IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oFOx41

This data sheet updated: 29th March 2005.

$CF_3O + H_2O \rightarrow CF_3OH + HO$

$\Delta H° = 43.4$ kJ mol^{-1}

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$<1 \times 10^{-16}$	298	Turnipseed et al., 1995	(a)
$<2 \times 10^{-16}$	381		
Relative Rate Coefficients			
$>2 \times 10^{-18}$	296	Wallington et al., 1993	(b)
$<4 \times 10^{-16}$	296		

Comments

(a) Pulsed laser photolysis/pulsed laser induced fluorescence technique. CF_3O radicals were generated by photolysis of CF_3OOCF_3 at 193 nm.

(b) Long path FTIR-based study. CF_3O radicals generated by chlorine-initiated oxidation of CF_3CFH_2 (HFC-134a) in photolytic mixture of Cl_2-CF_3CFH_2-H_2O in 1 bar air. Reaction rate studied in competition with the rate of $CF_3O + CF_3CFH_2$.

Preferred Values

$k < 2 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1} at 298 K.

$k < 3 \times 10^{-12} \exp(-3600/T)$ cm^3 molecule^{-1} s^{-1} over the temperature range 250-380 K.

Comments on Preferred Values

The A-factor is estimated by analogy with similar reactions of CF_3O and the activation energy is fitted to the upper limit at 381 K reported by Turnipseed et al. (1995). Note that this procedure results in a lower limit for E/R ($E/R > 3600$ K). The preferred value of k(298 K) is calculated from the Arrhenius parameters. The limits reported by Wallington et al. (1993) are consistent with this preferred value.

References

Turnipseed, A. A., Barone, S. B., Jensen, N. R., Hanson, D. R., Howard, C. J. and Ravishankara, A. R.: J. Phys. Chem., 99, 6000 , 1995.

Wallington, T. J., Hurley, M. D., Schneider, W. F., Sehested, J. and Nielsen, O. J.: J Phys. Chem., 97, 7606, 1993.