

## Cross-section of interlayer space, as one of the factors that determine the selectivity of intercalated montmorillonites in oligomerization reactions

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### Abstract

The intercalation process of layered silicates, for example, such as montmorillonite, by introducing into the interlayer space the polyoxocations produced by the cation hydrolysis reaction, is one of the promising ways to increase the catalytic activity of layered silicates. Indeed, montmorillonite (MON), characterized in its natural state by the expanding structural cell and thickness of the silicate layer 0.94 nm, is not sufficiently active. However, during intercalation, the interlayer space increases due to the substitution of interlayer cations for large oligomeric cations, and the activity of montmorillonite increases. It is important to note that the intercalation process does not lead to a violation of the primary structure of layered silicates.

Previously, the authors synthesized Fischer-Tropsch synthesis catalysts based on heteropolyacids applied to nanocomposite acid-activated montmorillonite. In this paper we present the results of modeling the processes of formation of the target products by the molecular dynamics method implemented in the Adsorption Locator module of Accelrys Material Studio 6.0. The effect of the cavity dimensions on the selectivity of the formation of C<sub>6</sub>-C<sub>12</sub> isoalkanes was estimated from the dependence of the adsorption energy on the pore sizes. Calculation of oligomer structures was carried out by the method of quantum-chemical modeling in the RM1 approximation.

The optimum structural characteristic (pore diameter) for heterogeneous porous materials was determined based on the results of the study with the aim of intensifying the oligomerization process of butane-butene and propane-propene fractions with the maximum yield of C<sub>6</sub>-C<sub>12</sub> isoolefins.

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