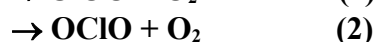


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet iClOx30

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 updated: 25th September 2003.



$$\Delta H^\circ(1) = -146.8 \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta H^\circ(2) = -149.7 \text{ kJ}\cdot\text{mol}^{-1}$$

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

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$k_2 < 1 \times 10^{-18}$	298	DeMore et al., 1975	DF-MS
$k_2 < 1 \times 10^{-18}$	298	Wongdontri-Stuper et al., 1979	FP-UVA (a)
$k_1 < 1.3 \times 10^{-17}$	233	Stevens and Anderson, 1990	(b)
$k_1 < 1.4 \times 10^{-17}$	298		
$k_1 = (4.0 \pm 2.0) \times 10^{-16}$	413		

Comments

- (a) Flash photolysis of Cl₂-O₃ mixtures. Upper limit to the rate coefficient obtained expected to really refer to k_2 (Stevens and Anderson, 1990).
- (b) Discharge flow system. Reaction channel (1) was followed by monitoring ClO produced from the thermal decomposition of the product ClOO in the presence of O₃. The product ClO was distinguished from the reactant ClO through isotopic labelling.

Preferred Values

$$k_1 < 1.5 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

$$k_2 < 1 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

Comments on Preferred Values

The preferred upper limit for k_1 is based on the results of the study of Stevens and Anderson (1990). The preferred upper limit for k_2 is based on the data of DeMore et al. (1975) and Wongdontri-Stuper et al. (1979). The upper limit of Stevens and Anderson (1990) at room temperature can be combined with their measured rate coefficient at 413 K to derive $A_1 = 2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $E_1/R > 3600 \text{ K}$. For k_2 one can estimate $A_2 = 1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and derive $E_2/R > 4000 \text{ K}$.

References

- DeMore, W. B., Lin, C. L. and Jaffe, S.: presented at ACS National Meeting, Philadelphia, PA, 1975.
- Stevens, P. S. and Anderson, J. G.: *Geophys. Res. Lett.* 17, 1287, 1990.
- Wongdontri-Stuper, W., Jayanty, R. K. M., Simonaitis, R. and Heicklen, J.: *J. Photochem.* 10, 163, 1979.