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Investiganion of molecular of clusters of petroleum asphaltenes

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Abstract

A study of the electronic and chemical structure of nanoclusters, consisting of molecular fragments of oil asphaltenes – "continental" type. The objects of study are asphaltenes residue of thermal cracking and tar Western-Siberian oil and asphaltenes of West Siberian oil. For experiments on the isolation and separation of asphaltenes was used the method of I.R. Khairudinov. The obtained electronic absorption spectra of solutions of asphaltenes West Siberian oil in the visible and UV region (280-780 nm). Processed spectra to a computer and calculating the effective potential of ionization and electron affinity of the studied objects by means of electronic phenomenological spectroscopy. The calculated values of the effective ionization potentials are in the range from 5.56 to 5.86 eV, electron affinity, from 1.68 m to 1.91 eV. Physico-chemical properties of petroleum asphaltenes determined by correlation of range-property: value srednetsenovoj molecular weight (from 2437 to 3884 e.m.), energy of activation of viscous flow (162.4 to 272.4 kJ/mol), concentration of paramagnetic centers of the carbon (from 145.6 to 273.4 1018 spin/cm^3). The calculated electronic structure of molecular nanoparticles of petroleum asphaltenes by the method DFT/B3LYP with basis set 6-31+G*.

According to the findings of the adiabatic first ionization potentials are in the range of 6.07 to 7.39 eV, the electron affinity is from 0.88 to 1.22 eV. The settlement data confirm the hypothesis that increased donor-acceptor abilities of asphaltic substances. The study of the structural characteristics of the nanoclusters petroleum asphaltenes using the method of molecular mechanics. The dihedral angle between the virtual planes of the alkyl ring and the plane of the ring is in the range from 0 to 108 1580. Thus the alkyl groups substituting hydrogen in the aromatic rings on the periphery of the substantially non-planar plane naphthenoaromatic rings. Confirmed deplanement structure naphthenoaromatic fragments of clusters. The dihedral angle between the plane of naphthenic rings and the plane of the aromatic rings in the structures of the nanoparticles has different values, being in the range from161^0 to 168^0. The distance h between the virtual planes naphthenoaromatic fragments of the nanocluster is in the range from 3.4 to 3.7 Å. The possibility of the formation of nanoclusters of petroleum asphaltenes, consisting of naphtene aromatic plates. The calculation results showed that the values of intermolecular interaction of molecular fragments are in the range from 7 to 226 kJ/mol. The results of the rheological studies indicate high values of activation energy of viscous flow.

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