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Influence of intramolecular ring-ring π,π-interaction on crystal building in ternary compound of nickel(II) chelates of 2,2'-{[2-(4-methylphenyl)ethyl]azanediyl} diacetic acid and 1,10-phenanthroline – Synthesis, spectral, optical and quantum chemical study

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The stoichiometric reaction between Ni(II) hydroxy-carbonate and N-(*p*-methyl-phenethyl)-Iminodiacetic acid ligand (H_2MEpheida) in aqueous media leads to binary complex of the type $[Ni(MEpheida)(H_2O)_3]\cdot xH_2O$ which gives ternary complex of the formula $[Ni(MEpheida)(phen)(H_2O)]\cdot 3H_2O$ on the addition of 1,10-phenanthroline (1,10-phen) in equimolar ratio. The compound has been characterized by means of elemental analysis, FTIR, UV-Vis, TGA and X-ray crystallography. The weak ring-ring intramolecular π,π-interaction between phen and benzene ring of MEpheida affects the crystal pattern of the complex (triclinic, space group P-1) reported herein. Crystallographic information reveals the distorted octahedral geometry of the type 1+2+2+1 (lesser Jahn-Teller distortion) around the Ni(II) ion with full and half occupancy of t_{2g}^6 and $3dx^2\text{-}y^2$, $3dz^2$ orbitals respectively. The iminodiacetate moiety of metal-chelate adopts *fac*-NO_2 conformation. Moreover, the quantum chemical calculations and HOMO-LUMO energy gap along with the other global descriptors have been performed for the H_2MEpheida and $[Ni(MEpheida)(phen)(H_2O)]$ complex using DFT/B3LYP methodology. The optical bandgap energy (E_g) for ligand and Ni(II) complex have been estimated through Tauc's equation, $\alpha h\nu = A(h\nu\text{-}E_g)^r$, where r = ½ for indirect and 2 for direct electronic transitions using electronic absorption data. The direct and indirect electronic transition bandgap calculated for Ni(II) complex 3.97 and 3.76 eV respectively, reflecting their semi-conducting nature.

Keywords: Nickel(II) ternary complex, Molecular structure, Supra-molecular chemistry, HOMO-LUMO calculations, Optical bandgap energy measurements