

Computational Study of Electronic Properties in Oligoacenes

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Abstract: *Calculations were performed for closed shell singlet states, open shell singlet states and open-shell triplet states using DFT and B3LYP functional in oligoacenes. 6-31+G(d,p) basis set was used to calculate energies for polyacenes in Hartrees at various levels of spin-state configuration. For systems beyond pentacene, open shell singlet state is more stabilized for hexacene, heptacene, octacene and nonacene and singlet triplet gap decreases as size of polyacene increases. This work is used to describe unrestricted DFT calculations, spin contamination and quantum mechanical applications..*

Keywords: Electronic Properties in Oligoacenes

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