IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oFOx6

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$O(^1D) + CH_3CHF_2$(HFC-152a) $\rightarrow O(^3P) + CH_3CHF_2$ (1)
$\rightarrow$ HO + products (2)
$\rightarrow$ other products (3)

$\Delta H°(1) = -190$ kJ mol^{-1}

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

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$k = (2.02 \pm 0.15) \times 10^{-10}$	298	Warren et al., 1991	PLP-RF
$k = (1.5 \pm 0.2) \times 10^{-10}$	298	Kono and Matsumi, 2001	PLP-LIF (a)
Branching Ratios			
$k_1/k = 0.54 \pm 0.07$	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

(a) Rate constant for the overall reaction ($k_1 + k_2 + k_3$) determined by monitoring the rate of formation of $O(^3P)$ atoms from the $O(^1D) + CH_3CHF_2$ reaction.
(b) Branching ratio was determined from the ratio of the $O(^3P)$ yield from $O(^1D) + CH_3CHF_2$ relative to that for $O(^1D) + N_2$.
(c) Branching ratio determined by monitoring the yield of $O(^3P)$ atoms (using LIF at 130.22 nm) from $O(^1D) + CH_3CHF_2$ relative to that for $O(^1D) + N_2$.
(d) Branching ratio determined by monitoring the yield of OH radicals (using LIF at 282 nm) from $O(^1D) + CH_3CHF_2$ relative to that for $O(^1D) + H_2O$.
(e) Inferred from $k_3/k = 1 - (k_1/k + k_2/k)$

Preferred Values

$k = 1.8 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1} at 298 K.
$k_1/k = 0.44$ at 298 K.
$k_2/k = 0.13$ at 298 K.
$k_3/k = 0.44$ at 298 K.

Reliability

$\Delta \log k = \pm 0.20$ at 298 K.
$\Delta(k_1/k) = \pm 0.10$ at 298 K.
$\Delta(k_2/k) = \pm 0.05$ at 298 K.

$\Delta(k_3/k) = \pm\ 0.10$ 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 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.