Quantum-Chemical and Experimental Estimation of Non-Bonding Level (Fermi Level) and π-Electron Afinity of Conjugated Systems

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Abstract

Method of quantitative estimation of the π-electron affinity for conjugated molecules, which is directly related to donor/acceptor properties is presented. The index φ_0 is proposed, it is determined by disposition of the frontier levels in respect to the non-bonding π-level (Fermi level). It is shown that this index/parameter can be estimated not only by quantum-chemical calculation, but also experimentally using the ionization potentials and electron affinity or/and the electron transition energy. The non-bonding level energy can be estimated basing on the parity theorem: in the alternant conjugated molecules, the occupied and vacant levels (including the highest occupied and lowest vacant levels) are disposed symmetrically in respect to the non-bonding levels. The proposed parameter is convenient for quantitative analysis of the donor/acceptor properties as well as the affinity of any conjugated molecule.