Thanita Sonthisawate 2006: Investigation on Transesterification of Biodiesel by Molecular Modelling. Master of Engineering (Chemical Engineering),
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Transesterification of alkyl esters plays an important industrial role with the production of biodiesel. One of the critical substances in transesterification mechanism of biodiesel production is triglyceride, triolein. Molecular modeling technique was used in this study to determine the geometrical parameter of triolein by semiempirical AM1, PM3 and *ab initio* Hartree-Fock based on GaussViewW and GAUSSAIN 03W softwares. The results obtained from AM1, PM3 and *ab initio* Hartree-Fock with 6-31G basis set show that the geometrical parameters of triolein molecule are in the same range. Hence, the model of triolein molecule can be used in the simulation of transesterification mechanism. Next step, the transesterification mechanism with an exact triolein molecule from the previous study is simulated. All possible mechanisms were proposed in this study to find reasonable mechanisms of the transesterification. The six types of transesterification mechanism or thirty six reactions were studied. The simulations were determined by an *ab initio* HF6-31G. From the simulations, it was found that the types of the reactions were divided into six types; the first type is irreversible reaction that the output molecule structure is product, the second type is irreversible reaction that the output molecule structures are reactants instead of product, the third type is irreversible reaction that the output molecule structure is similar to the product but the active site bond wasn't shown, the forth type is reversible reaction that the output molecule structures are reactants instead of product, the fifth type is reversible reaction that in the final the reaction doesn't give product, the sixth type is reversible reaction that the output molecule structure is similar to the product but the active site bond wasn't shown. The energy of the reactant in each step of transesterification mechanism is higher than the energy of the product. The energy in each type of the reaction in transesterification mechanism is similar to the others. The possible transesterification mechanisms are found in all types of transesterification mechanisms.

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