IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation - Data Sheet oFOx84; VII.A5.1

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$$HO + CH_2FCH_2OH \rightarrow CHFCH_2OH + H_2O \quad (1)$$
$$\rightarrow CH_2FCHOH + H_2O \quad (2)$$
$$\rightarrow CH_2FCH_2O + H_2O \quad (3)$$

Rate coefficient data ($k = k_1 + k_2 + k_3$)

k/cm^3 molecule^{-1} s^{-1}	T/K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(5.15\pm0.88) \times 10^{-12} \exp[-(330\pm45)/T]$	238-355	Rajakumar et al. (2005)	PLP-LIF (a)
$(1.63 \pm 0.09) \times 10^{-12}$	297		
Relative Rate Coefficients			
$(1.39 \pm 0.05) \times 10^{-12}$	298	Sellevåg et al. (2004)	RR (b)

Comments

(a) HO radicals were generated by the 248 nm (KrF laser) photolysis of H_2O_2 in 60-100 Torr (80-133 mbar) of helium diluent. Additional experiments were performed at 355 K using DO radicals (formed via O_3 photolysis in the presence of D_2O). The rate coefficients for the reactions of DO and HO radicals with CH_2FCH_2OH were indistinguishable. There was no evidence for the formation of HO radicals following reaction of DO radicals with CH_2FCH_2OH.

(b) HO radicals were generated by the photolysis of O_3 in the presence of H_2O in 1013 mbar of air diluent at 298 K. A rate coefficient ratio of $k(HO+CH_2FCH_2OH)/k(HO+C_2H_6) = 5.81 \pm 0.19$ was measured. Placing this on an absolute basis using $k(HO+C_2H_6) = 2.4 \times 10^{-13}$ (Atkinson et al., 2006) gives $k(HO+CH_2FCH_2OH) = (1.39 \pm 0.05) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}.

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	1.5×10^{-12}	298
k /cm^3 molecule^{-1} s^{-1}	$4.57 \times 10^{-12} \exp(-330/T)$	240-360
Reliability		
$\Delta \log k$	± 0.15	298
$\Delta E/R$	± 200	240-360

Comments on Preferred Values

The results from the relative rate study by Sellevåg et al. (2004) and the absolute rate study of Rajakumar et al. (2005) at ambient temperature are indistinguishable within the likely combined experimental uncertainties. Taking an average of the values reported by Sellevåg et al. (2004) and Rajakumar et al. (2005) at 298 K gives $k = 1.5 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}. Adopting the temperature dependence from Rajakumar et al. (2005) gives $k = 4.57 \times 10^{-12} \exp(-330/T)$ cm^3

molecule^{-1} s^{-1}

References

Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., and Troe, J.: Atmos. Chem. Phys., 6, 3625, 2006; IUPAC Subcommittee for Gas Kinetic Data Evaluation, http://iupac.pole-ether.fr.

Rajakumar, B., Burkholder, J. B., Portmann, R. W., and Ravishankara, A.R.: Phys. Chem. Chem. Phys., 7, 2498, 2005.

Sellevåg, S. R., Nielsen, C. J., Søvde, O. A., Myhre, G., Sundet, J. K., Stordal, F., and Isaksen, I. S. A.: Atmos. Environ., 38, 6725, 2004.