

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation Data Sheet oClOx92; VII.A5.24

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

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	T/K	Reference	Technique/ Comments
<i>Relative Rate Coefficients</i> $(4.38 \pm 0.29) \times 10^{-13}$	298	Carr et al. (2003)	RR (a)

Comments

- (a) OH radicals were generated by the photolysis of O_3 at 254 nm in the presence of H_2O vapour in 1 bar of O_2 diluent. $\text{CH}_2\text{ClCH}_2\text{Cl}$ was used as the reference compound. Chemical analysis was achieved using FTIR spectroscopy and GC techniques and a rate coefficient ratio of $k(\text{HO}+\text{CH}_2\text{ClC}(\text{O})\text{CH}_3)/k(\text{HO}+\text{CH}_2\text{ClCH}_2\text{Cl}) = 1.81 \pm 0.12$ was obtained. Using $k(\text{HO}+\text{CH}_2\text{ClCH}_2\text{Cl}) = 2.42 \times 10^{-13}$ (Calvert et al., 2008) gives $k(\text{HO}+\text{CH}_2\text{ClC}(\text{O})\text{CH}_3) = (4.38 \pm 0.29) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$.

Preferred Values

Parameter	Value	T/K
$k / \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	4.4×10^{-13}	298
<i>Reliability</i> $\Delta \log k$	0.15	298

Comments on Preferred Values

The recommendation is based on the study by Carr et al. (2003). The chlorine atom initiated oxidation of $\text{CH}_2\text{ClC}(\text{O})\text{CH}_3$ was studied by Carr et al. (2003) in one atmosphere of O_2 and the formation of CO , CO_2 , and $\text{HC}(\text{O})\text{Cl}$ products were reported. Carr et al (2003) did not provide any information on the magnitude of the consumption of $\text{CH}_2\text{ClC}(\text{O})\text{CH}_3$ and the precise mechanism by which these products form is not clear. As discussed by Calvert et al. (2011), photolysis leading to the formation of CO , CO_2 , and $\text{HC}(\text{O})\text{Cl}$ is probably the major atmospheric fate of $\text{CH}_2\text{ClC}(\text{O})\text{CH}_3$.

References

Calvert, J. G., Derwent, R. G., Orlando, J. J., Tyndall, G. S., and Wallington T. J.: Mechanisms of Atmospheric Oxidation of the Alkanes, Oxford University Press, New York, NY, 2008.

Calvert, J. G., Mellouki, A., Orlando, J. J., Pilling, M. J., and Wallington T. J.: *The Mechanisms of Atmospheric Oxidation of the Oxygenates*, Oxford University Press, New York, NY, 2011.

Carr, S., Shallcross, D.E., Canosa-Mas, C.E., Wenger, J.C., Sidebottom, H.W., Treacy, J.J., and Wayne, R.P.: *Phys. Chem. Chem. Phys.*, 5, 3874, 2003.