IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet X_VOC27

This data sheet updated: 12th November 2002.

$Cl + CH_3C(O)OONO_2 \rightarrow$ products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(3.7 \pm 1.7) \times 10^{-13}$	298	Tsalkani *et al*., 1988[1]	DF-EPR
Relative Rate Coefficients			
$< 7 \times 10^{-15}$	295 ± 2	Wallington *et al*., 1990[2]	RR (a)

Comments

(a) Cl atoms were generated by the photolysis of Cl_2 in Cl_2-air-$CH_3C(O)OONO_2$-CH_4 mixtures at 930 mbar (700 Torr) total pressure, with the $CH_3C(O)OONO_2$ and CH_4 concentrations being monitored by FTIR absorption spectroscopy. Upper limit to relative rate coefficient ratio placed on an absolute basis by use of $k(Cl + CH_4) = 9.9 \times 10^{-14}$ cm^3 molecule^{-1} s^{-1}.[3]

Preferred Values

$k < 2 \times 10^{-14}$ cm^3 molecule^{-1} s^{-1} at 298 K.

Comments on Preferred Values

The preferred value is based on the relative rate coefficient measurement of Wallington *et al*.,[2] in which no reaction of $CH_3C(O)OONO_2$ was observed in the presence of Cl atoms. In both the relative rate study of Wallington *et al*.[2] and the absolute rate study of Tsalkani *et al*.,[1] the major impurity in the $CH_3C(O)OONO_2$ samples would be the C_{12} or C_{13} alkane solvent, respectively. While this was of no consequence in the relative rate study of Wallington *et al*.,[2] the presence of ~0.1% tridecane in the $CH_3C(O)OONO_2$ sample used by Tsalkani *et al*.[1] could account for the Cl reaction rate observed; their $CH_3C(O)OONO_2$ sample was >99% pure from IR measurements. The upper limit cited here is a factor of ~3 higher than measured by Wallington *et al*.[2] to allow for greater uncertainties.

References

[1] N. Tsalkani, A. Mellouki, G. Poulet, G. Toupance, and G. Le Bras, J. Atmos. Chem. **7**, 409 (1988).

[2] T. J. Wallington, J. M. Andino, J. C. Ball, and S. M. Japar, J. Atmos. Chem. **10**, 301 (1990).

[3] IUPAC (2013), http://iupac.pole-ether.fr