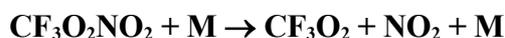


## IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet IV.A1.63 of FOx64

Datasheets can be downloaded for personal use only and must not be retransmitted or disseminated either electronically or in hardcopy without explicit written permission. The citation for this data sheet is: IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation, (<http://iupac.pole-ether.fr>).

This datasheet last evaluated: 24<sup>th</sup> January 2006.



$$\Delta H^\circ = 105 \text{ kJ mol}^{-1}$$

### Low-pressure rate coefficients Rate coefficient data

$k_0/\text{s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$2.4 \times 10^{-5} \exp(-9430/T) [\text{N}_2]$	264-297	Mayer-Figge, Zabel and Becker, 1996	(a)

### Comments

- (a) Preparation of  $\text{CF}_3\text{O}_2\text{NO}_2$  by *in situ* photolysis of  $\text{CF}_3\text{I}/\text{O}_2/\text{NO}_2/\text{N}_2$  mixtures in a 420 l reactor. Time dependence of  $\text{CF}_3\text{O}_2\text{NO}_2$  decay monitored by IR absorption. Measurements in 3.7-1013 mbar of  $\text{N}_2$  evaluated with  $F_c = 0.31$ ,  $N_c = 1.19$ , and  $k_\infty = 1.49 \times 10^{16} \exp(-11940/T) \text{ s}^{-1}$ . Similar results in  $\text{O}_2$ . Analysis of equilibrium constant gives  $\Delta H^\circ = 102.7 (\pm 2.0) \text{ kJ mol}^{-1}$ .

### Preferred Values

$$k_0 = 2.5 \times 10^{-5} \exp(-9430/T) [\text{N}_2] \text{ s}^{-1} \text{ over the temperature range 260-300 K.}$$

### Reliability

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

$$\Delta(E/R) = \pm 250 \text{ K.}$$

### Comments on Preferred Values

The single measurement falls in line with data for related reactions. In addition, it could be evaluated theoretically leading to realistic molecular parameters. Because no unusual complications were observed, the data appear reliable. The observed part of the falloff curve could well be represented with  $F_c$  and  $k_\infty$  such as given in comment (a) for  $k_0$ .

## High-pressure rate coefficients Rate coefficient data

$k_{\infty}/s^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$1.49 \times 10^{16} \exp(-11940/T)$	264-297	Mayer-Figge, Zabel and Becker, 1996	(a)

### Comments

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

### Preferred Values

$k_{\infty} = 1.5 \times 10^{16} \exp(-11940/T)$  over the temperature range 260-300 K.

#### *Reliability*

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

$\Delta(E/R) = \pm 250$  K.

#### *Comments on Preferred Values*

See Comments on Preferred Values for  $k_0$ . The theoretical analysis by Mayer-Figge et al. (1996) supersedes the more speculative earlier analysis by Destriau and Troe (1990). The falloff curve is constructed with the fitted  $F_c = 0.31$  and  $N_c = 1.19$  in good agreement with the recommendation given in the Introduction.

The following text-line combines the preferred values for the high and low pressure limiting rate coefficients to generate a single, cut-and-paste expression for calculation of  $k$ :

```
=((2.5e-5*exp(-9430/T))*M*(1.5e16 *exp(-11940/T)))/((2.5e-5*exp(-9430/T))*M+(1.5e16 *exp(-11940/T)))*10^(log10(0.31)/(1+(log10((2.5e-5*exp(-9430/T))*M/(1.5e16 *exp(-11940/T)))/(0.75-1.27*log10(0.31)))^2))
```

The molecular density,  $M = 7.243 \times 10^{21} P(\text{bar})/T(\text{K})$

### References

- Destriau, M. and Troe, J.: Int. J. Chem. Kinet., 22, 915, 1990.  
Mayer-Figge, A., Zabel, F. and Becker, K.H.: J. Phys. Chem., 100, 6587, 1996.