IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet X_VOC11

This data sheet updated: 9th August 2002.

$Cl + C_2H_5CHO \rightarrow$ products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Relative Rate Coefficients			
$(1.17 \pm 0.10) \times 10^{-10}$	295 ± 2	Wallington *et al*., 1988[1]	RR (a)
$(1.45 \pm 0.08) \times 10^{-10}$	298 ± 3	Thévenet, Mellouki and LeBras, 2000[2]	RR(b)
$(1.20 \pm 0.07) \times 10^{-10}$	298 ± 3		(c)
$(1.25 \pm 0.06) \times 10^{-10}$	298 ± 3		(d)
$(1.41 \pm 0.10) \times 10^{-10}$	298 ± 3		(e)

Comments

(a) Cl atoms were generated by the photolysis of Cl_2 in Cl_2-air mixtures, and the decay rates of C_2H_5CHO and C_2H_6 monitored by GC. 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}.[3]

(b) Cl atoms were generated by the photolysis of Cl_2 in Cl_2-air mixtures, and the decay rates of C_2H_5CHO and C_2H_6 monitored by GC. The measured rate coefficient ratio (2.46 ± 0.08) 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}.[3]

(c) Method as (b) but C_3H_8 as reference gas. The measured rate coefficient ratio (0.85 ± 0.05) is placed on an absolute basis by use of $k(Cl + C_3H_8) = 1.4 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1}.[3]

(d) Method as (b) but n-C_4H_{10} as reference gas. The measured rate coefficient ratio (0.61 ± 0.03) is placed on an absolute basis by use of $k(Cl + C_4H_{10}) = 2.05 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1}.[3]

(e) Method as (b) but n-hexane as reference gas. The measured rate coefficient ratio (0.44 ± 0.02) is placed on an absolute basis by use of $k(Cl + n\text{-hexane}) / k(Cl + n\text{-butane}) = 1.56$ (average value from references 4 and 5) and $k(Cl + n\text{-butane}) = 2.05 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1}.[3]

Preferred Values

$k = 1.3 \times 10^{-10}$ 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 value uses data from the relative rate studies of Wallington *et al*.,[1] and Thévenet, Mellouki and LeBras, 2000.[2] and is an average of the rate constants obtained in experiments in which, C_2H_6 , C_3H_8 and n-C_4H_{10} were used as reference gases, which have well defined rate coefficients for reaction with Cl.

References

[1] T. J. Wallington, L. M. Skewes, W. O. Siegl, C.-H. Wu, and S. M. Japar, Int. J. Chem. Kinet. **20**, 867 (1988).

[2] R. Thévenet, A. Mellouki and G. LeBras, Int. J. Chem. Kinet. **32**, 676 (2000).

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

[4] G.S. Tyndall, J.J. Orlando, T.J. Wallington, M. Dill and E.W. Kaiser, Int. J. Chem. Kinet. **29**, 43 (1999).

[5] P.A. Hooshiyar and H. Niki, Int. J. Chem. Kinet. **27**, 1197 (1995).