IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx95

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

$OH + CCl_3C(O)CH_3 \rightarrow CCl_3C(O)CH_2 + H_2O$ **(1)**

Rate coefficient data ($k = k_1$)

k/cm^3 molecule^{-1} s^{-1}	T/K	Reference	Technique/ Comments
Relative Rate Coefficients			
$(1.54 \pm 0.15) \times 10^{-14}$	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. CH_3CN was used as the reference compound. Chemical analysis was achieved using FTIR spectroscopy and GC techniques and a rate coefficient ratio of $k(HO+CCl_3C(O)CH_3)/k(HO+CH_3CN) = 0.70 \pm 0.07$ was obtained. Using $k(HO+CH_3CN) = 2.2 \times 10^{-14}$ (Atkinson et al., 2006) gives $k(HO+CCl_3C(O)CH_3) = (1.54 \pm 0.15) \times 10^{-14}$ cm^3 molecule^{-1} s^{-1}.

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	1.5×10^{-14}	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 $CCl_3C(O)CH_3$ was studied by Carr et al. (2003) in one atmosphere of O_2 and the formation of CO, CO_2, and $COCl_2$ products were reported. Carr et al (2003) did not provide any information on the magnitude of the consumption of $CCl_3C(O)CH_3$ and the precise mechanism by which these products form is not clear. As discussed by Calvert et al. (2010), photolysis leading to the formation of CO, CO_2, and $COCl_2$ is probably the major atmospheric fate of $CCl_3C(O)CH_3$.

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.

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.