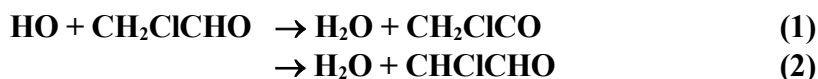


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx64

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This data sheet last evaluated: June 2015; last change in preferred values: November 2000.



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>			
$(3.0 \pm 0.6) \times 10^{-12}$	298	Balestra-Garcia et al., 1992	PLP-RF
<i>Relative Rate Coefficients</i>			
$(3.2 \pm 0.2) \times 10^{-12}$	298 ± 2	Scollard et al., 1993	RR (a)

Comments

- (a) HO radicals were generated by the photolysis of CH_3ONO or $\text{C}_2\text{H}_5\text{ONO}$ in CH_3ONO (or $\text{C}_2\text{H}_5\text{ONO}$)-NO- CH_2ClCHO - $\text{CH}_3\text{C}(\text{O})\text{CH}_2\text{CH}_3$ -air mixtures at 987 ± 13 mbar pressure. The concentrations of CH_2ClCHO and 2-butanone were measured by GC and/or FTIR spectroscopy. Scollard et al. (1993) did not report a value for the rate coefficient ratio $k(\text{HO} + \text{CH}_2\text{ClCHO})/k(\text{HO} + 2\text{-butanone})$. Dividing the reported value of $k(\text{HO} + \text{CH}_2\text{ClCHO})$ by the value of $k(\text{HO} + 2\text{-butanone})$ used by Scollard et al. (1993) gives $k(\text{HO} + \text{CH}_2\text{ClCHO})/k(\text{HO} + 2\text{-butanone}) = 2.70 \pm 0.18$ which is placed on an absolute basis in the table above using $k(\text{HO} + 2\text{-butanone}) = 1.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson et al., 2006).

Preferred Values

Parameter	Value	T/K
$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	3.1×10^{-12}	298
<i>Reliability</i>		
$\Delta \log k$	± 0.15	298

Comments on Preferred Values

The preferred 298 K rate coefficient is the average of those of Balestra-Garcia et al. (1992) and Scollard et al. (1993), which are in excellent agreement. The reaction is expected to proceed essentially totally by channel (1) at 298 K.

References

Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., and Troe, J.: Atmos. Chem. Phys., 6, 3625, 2006; IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation, <http://iupac.pole-ether.fr>
Balestra-Garcia, C., Le Bras, G. and Mac Leod, H.: J. Phys. Chem., 96, 3312, 1992.
Scollard, D. J., Treacy, J. J., Sidebottom, H. W., Balestra-Garcia, C., Laverdet, G., LeBras, G., MacLeod, H. and Téton, S.: J. Phys. Chem., 97, 4683, 1993.