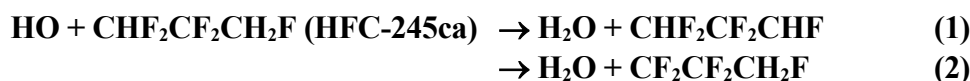


## IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet of FOx22

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### Rate coefficient data ( $k = k_1 + k_2$ )

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/Comments
<i>Absolute Rate Coefficients</i>			
$2.87 \times 10^{-12} \exp[-(1661 \pm 170)/T]$	260-365	Zhang et al., 1994	FP-RF
$(1.09 \pm 0.03) \times 10^{-14}$	298		
<i>Relative Rate Coefficients</i>			
$1.24 \times 10^{-20} T^{2.82} \exp[-(823 \pm 34)/T]$	286-364	Hsu and DeMore, 1995	RR (a)
$7.44 \times 10^{-15}$	298		

### Comments

- (a) Relative rate method. HO radicals were generated by 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 H<sub>2</sub>O-O<sub>3</sub>)-CHF<sub>2</sub>CF<sub>2</sub>CH<sub>2</sub>F-CH<sub>4</sub>-O<sub>2</sub>-N<sub>2</sub> mixtures. The concentrations of CHF<sub>2</sub>CF<sub>2</sub>CH<sub>2</sub>F and CH<sub>4</sub> were measured by FTIR absorption spectroscopy. The measured rate coefficient of  $k(\text{HO} + \text{CHF}_2\text{CF}_2\text{CH}_2\text{F})/k(\text{HO} + \text{CH}_4) = (0.67 \pm 0.07) \exp[(164 \pm 34)/T]$  is placed on an absolute basis by use of a rate coefficient of  $k(\text{HO} + \text{CH}_4) = 1.85 \times 10^{-20} T^{2.82} \exp(-987/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (IUPAC, current recommendation).

### Preferred Values

$k = 7.7 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K.

$k = 2.2 \times 10^{-12} \exp(-1685/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  over the temperature range 285-365 K.

#### Reliability

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

$\Delta(E/R) = \pm 300$  K.

#### Comments on Preferred Values

The relative rate coefficients of Hsu and DeMore (1995) are uniformly a factor of 1.5 lower than the absolute rate coefficients of Zhang et al. (1994) over the temperature range common to both studies (286-364 K). This suggests the presence of reactive impurities or of secondary reactions in the study of Zhang et al. (1994). The relative rate coefficients of Hsu and DeMore (1995) were used to derive the preferred values. These data were fitted to the three parameter equation,  $k = CT^2 \exp(-D/T)$ , resulting in  $k = 2.84 \times 10^{-18} T^2 \exp(-1045/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  over the temperature range 285-365 K. The preferred Arrhenius expression,  $k = A \exp(-B/T)$ , is centered at 320 K and is derived from the three parameter equation,  $k = CT^2 \exp(-D/T)$  with  $A =$

$C e^2 T^2$  and  $B = D + 2T$ .

### References

Zhang, Z., Padmaja, S., Saini, R. D., Huie, R. E. and Kurylo, M. J.: J. Phys. Chem. 98, 4312, 1994.

Hsu, K.-J. and DeMore, W. B.: J. Phys. Chem. 99, 1235, 1995.

IUPAC: <http://iupac.pole-ether.fr>, 2013.