IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation - Data Sheet oFOx73; VII.A1.2

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HO + CF_3CHFCH_2F (HFC-245eb) → $CF_3CHFCHF$ + H_2O (1)
→ CF_3CFCH_2F + 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			
$(1.37 \pm 0.03) \times 10^{-14}$	294	Nelson et al. (1995)	DF-LIF (a)
$1.23 \times 10^{-12} \exp[-(1250 \pm 40)/T]$	238-374	Rajakumar et al. (2006)	PLP-LIF (b)
1.80×10^{-14}	297		

Comments

(a) HO radicals produced via the H + NO_2 reaction. Experiments were performed in 1.4-2.9 Torr (1.9-3.9 mbar) of helium diluent.

(b) HO radicals produced by 248 nm photolysis of H_2O_2. Experiments were performed in 49-210 Torr (65-280 mbar) of helium diluent. The value given at 297 K is the average of the four determinations reported.

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	1.6×10^{-14}	298
k /cm^3 molecule^{-1} s^{-1}	1.1×10^{-12} exp (-1250/T)	240-380
Reliability		
$\Delta \log k$	0.15	298
Δ E/R	± 300	240-380

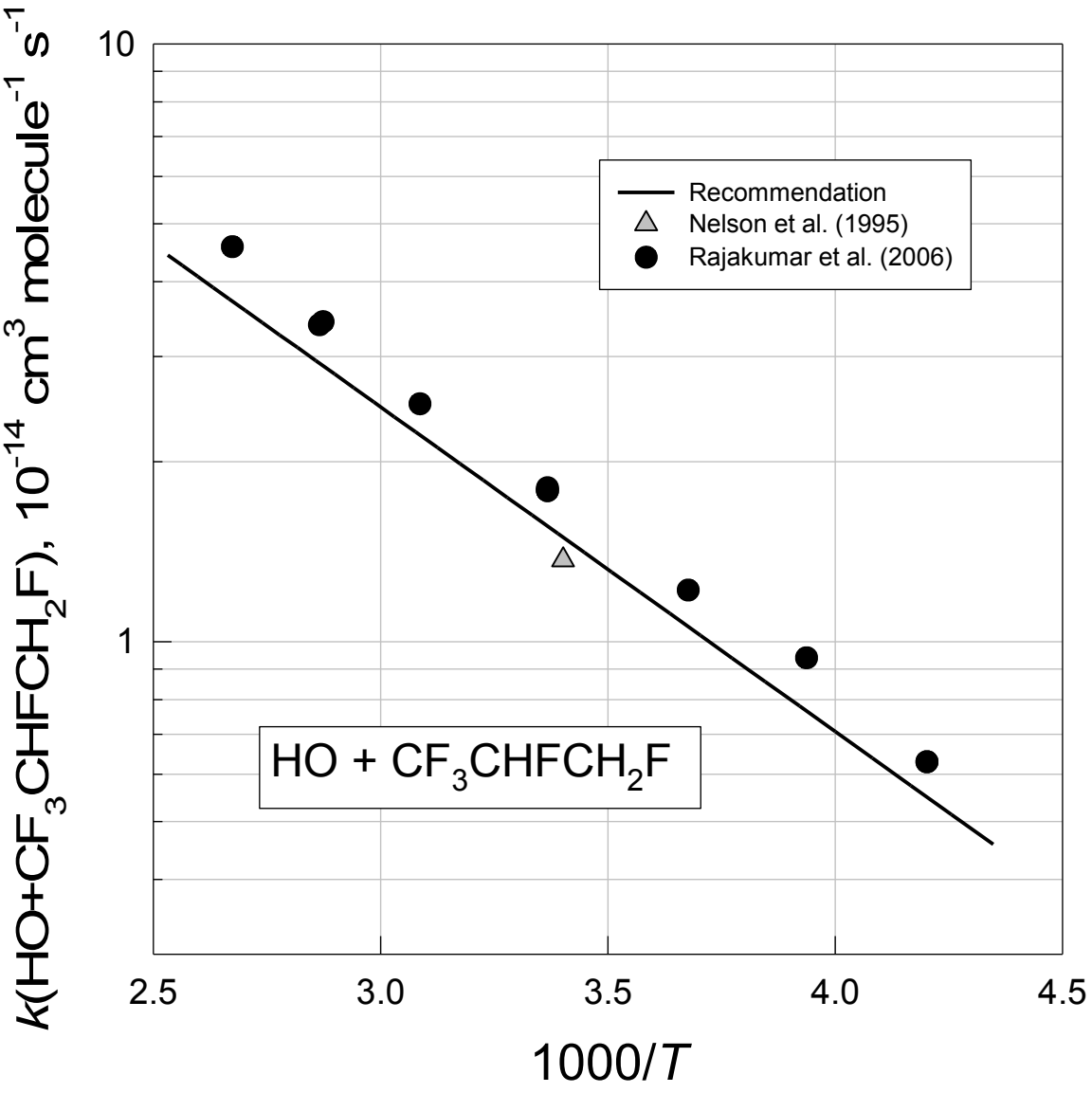
Comments on Preferred Values

The rate coefficient reported by Nelson et al. (1995) at 294 K is approximately 25% below that reported by Rajakumar et al. (2006) at 297 K. Adjusting both rate coefficients to values expected at 298 K using the temperature dependence reported by Rajakumar et al. (2006) reduces the difference between the studies to approximately 20%. Such a difference is likely just within the combined uncertainties from the two studies. The preferred value at 298 K is the average of the values derived from Nelson et al. (1995) and Rajakumar et al. (2006). The temperature dependence is taken from Rajakumar et al. (2006) with the pre-exponential A factor adjusted to be consistent with the k(298 K) value.

References

Nelson Jr., D. D., Zahniser, M. S., Kolb, C. E. and Magid, H.: J. Phys. Chem., 99, 16301, 1995.
Rajakumar, B., Portmann, R.W., Burkholder, J. B. and Ravishankara, A. R.: J. Phys. Chem. A, 110, 6724,

2006.


10
1
2.5
3.0
3.5
4.0
4.5
1000/T
k(HO+CF3CHFCH2F), 10-14 cm3 molecule-1 s-1
Recommendation
Nelson et al. (1995)
Rajakumar et al. (2006)
HO + CF3CHFCH2F