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$$\begin{aligned} HO + CH_3O_2 &\rightarrow HCHO + H_2O_2 && (1)\\ &\rightarrow CH_3O + HO_2 && (2)\\ &\rightarrow CH_3OH + O_2 && (3)\\ &\rightarrow CH_2O_2 + H_2O && (4)\\ &\rightarrow CH_3OOOH && (5) \end{aligned}$$

$\Delta H°(1) = -291$ kJ mole^{-1}
$\Delta H°(2) = -13$ kJ mole^{-1}
$\Delta H°(3) = -248$ kJ mole^{-1}

Rate coefficient data ($k = k_1 + k_2 + k_3 + k_4$)

k/cm^3 molecule^{-1} s^{-1}	Temp./K	*Reference*	Technique/ Comments
Absolute Rate Coefficients			
(2.8 ± 1.4) x 10^{-10}	294	Bossolasco et al., 2014	LP-LIF/CRD (a)

Comments

(a) HO was generated by the 248 nm photolysis of H_2O_2 or O_3 / H_2O, and detected by LIF. CH_3O_2 (excess reactant) was generated by the photolysis of CH_3I in the presence of O_2 and detected by CW- CRDS. Bath gas was He and no pressure dependence (67 or 133 mbar) was observed.

Preferred Values

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	2 x 10^{-10}	298
Reliability		
$\Delta \log k$	± 0.3	298

Comments on Preferred Values

There is only one experimental study of this reaction. The uncertainty in the rate constant reported by Bossolasco et al. (2014) stems mainly from uncertainty in the CH_3O_2 cross section at 7489 cm^{-1} which was derived from an analysis of CH_3O_2 self-reaction kinetics. The

authors assessed the role of I, IO and O(^{3}P) reactions via numerical simulation using an assumed reaction scheme. The complexity of the chemical system used, significant divergence (factor three) in the literature values for the cross section of CH_3O_2 at ~7489.16 cm^{-1} and the fact that this is the only study to date, lead us to prefer a rate constant of 2×10^{-10} cm^3 $molecule^{-1}$ s^{-1} with extended error limits. There are no published experimental data on the products of this reaction.

A theoretical study (Bian et al, 2015) indicates that CH_3O and HO_2 (channel 2) are the favoured products on a singlet PES, with formation of CH_2O_2 + H_2O (channel 4) being formed via a triplet PES. In supplementary information to their calculations on CH_2O_2 formation in a related chemical system, Nguyen et al (2015) present a potential energy surface and reaction mechanism that indicates that the trioxide (channel 5) is expected to be the dominant product under atmospheric conditions.

References

Bian, H., Zhang, S. G., and Zhang, H. M., Int. J. Quantum Chem., 115, 1181-1186, 2015.

Bossolasco, A., Farago, E. P., Schoemaecker, C., and Fittschen, C., Chem. Phys. Lett., 593, 7-13, 2014.

Nguyen, T. L., McCarthy, M. C., and Stanton, J. F., J. Phys. Chem. A, 119, 7197-7204, 2015.