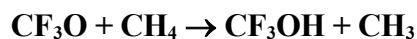


# IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet of FOx43

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: 29<sup>th</sup> March 2005.



$$\Delta H^\circ = -16.9 \text{ kJ mol}^{-1}$$

## Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$(2.2 \pm 0.2) \times 10^{-14}$	298	Saathoff and Zellner, 1993	LP/LIF(a)
$1.92 \times 10^{-12} \exp[-(1370 \pm 85)/T]$	247-360	Barone et al., 1994	PLP/LIF (b)
$(1.93 \pm 0.11) \times 10^{-14}$	298		
$3.1 \times 10^{-12} \exp[-(1470 \pm 250)/T]$	231-385	Jensen et al., 1994	FT/CIMS(c)
$(2.2 \pm 0.4) \times 10^{-14}$	298		
$4.49 \times 10^{-12} \exp[-(1606 \pm 84)/T]$	296-573	Bourbon et al., 1995	FT/LIF(d)
$(2.05 \pm 0.20) \times 10^{-12}$	298		
$3.3 \times 10^{-12} \exp[-(1430 \pm 150)/T]$	235--401	Bednarek et al., 1995	LP/LIF (e)
$2.5 \times 10^{-14}$	298		
<i>Relative Rate Coefficients</i>			
$<5 \times 10^{-15}$	297	Chen et al., 1992	(f)
$(1.2 \pm 0.1) \times 10^{-14}$	298	Kelly et al., 1993	(g)

## Comments

- (a)  $\text{CF}_3\text{O}$  radicals were generated by photolysis of  $\text{CF}_3\text{OF}$  at 248 nm.
- (b)  $\text{CF}_3\text{O}$  radicals were generated by photolysis of  $\text{CF}_3\text{OOCF}_3$  at 193 nm.
- (c)  $\text{CF}_3\text{O}$  radicals were generated by pyrolysis of  $\text{CF}_3\text{OOCF}_3$ .
- (d)  $\text{CF}_3\text{O}$  radicals were generated by the pyrolysis of  $\text{CF}_3\text{OOCF}_3$ .
- (e)  $\text{CF}_3\text{O}$  radicals were generated by photolysis of  $\text{CF}_3\text{OF}$  at 248 nm.
- (f) Long path FTIR-based product study of visible photolysis of  $\text{CF}_3\text{NO-NO-CH}_4$  mixtures in 700 torr air. Searched for  $\text{CH}_2\text{O}$  product from oxidation of  $\text{CH}_4$  initiated by reaction of  $\text{CF}_3\text{O}$  radicals with  $\text{CH}_4$ . Upper limit of  $k$  given in table is derived from the measured ratio  $k/k(\text{CF}_3\text{O+NO}) < 10^{-4}$  and the value of  $k(\text{CF}_3\text{O+NO})$  given in this evaluation.
- (g) Long-path FTIR-based study.  $\text{CF}_3\text{O}$  radicals were generated by photolysis of  $\text{CF}_3\text{OOCF}_3$ . The decay of the reactant hydrocarbon was compared with the decay of the reference hydrocarbon. The value of  $k$  given in table is derived from the measured ratio  $k/k(\text{CF}_3\text{O+C}_2\text{H}_6) = 0.010 \pm 0.001$  and the value of  $k(\text{CF}_3\text{O+C}_2\text{H}_6)$  (IUPAC, current evaluation).

## Preferred Values

$$k = 2.2 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

$$k = 2.6 \times 10^{-12} \exp(-1420/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ over the temperature range } 230\text{-}380 \text{ K.}$$

## Reliability

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

$$\Delta(E/R) = \pm 200 \text{ K.}$$

### *Comments on Preferred Values*

The preferred value at room temperature is the average of the values reported by Saathoff and Zellner (1993), Barone et al. (1994), Jensen et al. (1994), Bourbon et al. (1995) and Bednarek et al. (1994). Results of these direct studies are in excellent agreement at room temperature. The temperature dependence is based on the 247-360 K data of Barone et al. (1994) the 231-385 K data of Jensen et al. (1994) and the 235-401 K data of Bednarek et al. (1994). The temperature dependence of Bourbon et al. (1995) is thought to be high due to possible influence of wall reaction at high temperature. The relative rate measurements of Chen et al. (1992) and Kelly et al. (1993) are factors of 4 and 2, respectively, lower than the preferred value. Wallington and Ball (1995) reported  $k/k(\text{CF}_3\text{O} + \text{C}_2\text{H}_6) = 0.0152 \pm 0.0023$  at 296 K in good agreement with the recommended rate coefficients. Jensen et al. (1994) detected the product  $\text{CF}_3\text{OH}$  by chemical ionization mass spectrometer (CIMS) and observed its formation to correlate with the loss of the  $\text{CF}_3\text{O}$  reactant. The  $\text{CF}_3\text{OH}$  product of this reaction was also observed by Bevilacqua et al. (1993) and also by Bednarek et al. (1994), who used FTIR spectroscopy to show that  $\text{CF}_3\text{OH}$  is converted slowly to  $\text{CF}_2\text{O}$ .

### **References**

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