IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx58

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HO + $CHCl_2CF_2CF_3$ (HCFC-225ca) → H_2O + $CCl_2CF_2CF_3$

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/Comments
Absolute Rate Coefficients			
$2.3 \times 10^{-13} \exp[-(550 \pm 750)/T]$	251-393	Brown et al., 1990	DF-RF
$(3.7 \pm 0.8) \times 10^{-14}$	300		
$1.92 \times 10^{-12} \exp[-(1290 \pm 90)/T]$	270-400	Zhang et al., 1991	FP-RF
$(2.60 \pm 0.29) \times 10^{-14}$	298		
$6.5 \times 10^{-13} \exp[-(970 \pm 115)/T]$	295-364	Nelson et al., 1992	DF-LIF
$(2.41 \pm 0.24) \times 10^{-14}$	295		

Preferred Values

Parameter	Value	*T*/K
k /cm^3 molecule^{-1} s^{-1}	2.5×10^{-14}	298
k /cm^3 molecule^{-1} s^{-1}	$1.1 \times 10^{-12} \exp(-1130/T)$	270-400
Reliability		
$\Delta \log k$	± 0.15	298
$\Delta(E/R)$	± 300	270-400

Comments on Preferred Values

The rate coefficients measured by Zhang et al. (1991) and Nelson et al. (1992) over the temperature range 295-365 K are in good agreement within the experimental uncertainties. The rate coefficients measured by Brown et al. (1990) at 251 K and 300 K are significantly higher, and are not used in the evaluation. The preferred 298 K rate coefficient is the average of those calculated from the Arrhenius expressions of Zhang et al. (1991) and Nelson et al. (1992), and the preferred temperature dependence is the mean of those of Zhang et al. (1991) and Nelson et al. (1992) [a least-squares analysis of the rate coefficients of Zhang et al. (1991) and Nelson et al. (1992) yields $k = 1.56 \times 10^{-12} \exp(-1239/T)$ cm^3 molecule^{-1} s^{-1}, largely weighted by the 270 K

and 400 K rate coefficients of Zhang et al. (1991)]. The pre-exponential factor is adjusted to fit the preferred 298 K rate coefficient and the temperature dependence.

References

Brown, A. C., Canosa-Mas, C. E., Parr, A. D., Rothwell, K. and Wayne, R. P.: Nature, 347, 541, 1990.

Nelson, D. D., Jr., Zahniser, M. S. and Kolb, C. E.: J. Phys. Chem., 96, 249, 1992.

Zhang, Z., Liu, R., Huie, R. E. and Kurylo, M. J.: Geophys. Res. Lett., 18, 5, 1991.