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Thermochemical data of the oleic acid esterification reaction: a quantum mechanics approach

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Highlights

- DFT methods were used to predict thermochemical data of oleic acid esterification.
- Methanol, ethanol and propanol were used as alcohol for this reaction.
- An empirical equation was applied to correct values of energy calculated with the B3LYP functional.
- Results show that an increase in temperature favours the reactions.
- Reactions are not spontaneous and need extra energy to be accomplished.
- The obtained data will be useful when no experimental data are available.

Abstract

Biodiesel is an important renewable fuel that can be obtained from low cost oils once the esterification reaction of free fatty acids is carried out as a pretreatment. Scarcity of reliable thermochemical properties motivated the use of computational calculations to accurately predict these data for biodiesel compounds. The purpose of this study is to calculate thermochemical data of oleic acid esterification reactions with methanol, ethanol and propanol at several temperatures using the B3LYP hybrid functional with the standard 6-311+G(d,p) basis set. Calculated values of enthalpy of formation were corrected by applying a linear regression correction specifically developed for fatty acids and esters in order to decrease systematic errors related to the negligence of high order electron correlation energies in the B3LYP functional. Results showed that, although the esterification reactions are favoured by the temperature increase, these reactions are not spontaneous within the considered temperature range (from 273.15 to 373.15 K), which indicates