IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx83

This data sheet updated: 5th July 2005.

$CF_2Cl + O_2 + M \rightarrow CF_2ClO_2 + M$

$\Delta H° = -127.4$ kJ mol^{-1}

Low-pressure rate coefficients
Rate coefficient data

k_0/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients $1.4 \times 10^{-29} (T/298)^{-5.2} [N_2]$	200-300	Forst and Caralp, 1991	(a)

Comments

(a) Microcanonical variational theory with inversion of partition functions, used for interpolation between experimental data of the reactions O_2 + (CCl_3, CCl_2F, and CF_3).

Preferred Values

$k_0 = 1.4 \times 10^{-29} (T/300)^{-5} [N_2]$ cm^3 molecule^{-1} s^{-1} over the temperature range 200-300 K.

Reliability

$\Delta \log k_0 = \pm 0.5$ at 298 K.

$\Delta n = \pm 3$.

Comments on Preferred Values

There are no measurements for this reaction. However, the analysis by Forst and Caralp (1991), as well as a simple interpolation of k_0-values for $CF_3 + O_2$ and $CFCl_2 + O_2$ lead to the given preferred values. Unlike Forst and Caralp (1991), who prefer $F_c = 0.6$ we recommend $F_c = 0.4$.

High-pressure rate coefficients
Rate coefficient data

k_∞/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients $7.1 \times 10^{-12} (T/298)^{-0.56}$	200-300	Forst and Caralp, 1991	(a)

Comments

(a) See comment (a) for k_0.

Preferred Values

$k_\infty = 7 \times 10^{-12} (T/298)^{-0.6}$ cm^3 molecule^{-1} s^{-1} over the temperature range 200-300 K.

Reliability

$\Delta \log k_\infty = \pm 0.5$ at 298 K.

$\Delta n = \pm 0.5$.

Comments on Preferred Values

See Comments on Preferred Values for k_0.

References

Forst, W. and Caralp, F.: J. Chem. Soc. Faraday Trans.. 87, 2307, 1991.