End substituted thiahelicenes for electronic device applications

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April 28, 2020

Abstract

Minimum energy structures of neutral and radical cations of end substituted thia[n]helicenes (n=1-10) in DCM solvent are reported. For both neutral and radical cations of these helicenes, calculated structures are non-planar for n=3-10. Helical structures are obtained for higher helicenes and thia[8]helicene system has a helical structure with one complete turn. Equilibrium geometries are predicted applying B3LYP-D/6-311++G(d,p) method in conjunction with SMD solvent model. Single point energy calculations are also performed at MP2 level to improve certain energy parameters. Excited state calculations are performed using Time-Dependent Density Functional Theory (TDDFT) formalism to predict UV-Visible spectra of neutral and radical cations of thia[n]helicenes in DCM solvent. Thia[n]helicenes radical cation have strong absorption in the near IR region. Calculations also suggest that dimerization is not a favourable process in DCM solvent for the end substituted neutral and radical cation of thia[7]helicene. The present theoretical study examines the molecular and electronic properties of thia[n]helicenes in search of near infrared electronic devices.

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