, and the preferred values are based on these two studies. The upper limit to the rate coefficient measured by McLoughlin et al. (1993) is consistent with the preferred values.

References

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