IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oFOx39

This data sheet updated: 29th March 2005.

$CF_3O + O_2 \rightarrow COF_2 + FO_2$

$\Delta H°$= 47.0 kJ mol^{-1}

Rate coefficient data

k/cm^3 $molecule^{-1}$ s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute RateCoefficients			
<2 x 10^{-17}	298	Turnipseed et al., 1994	PLP/LIF(a)
<4 x 10^{-17}	373		

Comments

(a) CF_3O radicals were generated by photolysis of CF_3OOCF_3 at 193 nm.

Preferred Values

k < 1 x 10^{-18} cm^3 $molecule^{-1}$ s^{-1} at 298 K.
k < 1 x 10^{-10} exp(-5600/T) cm^3 $molecule^{-1}$ s^{-1} over the temperature range 250-370 K.

Comments on Preferred Values

The preferred values are based on the upper limit at 373 K reported by Turnipseed et al. (1994). Assuming that the activation energy barrier is at least equal to the reaction endothermicity (5600 K) leads to the preferred limits given for the A-factor and for k(298 K). This procedure using the high temperature limit yields a room temperature limit an order of magnitude lower than the upper limit to the rate coefficient directly determined at 298 K. Chen et al. (1992) in a long path FTIR study of the reaction of CF_3O with NO found no evidence for the reaction of CF_3O with O_2 in 1 bar of air at room temperature.

References

Chen, J., Zhu, T. and Niki, H.: J. Phys. Chem., 96, 6115, 1992.
Turnipseed, A. A., Barone, S. B. and Ravishankara, A. R.: J. Phys. Chem., 98, 4594, 1994.