IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oFOx44

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$CF_3O + C_2H_6 \rightarrow CF_3OH + C_2H_5$

$\Delta H° = -32.2$ kJ mol^{-1}

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(1.2 \pm 0.2) \times 10^{-12}$	298	Saathoff and Zellner, 1993	(a)
$4.84 \times 10^{-12} \exp[-(400 \pm 70)/T]$	233-360	Barone et al., 1994	(b)
$(1.30 \pm 0.11) \times 10^{-12}$	298		
$1.13 \times 10^{-11} \exp[-(642 \pm 113)/T]$	295-573	Bourbon et al, 1995	(c)
$(1.31 \pm 0.13) \times 10^{-12}$	298		
Relative Rate Coefficients			
$(1.1 \pm 0.6) \times 10^{-12}$	297	Chen et al., 1992	(d)

Comments

(a) Laser photolysis/laser induced fluorescence technique. CF_3O radicals were generated by the photolysis of CF_3OF at 248 nm.

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

(c) Fast flow tube (~1.3 mb pressure)/laser induced fluorescence. CF_3O radicals were generated by the pyrolysis of CF_3OOCF_3 at 193 nm.

(d) Long path FTIR-based product study of visible photolysis of CF_3NO-NO-C_2H_6 mixtures in 700 Torr air. The upper limit of k given in table is derived from measured ratio $k/k(CF_3O+NO) = 0.02 \pm 0.006$ and the value of $k(CF_3O+NO)$ (IUPAC, current recommendation).

Preferred Values

$k = 1.3 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K.

$k = 4.9 \times 10^{-12} \exp(-400/T)$ cm^3 molecule^{-1} s^{-1} over the temperature range 230-360 K.

Reliability

$\Delta \log k = \pm 0.1$ at 298 K.

$\Delta(E/R) = \pm 200$ K.

Comments on Preferred Values

The preferred value at room temperature is the average of the values reported by Saathoff and Zellner (1993), Barone et al. (1994) and Bourbon et al.(1995). Results of these direct studies are in excellent agreement. The temperature dependence is based on the 233-360 K data of Barone et al. (1994). The temperature dependence of Bourbon et al. (1995) is thought to be high due to possible influence of wall reaction at high temperature. The relative rate measurement of Chen et al. (1992) is in good agreement with the preferred value. Kelly et al. (1993) used a relative rate

method with FTIR detection to determine the rate of CF_3O reaction with a number of hydrocarbons relative to the rate of the reaction of CF_3O with C_2H_6. They reported $k(CF_3O + CH_4)/k = 0.010 \pm 0.001$ at 298 K and 1 bar pressure (Kelly et al., 1993). This is nearly a factor of 2 lower than the ratio of the preferred values given in this evaluation (0.017). Wallington and Ball (1995) reported $k(CF_3O + CH_4)/k = 0.0152 \pm 0.0023$ at 296 K in good agreement with the recommended rate coefficients.

References

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