IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation - Data Sheet oFOx88; VII.A5.5

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$$HO + C_2F_5CH_2OH \rightarrow C_2F_5CHOH + H_2O \quad\quad (1)$$
$$\rightarrow C_2F_5CH_2O + H_2O \quad\quad (2)$$

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

k/cm^3 molecule^{-1} s^{-1}	T/K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(1.40\pm0.27) \times 10^{-12}$ exp[-(780±60)/T]	250-430	Tokuhashi et al. (1999)	LP-LIF (a)
1.0×10^{-13}	298		FP-LIF (a)
			DF-LIF (a)
1.36×10^{-12} exp[-(730±43)/T]	263-358	Antinolo et al. (2012)	PLP-LIF (b)
$(1.19 \pm 0.03) \times 10^{-13}$	287		
Relative Rate Coefficients			
$(0.94 \pm 0.08) \times 10^{-14}$	296	Hurley et al. (2004)	RR (c)

Comments

(a) Three different absolute rate methods were employed by Tokuhashi et al. (1999): LP-LIF, FP-LIF, and DF-LIF. HO radicals in the LP-LIF experiments were generated by the photolysis (ArF laser) of N_2O to produce $O(^1D)$ atoms in the presence of H_2O in 15-70 Torr (20-93 mbar) of helium diluent. HO radicals in the FP-LIF experiments were generated by the photolysis (Xe flash lamp, $\lambda \geq 180$ nm) of H_2O in argon diluent. HO radicals in the DF-LIF experiments were generated by the reaction of H atoms with NO_2 in 4-6 Torr (5-8 mbar) of argon diluent. There was good agreement between the results from experiments using the three different techniques. The value at 298 K cited above is the average obtained using the different techniques.

(b) HO radicals were produced by 248 nm (KrF eximer laser) photolysis of H_2O_2 in 43-214 Torr (57-285 mbar) of helium diluent at 263-358 K. HO radicals were monitored by LIF. No effect of total pressure was reported over the range studied.

(c) HO radicals were generated by the photolysis of CH_3ONO in 700 Torr (933 mbar) of air. A rate coefficient ratio of $k(HO+C_2F_5CH_2OH)/k(HO+C_2H_2) = 0.12 \pm 0.01$ was reported. Using $k(HO+C_2H_2) = 7.8 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} (Atkinson et al., 2006) gives $k(HO+ C_2F_5CH_2OH) = (9.4 \pm 0.8) \times 10^{-14}$ cm^3 molecule^{-1} s^{-1}.

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	1.04×10^{-13}	298
k /cm^3 molecule^{-1} s^{-1}	1.28×10^{-12} exp $(-748/T)$	250-430
Reliability		
$\Delta \log k$	0.06	298
Δ E/R	± 200	250-430

Comments on Preferred Values

The room temperature rate coefficients measured by Tokuhashi et al. (1997), Hurley et al. (2004), and Antinolo et al. (2012) are in good agreement. Taking an average of the determinations in these three studies gives $k(HO + C_2F_5CH_2OH) = 1.04 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at 298 K. Fitting the Arrhenius expression to the data from Tokuhashi et al. (1997) and Antinolo et al. (2012) and adjusting the A-factor to reproduce the recommended value at 298 K gives $k(HO + C_2F_5CH_2OH) = 1.28 \times 10^{-12}$ exp (-748/T) cm^3 molecule^{-1} s^{-1}. The HO radical initiated oxidation of $C_2F_5CH_2OH$ is expected to lead to quantitative conversion into C_2F_5CHO (Calvert et al., 2011).

References

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