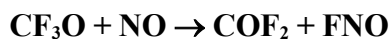


IUPAC Task group on Atmospheric chemical Kinetic Data Evaluation – Data Sheet of FOx42

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: 29th March 2005.



$$\Delta H^\circ = -135 \text{ kJ mol}^{-1}$$

Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$(5.2 \pm 2.7) \times 10^{-11}$	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

- Radicals generated by pulse radiolysis of CHF₃-O₂-NO-SF₆ mixtures. Value of k derived from simulations of FNO absorption transients at 310.5 nm.
- Pulsed laser photolysis/pulsed laser-induced fluorescence technique. CF₃O radicals were generated by photolysis of CF₃OOCF₃ at 193 nm.
- Flow tube reactor/chemical ionization mass spectrometer technique. CF₃O radicals were generated by pyrolysis of CF₃OOCF₃. A low value of k from the same laboratory reported earlier by Bevilacqua *et al.* (1993) is superseded by these results.
- CF₃O radicals were generated by DF technique in F/CF₃H/O₂/NO system.
- k obtained by modeling NO time dependence during secondary reactions in CF₃O₂ + NO reaction.
- CF₃O radicals were generated by photolysis of CF₃OOCF₃ at 193 nm. Time resolved formation of COF₂ using tunable diode laser absorption near 1950 cm⁻¹. FNO identified as major co-product with COF₂.

Preferred Values

$$k = 5.4 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

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

Reliability

$$\Delta \log k = \pm 0.1 \text{ at } 298 \text{ K.}$$

$$\Delta(E/R) = \pm 100 \text{ K.}$$

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.
Bhatnagar, A. and Carr, R.W.: Chem.Phys.Lett., 231, 454, 1994.
Bourbon, C., Briukov, 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.