IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet X_VOC24

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$Cl + n\text{-}C_3H_7ONO_2 \rightarrow$ products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Relative Rate Coefficients			
$(2.1 \pm 0.13) \times 10^{-11}$	295 ± 2	Wallington et al., 1990	RR (a)
$(2.28 \pm 0.14) \times 10^{-11}$	298 ± 2	Nielsen et al., 1991	RR (b)

Comments

(a) Cl atoms were generated by the photolysis of Cl_2 in Cl_2-*n*-propyl nitrate-C_2H_5Cl-air mixtures at 1 bar pressure. *n*-Propyl nitrate and C_2H_5Cl concentrations were measured by GC and a rate coefficient ratio of k(Cl + *n*-propyl nitrate) / k(Cl + C_2H_5Cl) = 2.67 ± 0.16 determined. Rate coefficient in table calculated using k(Cl + C_2H_5Cl) = 7.8×10^{-12} cm^3 molecule^{-1} s^{-1} (Wine et al, 1983 and Bryukov et al., 2003).

(b) Cl atoms were generated by the photolysis of Cl_2 in Cl_2-*n*-propyl nitrate-C_2H_6-N_2 mixtures at 1 bar pressure. Concentrations of *n*-propyl nitrate and C_2H_6 were measured by GC, and the rate coefficient ratio is placed on an absolute basis by use of k(Cl + C_2H_6) = 5.9×10^{-11} cm^3 molecule^{-1} s^{-1} (IUPAC, 2005).

Preferred Values

$k = 2.2 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 298 K.

Reliability

$\Delta \log k = \pm 0.2$ at 298 K.

Comments on Preferred Values

The preferred 298 K rate coefficient is the average of the data of Wallington et al. (1990) and Nielsen et al. (1991). The reaction probably proceeds by H-atom abstraction from the C-H bonds (1990).

References

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