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Investigation of molecular and electronic structure of polycyclic aromatic hydrocarbons of coal tar

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Abstract

The molecular and electronic structure of coal tar asphaltenes was investigated. The objects of the study are asphalt resins of coking Kuzbass coal. Solution absorption spectra in the range of 310-780 nm were recorded on a *СФ-2000* spectrophotometer. In the process of studying the absorption spectra of asphaltenes by optical spectroscopy, it has been found that the asphaltene fraction is a strong donor and electron acceptor. Effective ionization potential (6.64 eV), effective electron affinity (1.20 eV) and band gap width (5.44 eV) have been established.

The study of the electronic structure of molecules of polycyclic aromatic hydrocarbons (PAHs), which are nuclei of molecules of asphaltenes of the "continental" type, was carried out by the method of DFT/B3LYP with the basic set 6-31+G*, using the software package GAUSSIAN. Quantum-chemical calculations have shown that the first vertical ionization potential is equal to that the first vertical ionization potential is in the range of 6.41 to 6.71 eV, affinity to the electron – from 0.79 to 1.08 eV, values of the gap zone width – from 5.33 to 5.92 eV. Dipole moments of asphaltenes (0.32 to 0.46 D) were calculated. The calculation data confirm the hypothesis of increased donor-acceptor capacity of asphalt-resin substances.

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