IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation - Data Sheet oFOx89; VII.A5.6

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$$HO + CF_3CH(OH)CF_3 \rightarrow CF_3C(OH)CF_3 + H_2O \quad (1)$$
$$\rightarrow CF_3CH(O)CF_3 + H_2O \quad (2)$$

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

k/cm^3 molecule^{-1} s^{-1}	T/K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(6.99\pm1.56) \times 10^{-13}$ exp[-(990±70)/T]	250-430	Tokuhashi et al. (1999)	LP-LIF (a)
2.52×10^{-14}	298		FP-LIF (a)
			DF-LIF (a)

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.

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	2.5×10^{-14}	298
k /cm^3 molecule^{-1} s^{-1}	6.90×10^{-13} exp (-987/T)	250-430
Reliability		
$\Delta \log k$	0.12	298
Δ E/R	± 200	250-430

Comments on Preferred Values

The recommendation is based on a fit to the data from Tokuhashi et al. (1997) which gives k(HO+ $CF_3CH(OH)CF_3$) = 6.90×10^{-13} exp (-987/T) cm^3 molecule^{-1} s^{-1}. The HO radical initiated oxidation of $CF_3CH(OH)CF_3$ is expected to lead to quantitative conversion into $CF_3C(O)CF_3$ (Calvert et al., 2011).

$$HO + CF_3CH(OH)CF_3 \rightarrow CF_3C(OH)CF_3 + H_2O$$
$$CF_3C(OH)CF_3 + O_2 \rightarrow CF_3C(O)CF_3 + HO_2$$

References

Calvert, J. G., Mellouki, A., Orlando, J. J., Pilling, M., and Wallington T. J.: The Mechanisms of Atmospheric Oxidation of the Oxygenates, Oxford University Press, New York, NY, 2011.
Tokuhashi, K., Nagai, H., Takahashi, A., Kaise, M., Kondo, S., Sekiya, A., Takahashi, M., Gotoh,Y., and Suga, A.: J. Phys. Chem. A, 103, 2664, 1999.