

Thematic course: Quantum-chemical study of the transformation of triglycerides. Part 2.

Elementary acts of the hydrolysis reaction of triglycerides and catalytic role of intermediately authentic aliphatic carboxylic acids in the formation of their methyl esters in the physical conditions of supercritical fluids

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Abstract

By the quantum-chemical method DFT with the functional density PBE in the basis 3z (comparable basis set cc-pVTZ) using the program *Priroda 4.11* we studied the reactions of transesterification and hydrolyses of triglycerides in methanol at a promoter the assistance of the fatty acid analogues in the physical conditions of supercritical fluids, that is, when T = 623 K and P = 300 atm.

It is shown that in the conditions of a supercritical fluids the thermodynamic equilibrium of various reaction systems takes place that implements elementary acts of methanolysis and the hydrolysis of triglycerides to the side of accumulation of catalytically significant amounts of fatty acids. Thus associates of carboxylic acid – ethanol (or water) in a single reaction step of methanolysis (or hydrolysis) on the alkoxy carbonyl group of triglyceride analogues in supercritical fluids provide a promoter effect, which in combination with the presence of potential pitfalls, makes the directions of the reactions with their participation the main channel for accumulation of target products of the process of methanolysis of triglycerides, i.e. methyl esters of fatty acids.

It is noted that at high temperatures and pressures there is an unusual type of catalysis, due to a variety of thermodynamic equilibrium shift reaction systems realizing elementary acts of methanolysis and hydrolysis of triglycerides in the direction of the accumulation of catalytically significant amounts of fatty acids. In the transition to normal conditions the same thermodynamic equilibrium transfers fatty acids into their methyl esters.