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Synthesis, spectroscopic characterization of organic charge transfer complex of o-phenylenediamine with 2, 3-dichloro-5, 6-dicyano-1, 4-benzoquinone in solution and solid phases: Material prospects through DFT Analysis

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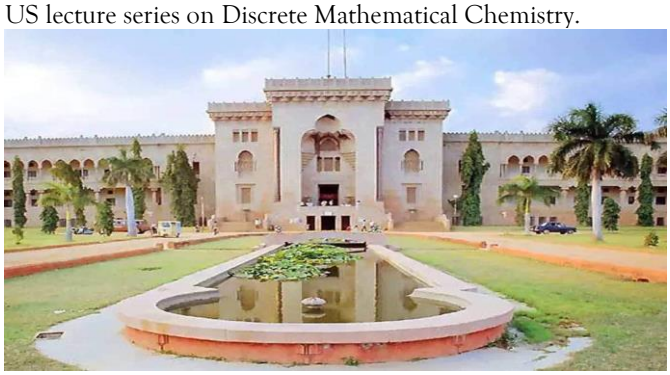
Abstract

The An exceptionally unique, easy to prepare, and economic charge transfer complex (CT-complex) of o-phenylenediamine (o-PD) with 2, 3-dichloro-5,6-dicyano benzoquinone (DDQ) is studied spectrophotometrically [1] in polar media. The stiochiometry of CT-complex is found to be 1:1. It is affirmed through Job's, conductivity [2] and photometric titration methods. The physical parameters; stability constant (KCT) and molar extinction coeffiecient (εCT) are assessed at the Benesi-Hildebrand condition. The resonance and standard Gibb's free energies are estimated. Highly negative standard free energy change and high formation constant infer the stable organic complex formation. The CT-complex is characterized by UV-Visible, XRD, FT-IR (ATR accessed), 1H NMR spectroscopic methods. The TGA-DTA studies reveal the CTC material is highly stable which favors the DNA binding through intercalative mode. The DFT (B3LYP-Gas phase/PCM) computational results support the mechanism of CT-complex formation [3]. The MEP maps demonstrate the exchange of electron stream from donor to the acceptor. The experimental and theoretical data with reference to electronic energy gap prompt us to develop the new semiconductor materials.

Biography

T Parthasarathy is professor at the Department of Chemistry, Osmania University since 2006. His research interests include Molecular Modeling and Drug Design with special reference to Virtual Screening, Docking, Homology, ADMET, Molecular Dynamics, QSAR, Semiemperical Methods - AMI and PM3, In vitro Spectrophotometric Antioxidant Study, Synthesis, Spectroscopic, Thermo dynamic Studies of Charge Transfer Complexes and DFT Computational Studies. His research group includes 14 Doctoral students who pursuing their Ph. D. degree. Eleven students were awarded Ph. D. degree under his guidance. He has completed two UGC Projects. He has reviewed several research articles and journals, J. of Chemical Education, USA, Indian J. of Chemistry, International Journal of Chemical Kinetics, Medicinal Chemistry Research and Chemical Science Transactions. He is the member of prestigious professional bodies such as American Chemical Society, Indian Science Congress and Indian Association of Chemistry Teachers. He has delivered invited lectures in First AP Science Congress and Fourth Indo-US lecture series on Discrete Mathematical Chemistry.



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