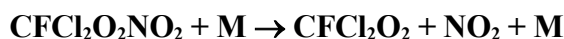


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oRCIOx44

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: 27th January 2006.



$$\Delta H^\circ = 107 \text{ kJ mol}^{-1}$$

Low-pressure rate coefficients

Rate coefficient data

k_0/s^{-1}	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$1.0 \times 10^{-2} \exp(-10860/T) [\text{N}_2]$	260-300	Köppenkastrop and Zabel, 1991	(a)

Comments

- (a) Reaction studied in a temperature-controlled 420 liter reaction chamber, monitoring the reactant by long-path IR absorption. Measurements at 11, 82, and 800 mbar pressure. Falloff extrapolations using $F_c = 0.28$ and $k_\infty = 6.6 \times 10^{16} \exp(-12240/T) \text{ s}^{-1}$.

Preferred Values

$$k_0 = 1.0 \times 10^{-2} \exp(-10860/T) [\text{N}_2] \text{ s}^{-1} \text{ over the temperature range 260-300 K.}$$

Reliability

$$\Delta \log k_0 = \pm 0.3 \text{ at 298 K.}$$

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

Comments on Preferred Values

The only available measurements are preferred with the employed $F_c = 0.28$. The data are consistent with related reactions.

High-pressure rate coefficients

Rate coefficient data

k_∞/s^{-1}	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$4.0 \times 10^{16} \exp(-12300/T)$	274-305	Simonaitis, Glavas and Heicklen, 1979	(a)
$6.6 \times 10^{16} \exp(-12240/T)$	260-300	Köppenkastrop and Zabel, 1991	(b)

Comments

- (a) Steady-state photolysis of $\text{Cl}_2\text{-CHFCl}_2\text{-O}_2\text{-NO-NO}_2$ mixtures at 1 bar. Simulation of the mechanism depending on the extent of various Cl-consuming reactions. k was assumed to be close to k_∞ .

(b) See comment (a) for k_0 .

Preferred Values

$k_\infty = 6.6 \times 10^{16} (-12240/T) \text{ s}^{-1}$ over the temperature range 260-300 K.

Reliability

$\Delta \log k_\infty = \pm 0.3$ at 298 K.

$\Delta(E/R) = \pm 500$ K.

Comments on Preferred Values

The agreement between the results from Simonatis et al. (1979) and Köppenkastrop and Zabel (1991) at 298 K and 1 bar within a factor of 1.5 appears satisfactory. The data from Köppenkastrop and Zabel (1991) are preferred.

References

Köppenkastrop, D. and Zabel F.: *Int. J. Chem. Kinet.*, 23, 1, 1991.

Simonaitis, R., Glavas, S. and Heicklen, J.: *Geophys. Res. Lett.*, 6, 385, 1979.