IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oFOx1

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This datasheet last evaluated: June 2015; last change in preferred values: June 2003.

$$O(^1D) + COF_2 \rightarrow O(^3P) + COF_2 \qquad (1)$$
$$\rightarrow \text{other products} \qquad (2)$$

$\Delta H°(1) = -190$ kJ mol^{-1}

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

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(7.4 \pm 1.2) \times 10^{-11}$	298	Wine and Ravishankara, 1983	PLP-RF
Branching Ratios			
$k_1/k = 0.7 \pm 0.07$	298	Wine and Ravishankara, 1983	PLP-RF (a)

Comments

(a) Branching ratio was determined from the ratio of the $O(^3P)$ yield from $O(^1D) + COF_2$ relative to that for $O(^1D) + N_2$.

Preferred Values

$k = 7.4 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 298 K.
$k_1/k = 0.7$ at 298 K.

Reliability

$\Delta \log k = \pm 0.3$ at 298 K.
$\Delta(k_1/k) = \pm 0.1$ at 298 K.

Comments on Preferred Values

The preferred value of k is based on the result of Wine and Ravishankara (1983). This study is much more direct than earlier studies. In that paper the authors state that the only chemical reaction involving COF_2 which might be important in the stratosphere is the reaction $O(^1D) + COF_2 \rightarrow F_2 + CO_2$ and that this reaction would have to proceed by a complex mechanism involving an intermediate adduct.

References

Wine, P. H. and Ravishankara, A. R.: Chem. Phys. Lett., 96, 129, 1983.