Articles

Topological Index of Conjugated Heterocyclic Compounds as Their Donor/Acceptor Parameter

Nataliya Obernikhina, Marina Kachaeva, Volodymir Shchodryi, Yaroslav Prostota, Oleksiy Kachkovsky, Volodymyr Brovarets & Zenoviy Tkachuk ...show less

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Abstract

The quantum-chemical analysis of donor–acceptor properties of the conjugated heterocyclic compounds is performed. For quantitative estimation of donor/acceptor ability, the topological index φ_0 is proposed; it connects with the positions of frontier levels and points on the shifting of the energy gap relative to the reference electron balanced system, for example, polyenes or polyacenes with the balanced donor and acceptor abilities. This index enables to the investigate the donor/acceptor properties of the heterocyclic compounds more detailed, taking into consideration the number of the cycles; presence, number and position of the heteroatoms as well as their type. The examples of the 5-, 6- and 7-membered heterocyclic compounds are studied, as well as the effects of the modification of the chemical constitution by replacing of the CH-fragments by atoms O, S and NH groups or by condensation with benzene. Proposed parameter could be useful for an analysis of the stability of the intermolecular stack's complex, for example, biological active complex.

Keywords: Donor/acceptor properties | energy gap middle | frontier levels | heterocyclic compounds | quantum-chemical calculations | tological index φ0