

# IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oRCIOx45

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This data sheet updated: 27<sup>th</sup> January 2006.



$$\Delta H^\circ = -105.6 \text{ kJ mol}^{-1}$$

## 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>			
$(9.2 \pm 3) \times 10^{-29} (T/298)^{-6.0} [\text{O}_2]$	233-373	Caralp et al., 1988	PLP-MS (a)

### Comments

- (a) Pulsed laser photolysis-MS study at pressures of 1.3-13 mbar. Falloff extrapolation with  $F_c = \exp(-T/260)$ , i. e.  $F_c = 0.32$  at 298 K, and  $k_\infty = 1.49 \times 10^{-12} (T/298)^{-0.3} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ .

### Preferred Values

$$k_0 = 9.2 \times 10^{-29} (T/298)^{-6.0} [\text{N}_2] \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ over the temperature range 230-380 K.}$$

### Reliability

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

$$\Delta n = \pm 2.$$

### Comments on Preferred Values

There is a single experimental study only. However, according to the analysis by Destriau and Troe (1990) it falls in line with related reactions. Equal values for  $k_0$  are assumed for the bath gases  $\text{O}_2$  and  $\text{N}_2$ . The  $F_c$  value should be used independent of the temperature.

## 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>			
$(1.49 \pm 0.8) \times 10^{-12} (T/298)^{-0.3}$	233-373	Caralp et al., 1988	PLP-MS (a)

### Comments

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

### Preferred Values

$k_{\infty} = 1.5 \times 10^{-12} (T/298)^{-0.7} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  over the temperature range 230-380 K.

*Reliability*

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

$\Delta n = \pm 0.5$ .

*Comments on Preferred Values*

See Comments on Preferred Values for  $k_0$ . Recommending a temperature-independent  $F_c = 0.32$  is consistent with changing  $n$  from -0.3 to -0.7 such as preferred for related reactions.

**References**

Caralp, F., Lesclaux, R., Rayez, M.-T., Rayez, J.-C. and Forst, W.: J. Chem. Soc. Faraday Trans. 2, 84, 569, 1988.

Destriau, M. and Troe, J.: Int. J. Chem. Kinet., 22, 915, 1990.