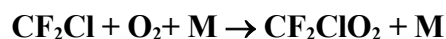


# IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx83

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: 5<sup>th</sup> July 2005.



$$\Delta H^\circ = -127.4 \text{ kJ mol}^{-1}$$

## Low-pressure rate coefficients Rate coefficient data

$k_0/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$1.4 \times 10^{-29} (T/298)^{-5.2} [\text{N}_2]$	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  $\text{O}_2 + (\text{CCl}_3, \text{CCl}_2\text{F}, \text{and } \text{CF}_3)$ .

## Preferred Values

$$k_0 = 1.4 \times 10^{-29} (T/300)^{-5} [\text{N}_2] \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ over the temperature range 200-300 K.}$$

### Reliability

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

$$\Delta n = \pm 3.$$

### 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  $\text{CF}_3 + \text{O}_2$  and  $\text{CFCl}_2 + \text{O}_2$  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

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

## Comments

- (a) See comment (a) for  $k_0$ .

## Preferred Values

$k_{\infty} = 7 \times 10^{-12} (T/298)^{-0.6} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  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.