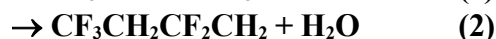
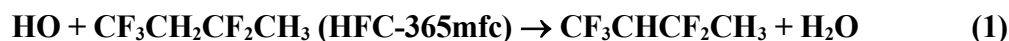


## IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation - Data Sheet of FOx76; VII.A1.5

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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>			
$1.68 \times 10^{-12} \exp[-(1585 \pm 80)/T]$	269-370	Mellouki et al. (1995)	PLP-LIF (a)
$8.69 \times 10^{-15}$	298		
<i>Relative Rate Coefficients</i>			
$1.39 \times 10^{-12} \exp[-1651/T]$	278-323	Barry et al. (1997)	RR (b)
$5.46 \times 10^{-15}$	298		

### Comments

- (a) HO radicals were produced by the 248 nm photolysis of  $\text{H}_2\text{O}_2$ . Experiments were performed in 100 Torr (133 mbar) of helium diluent.
- (b) HO radicals were produced by the 254 nm photolysis of  $\text{O}_3$  in the presence of  $\text{H}_2\text{O}$ . Experiments were performed in 1 bar of air diluent. Rate coefficient ratios were placed on an absolute basis using  $k(\text{OH}+\text{CH}_3\text{CCl}_3) = 1.2 \times 10^{-12} \exp(-1440/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (Atkinson et al., 2006).

### Preferred Values

Parameter	Value	$T/\text{K}$
$k$	$7.1 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	298
$k$	$1.6 \times 10^{-12} \exp(-1620/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	270-380
<i>Reliability</i>		
$\Delta \log k$	0.2	298
$\Delta E/R$	$\pm 200$	270-380

### Comments on Preferred Values

The rate coefficient at 298 K reported in the absolute rate study by Mellouki et al. (1995) is approximately 60% greater than that measured in the relative rate study by Barry et al. (1997). A possible explanation for this discrepancy is the presence of reactive impurities in the sample used by Mellouki et al. (1995). This explanation should lead to an increasing discrepancy between the two studies with decreasing temperature, but no such trend is evident. The temperature dependencies of the rate coefficients reported in the two studies are in good agreement. There being no obvious reason to prefer either study we recommend an average of the  $k(298\text{K})$  values and temperature dependencies from the two studies with the pre-exponential A factor chosen for consistency with the  $k(298\text{K})$ . As discussed by Barry et al. (1997) and Inoue et al. (2008), the OH radical initiated atmospheric oxidation of  $\text{CF}_3\text{CH}_2\text{CF}_2\text{CH}_3$  is expected to lead to the formation of  $\text{CF}_3\text{CH}_2\text{CF}_2\text{CHO}$  as the main primary product.

Oxidation of  $\text{CF}_3\text{CH}_2\text{CF}_2\text{CHO}$  will generate  $\text{CF}_3\text{CHO}$  and  $\text{COF}_2$  as secondary products. Oxidation of  $\text{CF}_3\text{CHO}$  will produce  $\text{COF}_2$ .

### References

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