IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oFOx18

The citation for this data sheet is: Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., Troe, J., and Wallington, T. J.: Atmos. Chem. Phys., 9, 4141, 2008; IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation, http://iupac.pole-ether.fr.

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

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$HO + CH_2FCHF_2$ (HFC-143) $\rightarrow H_2O + CH_2FCF_2$ (1)

$\rightarrow H_2O + CHFCHF_2$ (2)

$\Delta H°(1) = -78.0$ kJ mol^{-1}

$\Delta H°(2) = -80.1$ kJ mol^{-1}

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

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/Comments
Absolute Rate Coefficients			
$1.48 \times 10^{-12} \exp[-(1000 \pm 100)/T]$	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
Relative Rate Coefficients			
$4.97 \times 10^{-18} T^2 \exp[-1012/T]$	278-323	Barry et al., 1995	RR (a)
$(1.49 \pm 0.05) \times 10^{-14}$	298 ± 2		

Comments

(a) HO radicals were generated by the photolysis of O_3 in the presence of water vapor at ~250 nm at atmospheric pressure of air. Irradiations of O_3-H_2O-CH_2FCHF_2-CH_3CCl_3-air mixtures were carried out and the concentrations of CH_2FCHF_2 and CH_3CCl_3 measured by GC and FTIR spectroscopy. The measured rate coefficient ratio of $k(HO + CH_2FCHF_2)/k(HO + CH_3CCl_3) = 2.21 \exp(-102/T)$ is placed on an absolute basis by use of a rate coefficient of $k(HO + CH_3CCl_3) = 2.25 \times 10^{-18} T^2 \exp(-910/T)$ cm^3 molecule^{-1} s^{-1} (IUPAC, current recommendation).

Preferred Values

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

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

Reliability

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

$\Delta(E/R) = \pm 300$ 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 x 10^{-18} T^2 exp(-1012/T) cm^3 $molecule^{-1}$ 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.
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Martin, J.-P. and Paraskevopoulos, G.: Can. J. Chem. 61, 861, 1983.