# IUPAC Task group on Atmospheric chemical Kinetic Data Evaluation – Data Sheet oFOx42



This data sheet updated: 29th March 2005.

## $CF_3O + NO \rightarrow COF_2 + FNO$

$\Delta H° = -135$ kJ mol$^{-1}$

### Rate coefficient data

| $k$/cm$^3$ molecule$^{-1}$ s$^{-1}$ | Temp./K | Reference | Technique/ Comments |
|---|---|---|---|
| *Absolute Rate Coefficients* | | | |
| $(5.2 \pm 2.7) \times 10^{-11}$ | 295 | Sehested and Nielsen, 1993 | PR/UVA(a) |
| $3.34 \times 10^{-11} \exp[(160 \pm 45)/T]$ | 233-360 | Turnipseed et al., 1994 | PLP/LIF(b) |
| $(5.62 \pm 0.74) \times 10^{-11}$ | 298 | | |
| $4.1 \times 10^{-11} \exp[(60 \pm 100)/T]$ | 231-393 | Jensen, Hanson, and Howard, 1994 | (c) |
| $(5.0 \pm 1.0) \times 10^{-11}$ | 298 | | |
| $(4.7 \pm 0.9) \times 10^{-11}$ | 298 | Bourbon et al., 1996 | FT/LIF(d) |
| $(4.72 \pm 0.30) \times 10^{-11}$ | 293 | Bhatnagar and Carr, 1994 | FP/MS (e) |
| $4.1 \times 10^{-11} \exp[(60 \pm 100)/T]$ | 213-353 | Dibble et al., 1995 | LP/LAS(f) |

### Comments

(a) Radicals generated by pulse radiolysis of $CHF_3$-$O_2$-NO-$SF_6$ mixtures. Value of $k$ derived from simulations of FNO absorption transients at 310.5 nm.

(b) Pulsed laser photolysis/pulsed laser-induced fluorescence technique. $CF_3O$ radicals were generated by photolysis of $CF_3OOCF_3$ at 193 nm.

(c) Flow tube reactor/chemical ionization mass spectrometer technique. $CF_3O$ radicals were generated by pyrolysis of $CF_3OOCF_3$. A low value of $k$ from the same laboratory reported earlier by Bevilacqua *et al*. (1993) is superseded by these results.

(d) $CF_3O$ radicals were generated by DF technique in F/$CF_3H$/$O_2$/NO system.

(e) k obtained by modeling NO time dependence during secondary reactions in $CF_3O_2$ + NO reaction.

(f) $CF_3O$ radicals were generated by photolysis of $CF_3OOCF_3$ at 193 nm. Time resolved formation of $COF_2$ using tunable diode laserabsorption near 1950 cm-1. FNO identified as major co-product with $COF_2$.

### Preferred Values

$k = 5.4 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K.
$k = 3.7 \times 10^{-11} \exp(110/T)$ cm$^3$ molecule$^{-1}$ s$^{-1}$ over the temperature range 230-390 K.

*Reliability*

$\Delta \log k = \pm 0.1$ at 298 K.
$\Delta(E/R) = \pm 100$ K.

*Comments on Preferred Values*

The preferred values are based on the 233-360 K values of Turnipseed et al. (1994), the 231-393 K values of Jensen et al. (1994) and the 295 K value of Sehested and Nielsen (1993).

These results are in good agreement. The low value of $k$ reported by Bevilacqua et al. (1993) has been superseded by the results of Jensen et al. (1994). Room temperature results from Bourbon et al. (1996) and Bhatnagar and Carr (1994) and a temperature dependence study of Dibble et al (1995) are in good agreement with the recommendation. The reaction products have been reported by Chen et al. (1992), Bevilacqua et al. (1993) and Li and Francisco (1991).

## References


Bevilacqua, T. J., Hanson, D. R. and Howard, C. J.: J. Phys. Chem., 97, 3750, 1993.
Bhatagar, A. and Carr, R.W.: Chem.Phys.Lett., 231, 454, 1994.
Bourbon, C., Briuokov, M., Hanoune, B., Sawersyn, J. P. and Devolder, P.: Chem.Phys.Lett., 254, 203, 1996.
Chen, J., Zhu, T.and Niki, H.: J. Phys. Chem. 96, 6115, 1992.
Dibble, T. S., Maricq, M. M., Szente, J. J. and Francisco, J. S.: J. Phys. Chem., 99, 17394, 1995.
Jensen, N. R., Hanson, D. R. and Howard, C. J.: J. Phys. Chem., 98, 8574, 1994.
Li, Z. and Francisco, J. S.: Chem. Phys. Lett., 186, 336 , 1991.
Sehested, J. and Nielsen, O. J.: Chem. Phys. Lett., 206, 369, 1993.
Turnipseed, A. A., Barone, S. B. and Ravishankara, A. R.: J. Phys. Chem., 98, 4594, 1994.