IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet X_VOC19

This data sheet updated: 12th November 2002.

$$Cl + CH_3OOH \rightarrow HCl + CH_3O_2 \quad (1)$$
$$\rightarrow HCl + CH_2OOH \quad (2)$$

$\Delta H°(1) = -74$ kJ·mol^{-1}

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

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Relative Rate Coefficients $(5.9 \pm 0.3) \times 10^{-11}$	295 ± 2	Wallington *et al*., 1990[1]	RR (a)

Comments

(a) Cl atoms were generated by the photolysis of Cl_2 in Cl_2-N_2-CH_3OOH-C_2H_6 mixtures at 930 mbar (700 Torr) total pressure, and the CH_3OOH and C_2H_6 concentrations monitored by FTIR absorption spectroscopy. The measured rate coefficient ratio is placed on an absolute basis by use of $k(Cl + C_2H_6) = 5.9 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}.[2]

Preferred Values

$k = 5.9 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 298 K.

Reliability

$\Delta \log k = \pm 0.5$ at 298 K.

Comments on Preferred Values

The sole study carried out to date is that of Wallington *et al*.[1] The reaction may occur by the two pathways listed and the formation of HO radicals via decomposition of CH_2OOH may have led to secondary reactions involving HO radicals. Since the room temperature rate coefficient for the Cl atom reaction with H_2O_2 is two orders of magnitude lower than that for $Cl + CH_3OOH$,[2] it is expected that channel (2) will dominate. Wallington *et al*.[1] concluded that secondary reactions involving HO radicals did not contribute >15% to the observed CH_3OOH consumption. The cited uncertainty limits on the preferred values reflect this possibility.

References

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

2 IUPAC (2013), http://iupac.pole-ether.fr