

# Experimental and Computational Studies on Reaction Kinetics of Cl Atom with Methyl Propionate

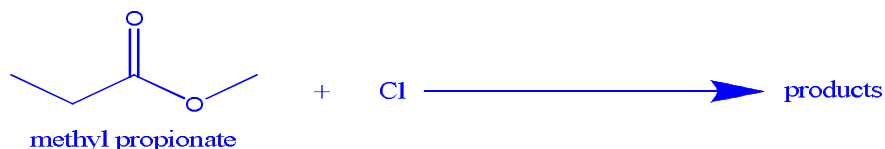
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Esters are volatile oxygenated organic compounds that are emitted into the atmosphere from biogenic and anthropogenic sources. Methyl propionate, also known as methyl propanoate C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>, is a volatile ester with a sweet fruity smell. Esters are used as industrial solvents and as reagents during the manufacture of perfumes and food flavoring. Esters are emitted into the atmosphere from natural sources (i.e., vegetation) and are also formed in the atmosphere as oxidation products of ethers used as automotive fuel additives. Moreover, methyl propionate and the corresponding radicals produced in the reaction of Cl atom/ OH radical were observed to be important intermediates in the pyrolysis of biodiesel.

In the present study, the gas phase kinetics of methyl propionate with Cl atoms were measured as a function of temperature (263-363 K) at pressure ~760 Torr using the relative rate technique, with ethane and ethyl chloride as reference compounds. An Arrhenius expression:  $k(T) = (2.53 \pm 1.5) \times 10^{-10} \exp [-(674 \pm 147)/T] \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  was obtained. Theoretical calculations were also performed using variational transition state theory (VTST) with small curvature tunneling (SCT) and the kinetic data was obtained over the temperature range of 200-3000 K which gave an Arrhenius expression:  $k(T) = [(9.68 \pm 5.8) \times 10^{-21}] T^{3.2} \exp [-(821 \pm 31)/T] \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ . The product analysis was performed by using GC-MS. The branching ratios, thermo chemistry, atmospheric implications, absorption cross-section and degradation path ways of methyl propionate were also studied. The detailed studies of the title reaction will be presented in the conference.



## References

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