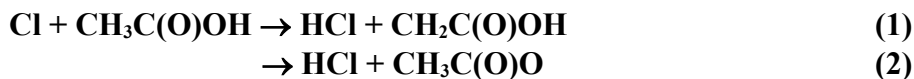


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet X_VOC21

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: 18th November 2005.



$$\Delta H^\circ(2) = 11 \text{ kJ}\cdot\text{mol}^{-1}$$

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>			
$(2.8 \pm 0.4) \times 10^{-14}$	298 ± 1	Koch and Moortgat, 1990	RR (a)
$(2.5 \pm 0.3) \times 10^{-14}$	295	Crawford et al., 1999	RR (b)

Comments

- (a) Cl atoms were generated by the photolysis of Cl_2 in Cl_2 - $\text{CH}_3\text{C}(\text{O})\text{OH}$ - CH_4 - N_2 mixtures at 1 bar total pressure. The concentrations of $\text{CH}_3\text{C}(\text{O})\text{OH}$ and CH_4 were measured by IR absorption spectroscopy. The rate coefficient ratio $k(\text{Cl} + \text{CH}_3\text{C}(\text{O})\text{OH}) / k(\text{Cl} + \text{CH}_4) = 0.28 \pm 0.04$ is placed on an absolute basis by use of $k(\text{Cl} + \text{CH}_4) = 1.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (IUPAC, 2005). An analogous experiment using $\text{CD}_3\text{C}(\text{O})\text{OH}$ yielded a rate coefficient of $k(\text{Cl} + \text{CD}_3\text{C}(\text{O})\text{OH}) = (7.5 \pm 0.2) \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, indicating that the reaction proceeds mainly by channel (1).
- (b) Cl atoms were generated by the photolysis of Cl_2 in Cl_2 - $\text{CH}_3\text{C}(\text{O})\text{OH}$ - CH_4 mixtures in N_2 or air at 933 mbar total pressure. The concentrations of $\text{CH}_3\text{C}(\text{O})\text{OH}$ and CH_4 were measured by IR absorption spectroscopy. The rate coefficient ratio $k(\text{Cl} + \text{CH}_3\text{C}(\text{O})\text{OH}) / k(\text{Cl} + \text{CH}_4) = 0.25 \pm 0.03$ is placed on an absolute basis by use of $k(\text{Cl} + \text{CH}_4) = 1.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (IUPAC, 2005).

Preferred Values

$$k = 2.65 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

Reliability

$$\Delta \log k = \pm 0.2 \text{ at } 298 \text{ K.}$$

Comments on Preferred Values

The preferred 298 K rate coefficient is an average of the similar studies of Koch and Moortgat (1990) and Crawford et al. (1999). The measured rate coefficient ratio of $k(\text{Cl} + \text{CH}_3\text{C}(\text{O})\text{OH})/k(\text{Cl} + \text{CD}_3\text{C}(\text{O})\text{OH}) = 3.7$ at (298 ± 1) K indicates that channel (1) dominates at 298 K (Koch and Moortgat, 1990).

References

Crawford, M. A., Wallington, T. J., Szente, J. J., Maricq, M. M., and Francisco, J. S.: J. Phys. Chem. A 103, 365, 1999.

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

Koch, S. and Moortgat, G. K.: Chem. Phys. Lett. 173, 531, 1990.