IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation - Data Sheet oFOx75; VII.A1.4

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$HO + CF_3CH_2CHF_2$ (HFC-245fa) $\rightarrow CF_3CH_2CF_2 + H_2O$ (1)
$\rightarrow CF_3CHCHF_2 + H_2O$ (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)
$6.32 \times 10^{-12} \exp[-(1331 \pm 43)/T]$	273-370	Orkin et al. (1996)	FP-RF (b)
$(7.24 \pm 0.02) \times 10^{-15}$	298		

Comments

(a) HO radicals produced via the H + NO_2 reaction. Experiments were performed in 2.2-3.1 Torr (0.3-0.4 kPa) of helium diluent.

(b) HO radicals were produced from the photolysis of H_2O vapor using a xenon flash lamp. HO radicals were monitored by their resonance fluorescence near 308 nm using microwave discharge resonance lamp. Experiments were performed in 100 Torr (13.33 kPa) of argon diluent.

Preferred Values

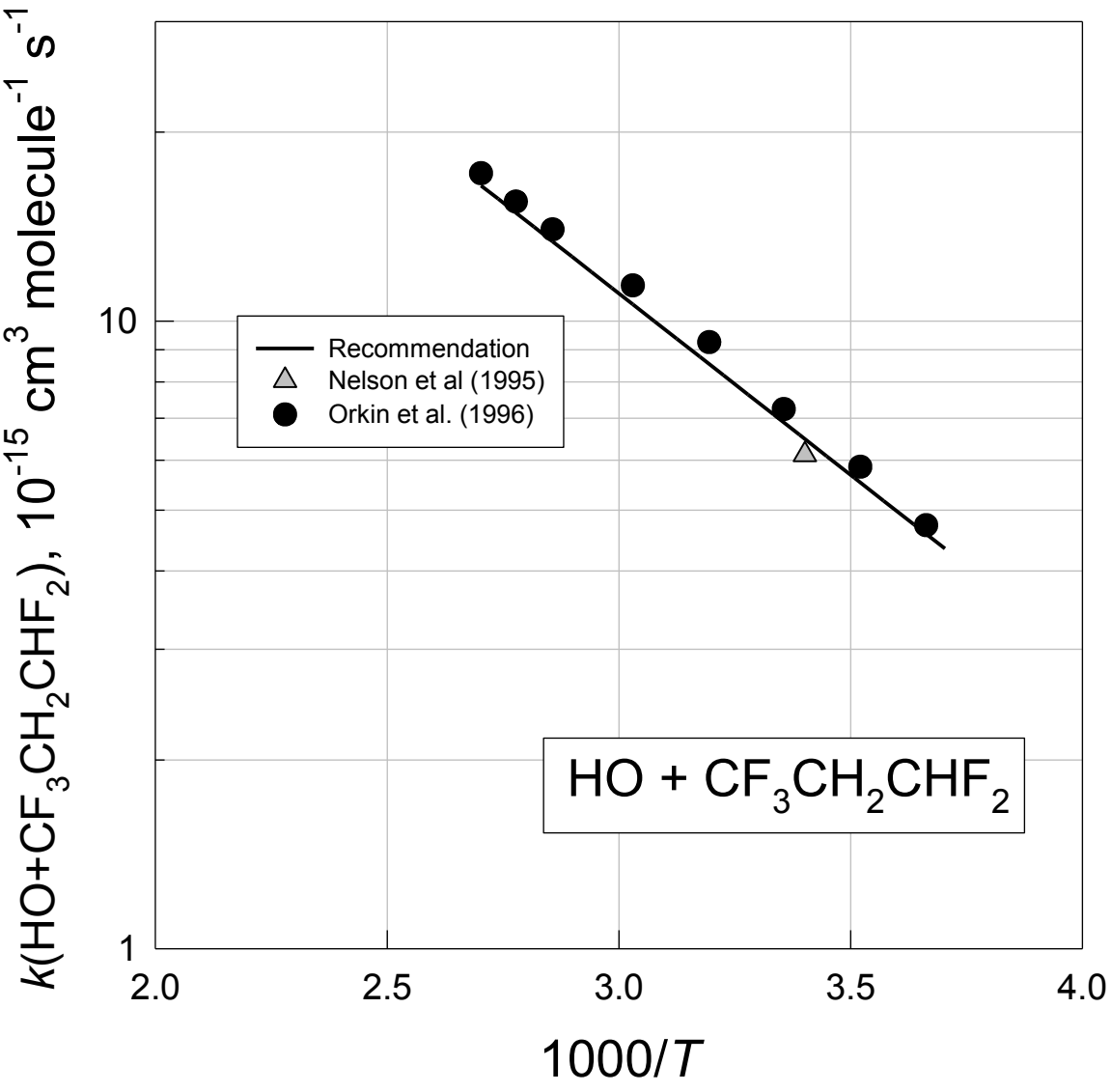
Parameter	Value	T/K
k	6.9×10^{-15} cm^3 molecule^{-1} s^{-1}	298
k	$6.0 \times 10^{-13} \exp(-1331/T)$ cm^3 molecule^{-1} s^{-1}	270-370
Reliability		
$\Delta \log k$	± 0.12	298
$\Delta E/R$	± 300	270-370

Comments on Preferred Values

Adjusting the rate coefficient at 294 K reported by Nelson et al. (1995) to the value expected at 298 K using the temperature dependence reported by Orkin et al. (1996) gives k(298K) = 6.50×10^{-15} cm^3 molecule^{-1} s^{-1} which is 10% below the k(298K) value reported by Orkin et al. (1996). Such a difference is well within the combined uncertainties from the two studies. The preferred value at 298 K is the average of the values from Nelson et al. (1995) and Orkin et al. (1996). The temperature dependence is taken from Orkin et al. (1996) with the pre-exponential A factor adjusted to be consistent with the k(298K) value.

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.


k(HO+$CF_3CH_2CHF_2$), 10^{-15} cm^3 $molecule^{-1}$ s^{-1}
10
1
2.0
2.5
3.0
3.5
4.0
1000/T
Recommendation
Nelson et al (1995)
Orkin et al. (1996)
HO + $CF_3CH_2CHF_2$