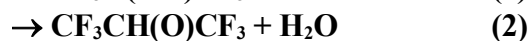


# IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation - Data Sheet of O<sub>x</sub>89; VII.A5.6

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The citation for the preferred values in this data sheet is: IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation, <http://iupac.pole-ether.fr>.

This datasheet last evaluated: June 2015; last change in preferred values: June 2009.



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

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$T/\text{K}$	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$(6.99 \pm 1.56) \times 10^{-13} \exp[-(990 \pm 70)/T]$	250-430	Tokuhashi et al. (1999)	LP-LIF (a)
$2.52 \times 10^{-14}$	298		FP-LIF (a)
			DF-LIF (a)

## Comments

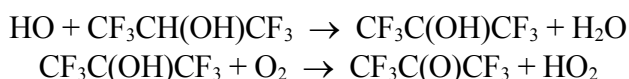
- (a) Three different absolute rate methods were employed by Tokuhashi et al. (1999): LP-LIF, FP-LIF, and DF-LIF. HO radicals in the LP-LIF experiments were generated by the photolysis (ArF laser) of N<sub>2</sub>O to produce O(<sup>1</sup>D) atoms in the presence of H<sub>2</sub>O in 15-70 Torr (20-93 mbar) of helium diluent. HO radicals in the FP-LIF experiments were generated by the photolysis (Xe flash lamp,  $\lambda \geq 180$  nm) of H<sub>2</sub>O in argon diluent. HO radicals in the DF-LIF experiments were generated by the reaction of H atoms with NO<sub>2</sub> in 4-6 Torr (5-8 mbar) of argon diluent. There was good agreement between the results from experiments using the three different techniques. The value at 298 K cited above is the average obtained using the different techniques.

## Preferred Values

Parameter	Value	T/K
$k / \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$2.5 \times 10^{-14}$	298
$k / \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$6.90 \times 10^{-13} \exp(-987/T)$	250-430
<i>Reliability</i>		
$\Delta \log k$	0.12	298
$\Delta E/R$	$\pm 200$	250-430

## Comments on Preferred Values

The recommendation is based on a fit to the data from Tokuhashi et al. (1997) which gives  $k(\text{HO} + \text{CF}_3\text{CH}(\text{OH})\text{CF}_3) = 6.90 \times 10^{-13} \exp(-987/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ . The HO radical initiated oxidation of CF<sub>3</sub>CH(OH)CF<sub>3</sub> is expected to lead to quantitative conversion into CF<sub>3</sub>C(O)CF<sub>3</sub> (Calvert et al., 2011).



## References

Calvert, J. G., Mellouki, A., Orlando, J. J., Pilling, M., and Wallington T. J.: The Mechanisms of Atmospheric Oxidation of the Oxygenates, Oxford University Press, New York, NY, 2011.

Tokuhashi, K., Nagai, H., Takahashi, A., Kaise, M., Kondo, S., Sekiya, A., Takahashi, M., Gotoh, Y., and Suga, A.: J. Phys. Chem. A, 103, 2664, 1999.

