Quantum chemical modeling of desulfurization process

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1. Introduction

Progress in the development of quantum chemical methods and software, as well as the development of computer technology provided the use of computer modeling in various fields of chemistry [1, 2]. The study of the mechanisms of catalytic reactions with supercomputersis of particular interest, which allows to carry out the screening of substances by their catalytic properties for a relatively short period of time.

Ni-skeletal catalysts commonly used in hydrogenation processes in the chemical industry. [3] The application of these catalysts in hydrotreatingofr petroleum refinery products, particularly, in the removal of sulfur from diesel fuel.Thermodynamic calculations of the equilibrium compositions of sulfur-containing model compounds: mercaptans, thiophene derivatives, thioalkanesindicate that thiophene and its derivatives are the most thermodynamically stable.

In this work we investigate the characteristics of the synthesis and structure of nickel - skeletal catalysts and quantum-chemical modeling of intermolecular interaction of thiophene molecules withnickel - skeletal catalysts.

2. Experimental

We investigated the diffraction patterns of samples of nickel - skeletal catalysts on a DRON-3M with copper radiation. Shooting mode samples the following: X-ray tube voltage is 30 kV, tube current is 30 mA, step movement 0.05° 2θ goniometer and time measuring of the intensity of the point - 1.0 seconds. Sample rotation on its own plane is about 60 turnover / min. The main phase is nickel. Galo with a maximum angle of 2θ equal to 18.0° belongs ebony cell. Nickel crystallite size is L = 40 Å.

3. Results and discussion

The object of study was a Ni Raney catalyst obtained from the alloy -51.1% Ni, Al - 46,9%, Fe - 0.075%, Cr - 0.893%, Ti - 0.914%. For the preparation of skeletal nickel catalyst by a complete leaching, the alloy was pulverized in a mortar, and sieved. Then a certain fraction of powder weighing 1 g was treated in a Kjeldahl flask with 20% sodium hydroxide solution while heating in a water bath for 2 hours, then drained and obtained alkali powder was washed with distilled water by decantation. Freshly prepared Ni-Raney catalyst was investigated by X-ray phase analysis.

The analysis shows that nickel forms a face-centered cubic lattice with the period a = 0,35352 nm (space group Fm3m).