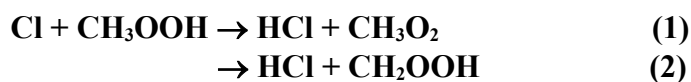


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet X_VOC19

Website: <http://iupac.pole-ether.fr>. See website for latest evaluated data. Data sheets can be downloaded for personal use only and must not be retransmitted or disseminated either electronically or in hardcopy without explicit written permission.

This data sheet updated: 12th November 2002.



$$\Delta H^\circ(1) = -74 \text{ kJ}\cdot\text{mol}^{-1}$$

Rate coefficient data ($k = k_1 + k_2$)

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Relative Rate Coefficients</i> (5.9 ± 0.3) $\times 10^{-11}$	295 \pm 2	Wallington <i>et al.</i> , 1990 ¹	RR (a)

Comments

- ^(a) Cl atoms were generated by the photolysis of Cl₂ in Cl₂-N₂-CH₃OOH-C₂H₆ mixtures at 930 mbar (700 Torr) total pressure, and the CH₃OOH and C₂H₆ concentrations monitored by FTIR absorption spectroscopy. The measured rate coefficient ratio is placed on an absolute basis by use of $k(\text{Cl} + \text{C}_2\text{H}_6) = 5.9 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$.²

Preferred Values

$$k = 5.9 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

Reliability

$$\Delta \log k = \pm 0.5 \text{ at } 298 \text{ K.}$$

Comments on Preferred Values

The sole study carried out to date is that of Wallington *et al.*¹ The reaction may occur by the two pathways listed and the formation of HO radicals via decomposition of CH₂OOH may have led to secondary reactions involving HO radicals. Since the room temperature rate coefficient for the Cl atom reaction with H₂O₂ is two orders of magnitude lower than that for Cl + CH₃OOH,² it is expected that channel (2) will dominate. Wallington *et al.*¹ concluded that secondary reactions involving HO radicals did not contribute >15% to the observed CH₃OOH consumption. The cited uncertainty limits on the preferred values reflect this possibility.

References

- ¹ T. J. Wallington, J. M. Andino, J. C. Ball, and S. M. Japar, *J. Atmos. Chem.* **10**, 301 (1990).
² IUPAC (2013), <http://iupac.pole-ether.fr>