IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx62

 The citation for this data sheet is: Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., Troe, J., and Wallington, T. J.: Atmos. Chem. Phys., 9, 4141, 2008; IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation, http://iupac.pole-ether.fr.
This data sheet last evaluated: June 2015; last change in preferred values: November 2003.

$HO + CH_3OCl \rightarrow$ products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$2.4 \times 10^{-12} \exp[-(360 \pm 100)/T]$	250-341	Crowley et al., 1996.	PLP-RF (a)
$(7.06 \pm 0.22) \times 10^{-13}$	294		

Comments

(a) HO radicals were generated from the pulsed laser photolysis of HNO_3 at 248 nm. CH_3OCl-Ar samples were shown to be stable with respect to decomposition over long time periods (up to 3 months). Each CH_3OCl-Ar sample used was analyzed for Cl_2 impurities by UV absorption before entering the reaction cell. At 294 K, no effect of total pressure of argon diluent (40-400 mbar) on the measured rate coefficient was observed, and the weighted average 294 K rate coefficient is given in the table.

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	7.2×10^{-13}	298
k /cm^3 molecule^{-1} s^{-1}	$2.4 \times 10^{-12} \exp(-360/T)$	250-350
Reliability		
$\Delta \log k$	± 0.3	298
$\Delta(E/R)$	± 300	250-350

Comments on Preferred Values

The preferred values are based on the sole study of this reaction by Crowley et al. (1996). The products have not been measured to date, but formation of $H_2O + CH_2OCl$ and $HOCl + CH_3O$ are possible.

References

Crowley, J. N., Campuzano-Jost, P. and Moortgat, G. K., J. Phys. Chem. 100, 3601, (1996).