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Strukturna zavisnost energije tripletnih stanja u konjugovanim molekulima

Slađana Đorđević, Slavko Radenković
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U ovom istraživanju smo pokazali da se efekat benzo-anelacije može primeniti za predviđanje energije tripletnih stanja derivata antracena, fluorantena i bifenilena. Razvijen je kvantitativni model zasnovan na broju angularno, linearno i geminalno aneliranih benzenovih prstena, koji veoma tačno predviđa energije tripletnih stanja ispitivanih molekula. Pokazali smo i da je energija tripletnih stanja povezana sa indeksima aromatičnosti centralnih prstenova u singletnom stanju proučavanih sistema. (Anti)aromatični karakter ovih molekula je procenjen uz pomoć energetskog efekta (ef), HOMA indeksa, multicentričnog delokalizacionog indeksa (MCI), gustine magnetno indukovanih struja (MICD) i indeksa NICS.

Revealing structural dependence of the triplet state excitation energies in conjugated molecules

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In this study we showed that the effect of benzo-annelation can be used to predict the triplet state excitation energies of anthracene, fluoranthene and biphenylene derivatives. A quantitative model based only on the number of angularly, linearly, and geminally annelated benzene rings was established, being able to accurately predict the triplet state excitation energies of the studied molecules. In addition, we showed that the triplet state excitation energy is correlated with the aromaticity indices of the central ring in the singlet state of the studied systems. The (anti)aromatic character of the examined molecules was studied using the energy effect (ef), harmonic oscillator model of aromaticity (HOMA), multicentre delocalization indices (MCI), magnetically induced current densities (MICDs) and nucleus independent chemical shifts (NICS).

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