IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet X_VOC23

This data sheet updated: 12th November 2002.

$Cl + C_2H_5ONO_2 \rightarrow$ products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Relative Rate Coefficients			
$(5.5 \pm 0.8) \times 10^{-12}$	295 ± 2	Wallington *et al*., 1990[1]	RR (a)
$(3.95 \pm 0.15) \times 10^{-12}$	298 ± 2	Nielsen *et al*., 1991[2]	RR (b)

Comments

(a) Cl atoms were generated by the photolysis of Cl_2 in Cl_2-ethyl nitrate-C_2H_5Cl-air mixtures at 1 bar pressure. Ethyl nitrate and C_2H_5Cl were measured by GC, and a rate coefficient ratio of k(Cl + ethyl nitrate) / k(Cl + C_2H_5Cl) = 0.46 ± 0.03 determined. Combined with k(Cl + C_2H_5Cl) / k(Cl + C_2H_6) = 0.201 ± 0.027 [3] and k(Cl + C_2H_6) = 5.9×10^{-11} cm^3 molecule^{-1} s^{-1},[4] the rate coefficient cited in the table is obtained.

(b) Cl atoms were generated by the photolysis of Cl_2-ethyl nitrate-C_2H_6-N_2 mixtures at atmospheric pressure. Concentrations of ethyl nitrate and ethane were measured by GC, and the rate coefficient ratio placed on an absolute basis by use of k(Cl + C_2H_6) = 5.9×10^{-11} cm^3 molecule^{-1} s^{-1}.[4]

Preferred Values

$k = 4.7 \times 10^{-12}$ 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*.[1] and Nielsen *et al*.,[2] The reaction probably proceeds by H atom abstraction from the C-H bonds.[2]

References

1 T. J. Wallington, M. M. Hinman, J. M. Andino, W. O. Siegl, and S. M. Japar, Int. J. Chem. Kinet. **22**, 665 (1990).

2 O. J. Nielsen, H. W. Sidebottom, M. Donlon, and J. Treacy, Chem. Phys. Lett. **178**, 163 (1991).

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

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