IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oRClOx59

This data sheet last evaluated: 28th June 2007; no revision of preferred values.

$O_3 + C_2Cl_4 \rightarrow$ products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$<2 \times 10^{-23}$	297	Mathias et al., 1974	(a)

(a) From experiments carried out at initial O_3 and tetrachloroethene concentrations of $\geq 10^{17}$ molecule cm^{-3} in the presence of excess O_2, using an assumed mechanism and monitoring the formation rate of $C(O)Cl_2$. From the data given in Mathias et al. (1974), a more conservative upper limit of $k < 8 \times 10^{-23}$ cm^3 molecule^{-1} s^{-1} can be derived by assuming that only one $C(O)Cl_2$ molecule is formed per tetrachloroethene reacted.

Preferred Values

$k < 10^{-21}$ cm^3 molecule^{-1} s^{-1} at 298 K.

Comments on Preferred Values

The upper limit to the preferred value is derived from the very limited amount of data reported by Mathias et al. (1974), with the upper limit to the rate coefficient being increased by a factor of 50 over that reported. This upper limit to the rate coefficient for tetrachloroethene is consistent with the kinetic data for the other chloroethenes (Atkinson and Carter, 1984), which show that Cl atom substitution markedly decreases the reactivity of the chloroethenes towards O_3, compared to that for ethene.

References

Atkinson. R. and Carter, W. P. L.: Chem. Rev. 84, 437, 1984.
Mathias, E., Sanhueza, E., Hisatsune, I. C. and Heicklen, J.: Can. J. Chem. 52, 3852, 1974.