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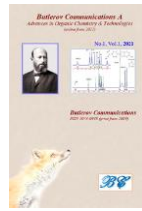

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Study of the molecular and electronic structure of asphaltenes type "archipelago"

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Abstract

The objects of research are the asphaltenes of West Siberian oil. For experiments on the isolation and separation of asphaltenes was used the method of I. R. Khairutdinov. The electronic structure of asphaltenes was investigated using electron spectroscopy by measuring a broad absorption signal in the UV and visible range of the range (280-780 nm). The values of the effective ionization potential (5.69 eV) and effective electron affinity (1.79 eV) of asphaltenes have been determined.

The elemental composition of petroleum asphaltenes was determined by X-ray fluorescence analysis. The number average molecular weight of the sample, obtained by cryoscopy in naphthalene, is 2557 a.m.u. The structural and chemical characteristics of asphaltenes have been studied by FTIR spectroscopy. Based on the data of elemental analysis, IR and UV spectroscopy, the structural and chemical characteristics of asphaltene molecules have been studied and model fragments of asphaltenes of the "archipelago" type, characteristic of oil and straight-run oil residues, have been constructed. Model molecules consist of 4-5 naphthenoaromatic condensed structures connected by aliphatic side chains with the number of carbon atoms from 4 to 6. The structures contain pyrrole rings, carbonyl, thiol and OH groups.

The calculation of the electronic structure of the model fragments of petroleum asphaltenes was performed by the 6-31G** method using the GAUSSIAN software package. It was found that molecular fragments of model molecules have ionization

potential (IP) values in the range from 6.14 to 6.77 eV, free radical fragments – from 4.78 to 5.24 eV. The values of the electron affinity (EA) of molecular fragments are in the range from -0.79 to 1.14 eV, for free radicals – from 2.10 to 2.30 eV. The values of the dipole moments of the model molecules are in the range from 3.97 to 7.05 D. The obtained refined IP and EA values are in good agreement with the data of electron spectroscopy. For molecular fragments of asphaltenes, the values of the quasi-Fermi level are in the range of 5.00-5.98 eV, for free radical fragments – 2.68-2.98 eV. According to spectroscopic data, the band gap of a sample of asphaltenes from West Siberian oil is 3.9 eV.

The hypothesis of an increased donor-acceptor ability of asphaltenes is confirmed. The presence of low IP and high EA suggests that asphaltenes can be used as organic materials with electrically conductive properties.

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