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Evaluation of donor-acceptor properties of polycyclic hydrocarbon molecules by the integral autocorrelation characteristics of the optical spectra

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Abstract

This study established a relationship between of the relative integral autocorrelation characteristics of the optical spectra and donor-acceptor properties of polycyclic aromatic hydrocarbon (PAH) molecules. It is shown that the identified patterns are to hydrocarbons of a certain groups of symmetry according to the system of notation, known as the classification of Schoenflies. For registration of optical spectra were clear and optically transparent solvents used. The energy spectra of the molecules we present in the form of integrals of autocorrelation functions (IACF), according to the technique adopted in statistical radio physics to describe random processes. The physical meaning of the relative IACFs is the relative interaction energy of the electronic states in the ultraviolet region and the quality of energy transition of electronic states of molecules at certain frequencies. Values of relative IACFs equal to the ratio of the energy in the UV part of the spectrum to the energy of the electronic spectrum. The values of ionization potential and electron affinity of molecules of organic semiconductors was determined by the density functional theory with the Becke's three parameter exchange functional along with the Lee–Yang–Parr correlation functional (B3LYP) with basis set 6-311+G (d,p). In the course of the experiment established a linear relationship between the relative IACF and the characteristics of the parameter of electron-donating ability of the PAH molecules for each symmetry group. Adequacy of the mathematical model is by mathematical statistics confirm. The resulting patterns suggests the possibility of determining donor-acceptor characteristics without quantum calculations and experiments using complex equipment.

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