INFLUENCE OF p^{-} π-CONJUGATION ON THE ENERGY STRUCTURE OF TETRATIO- AND TETRASELENTETRACEN

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S u m m a r y

The energy structure of neutral electron molecular states of TSeT is throughly examinated. We have found the TTT energy structure and shown the appearance of four *l*-levels filled with valence heteroatom electrons of S(Se) under $p-\pi$-conjugation of C– S(Se) bonds. Two of those levels are placed above the π-levels of the acen skeleton. For the TTT to TSeT transition, an increase of the size of heteroatomic valence orbitals has no essential impact on the bathochromic transition absorption spectrum rate. We claim that this transition depends on the geometry and the amount of conjugated system electrons. In TTT and TSeT, $l\pi^{*}$- and $\pi\pi^{*}$-states are observed.