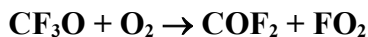


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet of FOx39

Website: <http://iupac.pole-ether.fr>. See website for latest evaluated data. Data sheets can be downloaded for personal use only and must not be retransmitted or disseminated either electronically or in hardcopy without explicit written permission.

This data sheet updated: 29th March 2005.



$$\Delta H^\circ = 47.0 \text{ kJ mol}^{-1}$$

Rate coefficient data

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

Comments

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

Preferred Values

$$k < 1 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

$$k < 1 \times 10^{-10} \exp(-5600/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ over the temperature range } 250\text{-}370 \text{ K.}$$

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 $k(298 \text{ K})$. 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.