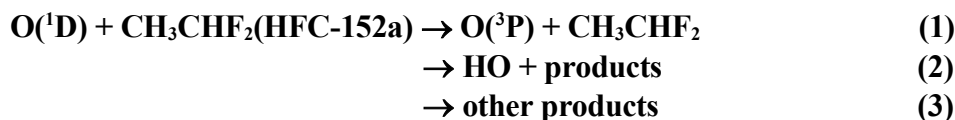


# IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet of FOx6

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This datasheet last evaluated: June 2015; last change in preferred values: July 2007.



$$\Delta H^\circ(1) = -190 \text{ kJ mol}^{-1}$$

## Rate coefficient data ( $k = k_1 + k_2 + k_3$ )

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$k = (2.02 \pm 0.15) \times 10^{-10}$	298	Warren et al., 1991	PLP-RF
$k = (1.5 \pm 0.2) \times 10^{-10}$	298	Kono and Matsumi, 2001	PLP-LIF (a)
<i>Branching Ratios</i>			
$k_1/k = 0.54 \pm 0.07$	298	Warren et al., 1991	PLP-RF (b)
$k_1/k = 0.34 \pm 0.06$	298	Kono and Matsumi, 2001	PLP-LIF (c)
$k_2/k = 0.15 \pm 0.02$			(d)
$k_3/k = 0.51 \pm 0.06$			(e)

## Comments

- Rate constant for the overall reaction ( $k_1 + k_2 + k_3$ ) determined by monitoring the rate of formation of O(<sup>3</sup>P) atoms from the O(<sup>1</sup>D) + CH<sub>3</sub>CHF<sub>2</sub> reaction.
- Branching ratio was determined from the ratio of the O(<sup>3</sup>P) yield from O(<sup>1</sup>D) + CH<sub>3</sub>CHF<sub>2</sub> relative to that for O(<sup>1</sup>D) + N<sub>2</sub>.
- Branching ratio determined by monitoring the yield of O(<sup>3</sup>P) atoms (using LIF at 130.22 nm) from O(<sup>1</sup>D) + CH<sub>3</sub>CHF<sub>2</sub> relative to that for O(<sup>1</sup>D) + N<sub>2</sub>.
- Branching ratio determined by monitoring the yield of OH radicals (using LIF at 282 nm) from O(<sup>1</sup>D) + CH<sub>3</sub>CHF<sub>2</sub> relative to that for O(<sup>1</sup>D) + H<sub>2</sub>O.
- Inferred from  $k_3/k = 1 - (k_1/k + k_2/k)$

## Preferred Values

$$k = 1.8 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

$$k_1/k = 0.44 \text{ at } 298 \text{ K.}$$

$$k_2/k = 0.13 \text{ at } 298 \text{ K.}$$

$$k_3/k = 0.44 \text{ at } 298 \text{ K.}$$

## Reliability

$$\Delta \log k = \pm 0.20 \text{ at } 298 \text{ K.}$$

$$\Delta(k_1/k) = \pm 0.10 \text{ at } 298 \text{ K.}$$

$$\Delta(k_2/k) = \pm 0.05 \text{ at } 298 \text{ K.}$$

$$\Delta(k_3/k) = \pm 0.10 \text{ at } 298 \text{ K.}$$

### *Comments on Preferred Values*

The preferred value of  $k$  and the preferred value of the branching ratio  $k_1/k$  are based on an average of the results of Warren et al. (1991) and Kono and Matsumi (2001).. The preferred values of  $k_2/k$  and  $k_3/k$  were derived by setting  $k_2/k + k_3/k = 1 - k_1/k$  and adopting the relative importance of  $k_2/k$  and  $k_3/k$  determined by Kondo and Matsumi (2001).

### **References**

- Kono, M. and Matsumi, Y.: J. Phys. Chem. A., 105, 65, 2001.  
Warren, R., Gierczak, T. and Ravishankara, A. R.: Chem. Phys. Lett., 183, 403, 1991.