IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oFOx5

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: July 2007.

$O(^1D) + CH_3CH_2F(HFC\text{-}161) \rightarrow O(^3P) + CH_3CH_2F$ (1)
$\rightarrow$ other products (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			
$(2.61 \pm 0.40) \times 10^{-10}$	298	Schmoltner et al., 1993	PLP-RF
Branching Ratios			
$k_1/k = 0.18 \pm 0.05$	298	Schmoltner et al., 1993	PLP-RF (a)

Comments

(a) Branching ratio was determined from the ratio of the $O(^3P)$ yield from $O(^1D) + CH_3CH_2F$ relative to that for $O(^1D) + N_2$.

Preferred Values

$k = 2.6 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1} at 298 K.
$k_1/k = 0.18$ 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 and the preferred value of the branching ratio k_1/k are based on the results of Schmoltner et al. (1993), the only published study of this reaction. In these experiments, only $O(^3P)$ was monitored and therefore no direct information relating to the products of the chemical reaction of $O(^1D) + CH_3CH_2F$ was obtained.

References

Schmoltner, A. M., Talukdar, R. K., Warren, R. F., Mellouki, A., Goldfarb, L., Gierczak, T., McKeen, S. A. and Ravishankara, A. R.: J. Phys. Chem., 97, 8976, 1993.