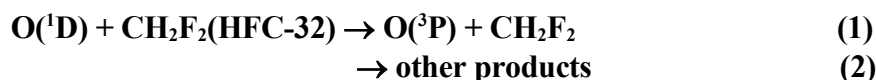


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet of FOx3

Website: <http://iupac.pole-ether.fr>. See website for latest evaluated data. Datasheets can be downloaded for personal use only and must not be retransmitted or disseminated either electronically or in hardcopy without explicit written permission. The citation for this data sheet is: Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., Troe, J., and Wallington, T. J.: Atmos. Chem. Phys., 9, 4141, 2008; 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 2013.



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

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

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$(5.13 \pm 0.33) \times 10^{-11}$	298	Schmoltner et al., 1993	PLP-RF
<i>Branching Ratios</i>			
$k_1/k = 0.70 \pm 0.11$	298	Schmoltner et al., 1993	PLP-RF (a)
<i>Relative Rate Coefficients</i>			
$k_2 = (4.6 \pm 2.3) \times 10^{-11}$	297	Green and Wayne, 1976	RR (b)
$k_2 = (4.78 \pm 1.03) \times 10^{-11}$	298	Nilsson et al., 2012	RR (c)

Comments

- (a) Branching ratio was determined from the ratio of the O(³P) yield from O(¹D) + CH₂F₂ relative to that for O(¹D) + N₂.
- (b) O(¹D) produced by photolysis of NO₂ at 229 nm. Δ(CH₂F₂)/Δ(N₂O) monitored by IR absorption spectroscopy. Measured rate coefficient ratio of $k_2/k(\text{O}(^1\text{D}) + \text{N}_2\text{O}) = 0.4 \pm 0.2$ is placed on an absolute basis by use of $k(\text{O}(^1\text{D}) + \text{N}_2\text{O}) = 1.16 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson et al., 2004). The cited rate coefficient refers to chemical reaction only and does not include physical quenching.
- (c) O(¹D) atoms were produced by the 254 nm photolysis of O₃ in the presence of CH₄ and CH₂F₂. The loss of CH₄ and CH₂F₂ was monitored using FTIR spectroscopy and chemical modeling was used to account for the secondary loss of CH₂F₂ via reaction with HO radicals produced in the system.

Preferred Values

$$k = 5.1 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

$$k_1/k = 0.7 \text{ at } 298 \text{ K.}$$

Reliability

$$\Delta \log k = \pm 0.1 \text{ at } 298 \text{ K.}$$

$$\Delta(k_1/k) = \pm 0.1 \text{ at } 298 \text{ K.}$$

Comments on Preferred Values

The preferred value of k and the preferred value of the branching ratio k_1/k are based on the results of Schmoltner et al. (1993). In these experiments, only O(³P) was monitored and therefore no direct information relating to the products of the chemical reaction of O(¹D) + CH₂F₂ was obtained. Burks and Lin (1981) have observed the appearance of stimulated emissions from vibrationally excited HF. The results from the relative rate study by Green and Wayne (1976) and Nilsson et al. (2012) are consistent with the preferred values.

References

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