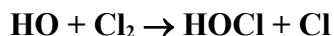


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet iClOx21

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 re-transmitted or disseminated either electronically or in hard copy without explicit written permission.

This data sheet last evaluated: 28th June 2007; no revision of preferred values.



$$\Delta H^\circ = 6 \text{ kJ mol}^{-1}$$

Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$(5.5 \pm 0.3) \times 10^{-14}$	298	Leu and Lin, 1979	DF-RF
$\sim 7.4 \times 10^{-14}$	298	Ravishankara et al., 1983	DF-RF
$(6.70 \pm 0.72) \times 10^{-14}$	298 ± 3	Loewenstein and Anderson, 1984	DF-RF
$1.7 \times 10^{-12} \exp[-(911 \pm 373)/T]$	253-333	Boodaghians et al., 1987	DF-RF
$(6.8 \pm 1.0) \times 10^{-14}$	293 ± 2		
$3.77 \times 10^{-12} \exp[-(1228 \pm 140)/T]$	231-354	Gilles et al., 1999	PLP-LIF
$(5.95 \pm 0.75) \times 10^{-14}$	298		
$3.09 \times 10^{-16} T^{1.35} \exp(-745/T)$	297-826	Bryukov et al., 2004	PLP-LIF (a)
$(6.34 \pm 0.18) \times 10^{-14}$	297		

Comments

- (a) The cited 297 K rate coefficient is a weighted average of the two determinations at this temperature. Combining rate coefficient calculations with their data and those of Gilles et al. (1999) resulted in the expression $1.35 \times 10^{-16} T^{1.50} \exp(-723/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, which was proposed to be applicable to the temperature range 200-3000 K (Bryukov et al., 2004).

Preferred Values

$$k = 6.5 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

$$k = 3.6 \times 10^{-12} \exp(-1200/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ over the temperature range } 230\text{-}360 \text{ K.}$$

Reliability

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

$$\Delta(E/R) = \pm 300 \text{ K.}$$

Comments on Preferred Values

The preferred values are based on the data of Loewenstein and Anderson (1984), Boodaghians et al. (1987), Gilles et al. (1999) and Bryukov et al. (2004), which are in good agreement concerning the room temperature rate coefficient. Because of the more atmospherically relevant temperature range covered, the preferred temperature dependence is that reported by Gilles et al. (1999), with the pre-exponential factor, A , being adjusted to fit the preferred 298 K rate coefficient. Loewenstein and Anderson (1984) determined that the exclusive products are HOCl + Cl.

References

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- Recommendation
- Lowenstein and Anderson (1984)
- Boodaghians et al. (1987)
- ▲ Gilles et al. (1999)
- ▼ Bryukov et al. (2004)

