

# IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet of FOx11

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$$\Delta H^\circ = -65.0 \text{ kJ mol}^{-1}$$

## Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/Comments
<i>Absolute Rate Coefficients</i>			
$(7.8 \pm 1.2) \times 10^{-15}$	296	Howard and Evenson, 1976	DF-LMR
$7.42 \times 10^{-12} \exp[-(2100 \pm 200)/T]$	293-429	Clyne and Holt, 1979	DF-RF
$(5.8 \pm 0.3) \times 10^{-15}$	293		
$(1.17 \pm 0.14) \times 10^{-14}$	297	Nip et al., 1979	FP-RA
$4.4 \times 10^{-12} \exp[-(1766 \pm 50)/T]$	250-492	Jeong et al., 1984	DF-RF (a)
$(1.12 \pm 0.075) \times 10^{-14}$	298		
$(8.8 \pm 1.4) \times 10^{-15}$	298	Bera and Hanrahan, 1988	PR-A
$1.57 \times 10^{-12} \exp[-(1470 \pm 100)/T]$	222-381	Talukdar et al., 1991	FP-LIF
$(1.13 \pm 0.10) \times 10^{-14}$	298		
$(2.52 \pm 0.25) \times 10^{-15}$	223	Schmoltner et al., 1993	PLP/FP-LIF
$(1.09 \pm 0.03) \times 10^{-14}$	298		
$(1.00 \pm 0.03) \times 10^{-14}$	298	Szilagyi et al., 2000	DF-RF
<i>Relative Rate Coefficients</i>			
$2.24 \times 10^{-18} T^2 \exp[-(857 \pm 24)/T]$	297-383	Hsu and DeMore, 1995	RR (b)
$1.12 \times 10^{-14}$	297		

## Comments

- (a) The rate expression cited in Jeong et al. (1984) supersedes that reported in Jeong and Kaufman (1982).
- (b) Relative rate method. HO radicals were generated from the photolysis of H<sub>2</sub>O at 185 nm or of O<sub>3</sub>-H<sub>2</sub>O mixtures in the UV in H<sub>2</sub>O (or O<sub>3</sub>-H<sub>2</sub>O)-CH<sub>2</sub>F<sub>2</sub>-CH<sub>3</sub>CHF<sub>2</sub>-O<sub>2</sub>-N<sub>2</sub> mixtures. The concentrations of CH<sub>2</sub>F<sub>2</sub> and CH<sub>3</sub>CHF<sub>2</sub> were measured by FTIR spectroscopy. The measured rate coefficient ratio of  $k(\text{HO} + \text{CH}_2\text{F}_2)/k(\text{HO} + \text{CH}_3\text{CHF}_2) = (0.80 \pm 0.06) \exp[-(277 \pm 24)/T]$  is placed on an absolute basis using a rate coefficient of  $k(\text{HO} + \text{CH}_3\text{CHF}_2) = 2.80 \times 10^{-18} T^2 \exp(-580/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (IUPAC, current recommendation).

## Preferred Values

$k = 1.1 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K.

$k = 2.3 \times 10^{-12} \exp(-1590/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  over the temperature range 220-300 K.

### Reliability

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

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

### Comments on Preferred Values

The absolute rate coefficients of Schmoltner et al. (1993) at 223 K and 298 K are in excellent agreement with the earlier, and much more extensive rate coefficient data of Talukdar et al. (1991). The room temperature rate coefficients of Nip et al. (1983), Jeong and Kaufman (1982), Jeong et al. (1984), Talukdar et al. (1991) and Schmoltner et al. (1993) are in good agreement, but are ~30% higher than those of Howard and Evenson (1976), Clyne and Holt (1979) and Bera and Hanrahan (1988). The data of Clyne and Holt (1979) are not considered reliable and that of Bera and Hanrahan (1988) may have been subject to secondary reactions. The rate coefficients measured by Jeong and Kaufman (1982) (250-492 K) and Talukdar et al. (1991) (222-381 K) are in good agreement over the temperature range where they overlap.

The rate coefficient data of Nip et al. (1983), Jeong and Kaufman (1982), Talukdar et al. (1991), Hsu and DeMore (1995), Schmoltner et al. (1993), and Szilagyi et al. (2000) have been fitted to the three parameter equation  $k = CT^2 \exp(-D/T)$ , resulting in  $k = 4.80 \times 10^{-18} T^2 \exp(-1080/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  over the temperature range 222-492 K. The preferred Arrhenius expression,  $k = A \exp(-B/T)$ , is centered at 255 K and is derived from the three-parameter equation with  $A = C e^2 T^2$  and  $B = D + 2T$ .

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- Howard and Evenson (1976)
- Jeong and Kaufman (1982)
- ▲ Nip et al. (1979)
- ▼ Talukdar et al. (1991)
- ◆ Schmoltnner et al. (1993)
- ◆ Szilagyi et al. (2000)
- △ Hsu and DeMore (1995) relative to  $\text{CH}_3\text{CHF}_2$

