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The donor-acceptor properties estimation of oxygen-containing compounds and band-gap energy for anthraquinone nanoclusters with integral characteristics of signals optical absorption spectra

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Abstract

As is known, the orbitally-controlled reactions are associated, which with the transfer of charge between reagents. This corresponds to the formation of molecular donor-acceptor complexes. Thus, the formation of molecular donor-acceptor complexes is carried out. Therefore, the equilibrium constants and the rates of the corresponding reactions are affected by the ionization potentials (IP) and the electron affinity (EA) of the reagents that characterize the ability to give and receive electrons. In addition, IP and EA are the most important factors influencing on semiconductors band-gap energy.

A linear correlation of the first vertical IP and EA of the oxygen-containing natural compounds and the integral characteristics of the absorption in the UV and the visible spectral ranges has supposed by the authors. IP and EA were calibrated by the RHF-6-31G** method.

To estimate the band-gap energy of dark conductivity E_g in nanoclusters of the anthraquinone organic semiconductors series, a semi-empirical approach is proposed, where a relationship between the calculated values of E_g and the autocorrelation integral characteristics of signal is constructed.

The nanoclusters band-gap energy was estimated as the difference of the band-gap energy of isolated molecule E_{g0}, the intermolecular energy and the electron-hole interactions energy. E_{g0} was calculated by the RHF-6-31G ** method as the difference between the IP and EA. The energy of the intermolecular interaction was taken into account by the MM2 method with the minimum of interparticle potentials.

The correlations of the IP and EA to estimate for oxygen-containing compounds is shown. In additional, exist possible estimation of the band-gap energy of dark conductivity for nanocluster semiconductors, using experimental data on integral absorption characteristics determined directly from optical absorption spectra in the UV and visible range, and also simple molecular models without using the quantum methods.

The result of research may be used in organic chemistry and molecular electronics by definition electron transport processes. The correlations has confirmed by calculations and data processing on specially developed algorithms and programs.

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