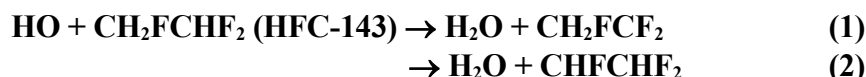


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet of FOx18

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This datasheet last evaluated: June 2015; last change in preferred values: March 2005.



$$\Delta H^\circ(1) = -78.0 \text{ kJ mol}^{-1}$$

$$\Delta H^\circ(2) = -80.1 \text{ kJ mol}^{-1}$$

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>			
$1.48 \times 10^{-12} \exp[-(1000 \pm 100)/T]$	293-425	Clyne and Holt, 1979	DF-RF
$(4.68 \pm 0.40) \times 10^{-14}$	294		
$(1.83 \pm 0.18) \times 10^{-14}$	298	Martin and Paraskevopoulos, 1983	FP-RA
<i>Relative Rate Coefficients</i>			
$4.97 \times 10^{-18} T^2 \exp[-1012/T]$	278-323	Barry et al., 1995	RR (a)
$(1.49 \pm 0.05) \times 10^{-14}$	298 \pm 2		

Comments

- (a) HO radicals were generated by the photolysis of O₃ in the presence of water vapor at ~250 nm at atmospheric pressure of air. Irradiations of O₃-H₂O-CH₂FCHF₂-CH₃CCl₃-air mixtures were carried out and the concentrations of CH₂FCHF₂ and CH₃CCl₃ measured by GC and FTIR spectroscopy. The measured rate coefficient ratio of $k(\text{HO} + \text{CH}_2\text{FCHF}_2)/k(\text{HO} + \text{CH}_3\text{CCl}_3) = 2.21 \exp(-102/T)$ is placed on an absolute basis by use of a rate coefficient of $k(\text{HO} + \text{CH}_3\text{CCl}_3) = 2.25 \times 10^{-18} T^2 \exp(-910/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (IUPAC, current recommendation).

Preferred Values

$$k = 1.5 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

$$k = 3.3 \times 10^{-12} \exp(-1610/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ over the temperature range } 270\text{-}330 \text{ K.}$$

Reliability

$$\Delta \log k = \pm 0.2 \text{ at } 298 \text{ K.}$$

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

Comments on Preferred Values

The rate coefficient of Martin and Paraskevopoulos (1983) at 298 K is ~25% higher than the 298 K value Barry et al. (1995). The preferred rate coefficients are therefore derived from the relative rate study of Barry et al. (1995). The preferred Arrhenius expression, $k = A \exp(-B/T)$,

is derived from the three parameter expression cited in the table ($k = 4.97 \times 10^{-18} T^2 \exp(-1012/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ over the temperature range 278-323 K) and is centered at 300 K with $A = C e^2 T^2$ and $B = D + 2T$.

References

- Barry, J., Sidebottom, H., Treacy, J. and Franklin, J. *Int. J. Chem. Kinet.* 27, 27, 1995.
Clyne, M. A. A. and Holt, P. M.: *J. Chem. Soc. Faraday Trans. 2*, 75, 582, 1979.
IUPAC: <http://iupac.pole-ether.fr>, 2013.
Martin, J.-P. and Paraskevopoulos, G.: *Can. J. Chem.* 61, 861, 1983.