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Ab Initio Study of Polarizabilities of Oligothiophene, Oligocyclopentadiene and Oligofulvene and their Cyano Substituted Oligomers[1]
JOLANTA LAGOWSKI, Memorial University of Newfoundland, SULTANA FERDOUS, Brigham Young University — Ab Initio polarizabilities of thiophene, fulvene and cyclopentadiene based conducting oligomers and polymers and their cyano derivatives have been calculated using the Hartree-Fock (HF), configuration interaction (singles) (CIS) and density functional (DF) theories with 3-21G* basis using Gaussian software. The main motivation of this investigation is to determine the correlation between the excitation energies and polarizabilities for the conjugated systems studied. It has been found that HF and DF approaches give similar magnitudes for polarizabilities whereas CIS theory provides results that are considerably different. All three methods predict similar trends in polarizabilities as a function of oligomer length and bond alternation along the backbone of the oligomers. It has also been observed that the end groups and the number of 'double' bonds have a significant effect on the magnitude of polarizability per C-C bond. Comparison with experimental results will be made where possible.

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