IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx93

This data sheet last evaluated: June 2011; last change in preferred values: June 2010.

$$HO + CH_2ClC(O)CH_3 \rightarrow CHClC(O)CH_3 + H_2O \quad (1)$$
$$\rightarrow CH_2ClC(O)CH_2 + H_2O \quad (2)$$

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

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

Comments

(a) HO 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. CH_2ClCH_2Cl was used as the reference compound. Chemical analysis was achieved using FTIR spectrocopy and GC techniques and a rate coefficient ratio of $k(HO+CH_2ClC(O)CH_3)/k(HO+CH_2ClCH_2Cl) = 1.81 \pm 0.12$ was obtained. Using $k(HO+CH_2ClCH_2Cl) = 2.42 \times 10^{-13}$ (Calvert et al., 2008) gives $k(HO+CH_2ClC(O)CH_3) = (4.38 \pm 0.29) \times 10^{-13}$ cm^3 molecule^{-1} s^{-1}.

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	4.4×10^{-13}	298
Reliability		
$\Delta \log k$	± 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 $CH_2ClC(O)CH_3$ was studied by Carr et al. (2003) in one atmosphere of O_2 and the formation of CO, CO_2, and HC(O)Cl products were reported. Carr et al (2003) did not provide any information on the magnitude of the consumption of $CH_2ClC(O)CH_3$ 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 HC(O)Cl is probably the major atmospheric fate of $CH_2ClC(O)CH_3$.

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, in press, 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.