IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oFOx24

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HO + $CF_3CHFCHF_2$ (HFC-236ea) → H_2O + CF_3CFCHF_2 (1)

→ H_2O + CF_3CHFCF_2 (2)

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

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/Comments
Absolute Rate Coefficients			
$2.0 \times 10^{-13} \exp[-(1007 \pm 151)/T]$	251-311	Garland et al., 1993	PLP-LIF
$(6.5 \pm 0.5) \times 10^{-15}$	294		
$1.05 \times 10^{-12} \exp[-(1434 \pm 161)/T]$	260-365	Zhang et al., 1994	FP-RF
$(8.51 \pm 0.26) \times 10^{-15}$	298		
$(4.93 \pm 0.25) \times 10^{-15}$	294	Nelson et al., 1995	DF-LIF
Relative Rate Coefficients			
$6.7 \times 10^{-21} T^{2.82} \exp[-(756 \pm 100)/T]$	298-380	Hsu and DeMore, 1995	RR (a)
5.0×10^{-15}	298		

Comments

(a) HO radicals were generated by the photolysis of H_2O at 185 nm or of O_3-H_2O mixtures in the UV, in H_2O (or O_3-H_2O)-$CF_3CHFCHF_2$-CH_4-O_2-N_2 mixtures. The concentrations of $CF_3CHFCHF_2$ and CH_4 were measured by FTIR absorption spectroscopy. The measured rate coefficient ratio of $k(HO + CF_3CHFCHF_2)/k(HO + CH_4) = (0.36 \pm 0.01) \exp[(231 \pm 12)/T]$ is placed on an absolute basis by using a rate coefficient of $k(HO + CH_4) = 1.85 \times 10^{-20} T^{2.82} \exp(-987/T)$ cm^3 molecule^{-1} s^{-1} (IUPAC, current recommendation).

Preferred Values

$k = 5.0 \times 10^{-15}$ cm^3 molecule^{-1} s^{-1} at 298 K.

$k = 1.4 \times 10^{-12} \exp(-1680/T)$ cm^3 molecule^{-1} s^{-1} over the temperature range 290-380 K.

Reliability

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

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

Comments on Preferred Values

The preferred values are derived from the relative rate coefficients of Hsu and DeMore (1995) and the absolute rate study by Nelson et al. (1995). These data were fitted to the three parameter equation, $k = CT^2 \exp(-D/T)$, resulting in $k = 1.76 \times 10^{-18} T^2 \exp(-1021/T)$ cm^3 molecule^{-1} s^{-1} over the temperature range 294-380 K. The preferred Arrhenius expression, $k = A \exp(-B/T)$, is centered at 330 K and is derived from the three parameter equation, $k = A \exp(-B/T)$ with $A = C e^2 T^2$ and $B = D + 2T$. The higher values of Garland et al. (1993) and Zhang et al. (1994) were

not used in this evaluation as their experiments may have been subject to problems arising from the presence of impurities.

References

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