IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oFOx109

This data sheet last evaluated: September 2011; last change in preferred values: September 2011.

$HO + CHF_2CH_2CF_3$ (HFC-245fa) $\rightarrow CF_2CH_2CF_3 + H_2O$ (1)

$\rightarrow CHF_2CHCF_3 + H_2O$ (2)

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

k/cm^3 molecule^{-1} s^{-1}	T/K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(6.12 \pm 0.22) \times 10^{-15}$	294	Nelson et al. (1995)	DF-LIF (a)
$6.32 \times 10^{-13} \exp[-(1331 \pm 43)/T]$	273-370	Orkin et al. (1996)	FP-RF (b)
$(7.24 \pm 0.02) \times 10^{-15}$	298		

Comments

(a) HO radicals were generated by the reaction of H atoms with NO_2. The experiments were conducted in 1.1-6.8 Torr (1.5-9.1 mbar) of helium diluent. The loss of HO radicals was monitored by LIF at 282 nm.

(b) HO radicals were generated by the flash photolysis of H_2O using a xenon lamp. The decay of HO radicals was monitored in the presence of $CHF_2CH_2CF_3$ in 100 Torr (133 mbar) of argon diluent.

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	6.85×10^{-15}	298
k /cm^3 molecule^{-1} s^{-1}	$5.96 \times 10^{-13} \exp(-1331/T)$	270-370
Reliability		
$\Delta \log k$	± 0.1	298
$\Delta E/R$	± 300	

Comments on Preferred Values

The results reported by Nelson et al. (1995) and Orkin et al. (1996) are in excellent agreement. We have used the temperature dependence reported by Orkin et al. (1996) to adjust the result reported by Nelson et al. (1995) at 294 K (6.12×10^{-15}) to give a value at 298 K of 6.50×10^{-15} cm^3 molecule^{-1} s^{-1}. The recommended value at 298 K is the average of this result and that reported by Orkin et al. (1996). The recommended temperature dependence is taken from Orkin et al. (1996).

References

Nelson Jr., D. D., Zahniser, M. S., Kolb, C. E., and Magid, H.: J. Phys. Chem., 99, 16301, 1995.

Orkin, V. L., Huie, R. E., and Kurylo, M. J.: J. Phys. Chem., 100, 8907, 1996.