IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet X_VOC6

This data sheet last evaluated: June 2003; last change in preferred values: June 2003

$Cl + C_3H_6 + M \rightarrow HCl + C_3H_6Cl + M$ (1)

$Cl + C_3H_6 + M \rightarrow C_3H_5 + HCl$ (2)

Low-pressure rate coefficients
Rate coefficient data (k_{1o})

k_{1o}/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Relative Rate Coefficients			
$(4.0 \pm 0.4) \times 10^{-28}$ [N_2]	298	Kaiser and Wallington, 1996	(a)

Comments

(a) Cl atoms were generated by photolysis of Cl_2 in the presence of C_3H_6, C_2H_6 and 1 mbar to 900 mbar of N_2. C_3H_6 consumption was determined by FTIR or GC analysis, the major products being 3-chloropropene and 1,2-dichloropropane. At low pressure (below 12 mbar) 3-chloropropene is the major product indicating that the abstraction of H by Cl from the C_3H_6 is the dominant channel. At pressures higher than 12 mbar, the primary product observed is 1,2-dichloropropane, indicating that addition of a Cl atom to the double bond is the major channel. The limiting rate coefficients were obtained using $F_c = 0.6$. A rate coefficient for the reference reaction $Cl + C_2H_6 \rightarrow C_2H_5 + HCl$ of 5.9×10^{-11} cm^3 molecule^{-1} s^{-1} was employed (Kaiser and Wallington, 1996; Atkinson et al. 2006).

Preferred Values

$k_{1o} = 4.0 \times 10^{-28}$ [N_2] cm^3 molecule^{-1} s^{-1} at 298 K.

Reliability

$\Delta \log k_{1o} = \pm 0.5$ at 298 K.

Comments on Preferred Values

The preferred value is based on the only value reported (Kaiser and Wallington, 1996). Due to this and to the uncertainty of the extrapolated k_{1o}, a large error limit is assigned.

High-pressure rate coefficients
Rate coefficient data ($k = k_1 + k_2$)

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Relative Rate Coefficients			
$(2.54 \pm 0.09) \times 10^{-10}$	296	Atkinson and Aschmann, 1985	(a)
$(2.94 \pm 0.13) \times 10^{-10}$	295	Wallington, Skewes and Siegl, 1988	(b)
$(2.68 \pm 0.13) \times 10^{-10}$	298	Kaiser and Wallington, 1996	(c)

Comments

(a) Cl atoms generated by the photolysis of Cl_2-*n*-C_4H_{10}-C_3H_6-air at 1 bar. The reaction was studied relative to the reaction Cl + *n*-$C_4H_{10} \rightarrow$ products for which a rate coefficient 2.05×10^{-10} cm^3 molecule^{-1} s^{-1} is used (Atkinson et al., 2006). C_3H_6 and *n*-C_4H_{10} were analyzed by GC.

(b) Cl atoms were formed by photolysis of Cl_2 in the presence of C_3H_6 and C_2H_6 or *n*-C_4H_{10} at atmospheric pressure of synthetic air. The decay rate of C_3H_6 was measured relative to that of *n*-C_4H_{10} and placed on an absolute basis using a rate coefficients of 2.05×10^{-10} cm^3 molecule^{-1} s^{-1} for the reference reaction, (Atkinson et al., 2006).

(c) See comment (a) for k_{1o}. Rate coefficient at 933 mbar (700 Torr) pressure of N_2 or air.

Preferred Values

$k = 2.7 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1} at 298 K and 1 bar of air.

Reliability

$\Delta \log k = \pm 0.3$ at 298 K.

Comments on Preferred Values

The preferred value at 1 bar of air is an average of earlier results from Atkinson and Aschmann (1985) and Wallington et al. (1988) and the more recent determination by Kaiser and Wallington (1996). At room temperature and atmospheric pressure, the addition of Cl atoms to the double bond accounts for approximately 90% of the reaction (Kaiser and Wallington, 1996). The H atom abstraction occurs from the C-H bonds of the methyl group (Kaiser and Wallington, 1996).

References

Atkinson, R. and Aschmann, S. M.: Int. J. Chem. Kinet. 17, 33, 1985.

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Kaiser, E. W. and Wallington, T. J.: J. Phys. Chem. **100**, 9788, 1996.

Wallington, T. J., Skewes, L. M., and Siegl, W. O.: J. Photochem. Photobiol. A: Chem., 45, 167, 1988.