# IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet X_VOC18

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This data sheet last evaluated January 2008.

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## Cl + *n*-$C_4H_9OH$ → products

### Rate coefficient data: *k*

| *k*/cm$^3$ molecule$^{-1}$ s$^{-1}$ | Temp./K | Reference | Technique/ Comments |
|---|---|---|---|
| *Absolute Rate Coefficients* | | | |
| (1.96 ± 0.19) x $10^{-10}$ | 298 | Garzón et al., 2006 | LP-RF (a) |
| 3.12 x $10^{-11}$ exp[(548 ± 65)/*T*] | 266-382 | | |
| *Relative Rate Coefficients* | | | |
| (2.14 ± 0.11) x $10^{-10}$ | 298 ± 2 | Nelson et al., 1990 | RR (b) |
| (2.25 ± 0.11) x $10^{-10}$ | 295 | Wu et al., 2003 | RR (c) |
| (2.37 ± 0.11) x $10^{-10}$ | 295 | Wu et al., 2003 | RR (d) |

### Comments

(a) Cl atoms generated by $Cl_2$ photolysis at 308 nm and detected by RF at ≈ 135 nm. All experiments in He bath gas (26.7-266.7 mbar) with traces of $O_2$ to scavenge organic radicals. *k* was independent of pressure.

(b) Cl atoms were generated by photolysis of $Cl_2$ or $COCl_2$ in $Cl_2$ (or $COCl_2$)-$N_2$ (or $O_2$)-*n*$C_4H_9OH$-cyclohexane mixtures at 1 bar pressure. Concentrations of *n*$C_4H_9OH$ and cyclohexane were measured by GC, and the rate coefficient ratio *k*(Cl + *n*$C_4H_9OH$) / *k*(Cl + cyclohexane) = (0.656 ± 0.045) was placed on an absolute basis by use of *k*(Cl + cyclohexane) / *k*(Cl + *n*-butane) = 1.59 (Aschmann and Atkinson, 1995) and *k*(Cl + *n*-butane) = 2.05 x $10^{-10}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (IUPAC, 2008).

(c) Photolysis of $Cl_2$ in presence of *n*$C_4H_9OH$ using propane as reference reactant and 1 atmosphere pressure of air as bath gas. Reactants analysed by GC. Rate coefficient ratio *k*(Cl + *n*$C_4H_9OH$) / *k*(Cl + $C_3H_8$) = (1.61 ± 0.08) was put on an absolute basis using *k*(Cl + $C_3H_8$) = 1.4 × $10^{-10}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (IUPAC, 2008).

(d) Photolysis of $Cl_2$ in presence of *n*$C_4H_9OH$ using cyclohexane as reference reactant and 1 atmosphere pressure of air as bath gas. Reactants analysed by GC. Rate coefficient ratio *k*(Cl + *n*$C_4H_9OH$) / *k*(Cl + cyclohexane) = (0.726 ± 0.033) was put on an absolute basis using *k*(Cl + cyclohexane) = 3.26 × $10^{-10}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ which was derived using *k*(Cl + cyclohexane) / *k*(Cl + *n*-butane) = 1.59 (Aschmann and Atkinson, 1995) and *k*(Cl + *n*-butane) = 2.05 x $10^{-10}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (IUPAC, 2008).

### Preferred Values

*k* = 2.2 x $10^{-10}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K.
*k* = 3.5 x $10^{-11}$ exp(550/*T*) cm$^3$ molecule$^{-1}$ s$^{-1}$ over the temperature range 260 - 390 K.

*Reliability*

$\Delta \log k = \pm 0.08$ at 298 K.

$\Delta(E/R) = \pm 200$ K.

*Comments on Preferred Values*

The preferred room temperature rate coefficient is an average value from the four studies of this reaction, which are in good agreement. The temperature dependence is taken from Garzón et al. (2006) with the pre-exponential factor adjusted to return the preferred value of $k$ at 298 K.

## References


Garzón, A. G., Cuevas, C. A., Ceacero, A. A., Notario, A., Albaladejo, J. and Fernández-Gómez, M.: J. Chem. Phys. 125, article. 104305, 2006.

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

Nelson, L., Rattigan, O., Neavyn, R., Sidebottom, H, Treacy, J. and Nielsen, O. J.: Int. J. Chem. Kinet. 22, 1111, 1990.

Wu, H., Mu, Y., Zhang, X. and Jiang, G.: Int. J. Chem. Kin. 35, 81, 2003.