# IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet IV.A1.63 oFOx64



This datasheet last evaluated: 24th January 2006.

**$CF_3O_2NO_2 + M \rightarrow CF_3O_2 + NO_2 + M$**

$\Delta H° = 105$ kJ mol$^{-1}$

## Low-pressure rate coefficients
## Rate coefficient data

| $k_0$/s$^{-1}$ | Temp./K | Reference | Technique/ Comments |
|---|---|---|---|
| *Absolute Rate Coefficients* | | | |
| 2.4 x 10$^{-5}$ exp(-9430/$T$) [$N_2$] | 264-297 | Mayer-Figge, Zabel and Becker, 1996 | (a) |

## Comments

(a) Preparation of $CF_3O_2NO_2$ by *in situ* photolysis of $CF_3I/O_2/NO_2/N_2$ mixtures in a 420 l reactor. Time dependence of $CF_3O_2NO_2$ decay monitored by IR absorption. Measurements in 3.7-1013 mbar of $N_2$ evaluated with $F_c = 0.31$, $N_c = 1.19$, and $k_\infty = 1.49 \times 10^{16}$ exp(-11940/$T$) s$^{-1}$. Similar results in $O_2$. Analysis of equilibrium constant gives $\Delta H° = 102.7$ (± 2.0) kJ mol$^{-1}$.

## Preferred Values

$k_0 = 2.5 \times 10^{-5}$ exp(-9430/$T$) [$N_2$] s$^{-1}$ over the temperature range 260-300 K.

*Reliability*

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

$\Delta(E/R) = \pm 250$ 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 |
|---|---|---|---|
| *Absolute Rate Coefficients* | | | |
| 1.49 x $10^{16}$ 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 x $10^{16}$ 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 = $7.243\times10^{21}$P(bar)/T(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.