Theoretical study of thermal decomposition of biodiesel fuels

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The use of petroleum-based fuels in the transport sector has raised issues such as air pollution, energy security, and substantial emission of CO_2, which is linked to climate change. Due to the extensive use of these fuels, researchers are motivated to look for alternative solutions. One of the potential alternative fuels that has been suggested is biofuels. Biofuels are comprised of a mixture of saturated and unsaturated alkyl esters, containing long carbon chains with 16-18 carbon atoms, which are typically derived from vegetable oils and animal fats. These fuels introduce new challenges for the development of chemical reaction mechanisms. Namely, due to the complexity of biofuels molecules, a very large number of reactions are usually required to create kinetic mechanisms for these fuels directly. As a result, simpler molecules are typically chosen to represent the chemical properties of real fuels. Methyl butanoate (MB), is an example of a simple methyl ester that has been suggested to be a convenient alternative for large biofuel molecules. Ab initio methods, namely, high level quantum composite G3B3 and CASSCF methods calculated accurate energies; Variational Transition State Theory, Rice-Ramsperger-Kassel-Marcus (RRKM) and master equation (ME) simulations provided temperature and pressure dependent reaction rate constants.

References

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