ABSTRACT

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Title: ''Investigation on Synthesis: Structure & Characterization of Some Novel Copper (II) and Iridium (III) complexes: Biological activities and DFT studies''

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This thesis comprises of work regarding the synthesis and characterization of some iridium and copper complexes having *N, N, O* donor sites having azo and schiff base moieties.

This thesis consists of five chapters. **Chapter I** contains summary of the work presented in this thesis with short description of the physical methods and equipment employed.

Chapter-II describes the synthesis and characterization of a heteroleptic iridium(III) complex, $[Ir(2\text{-}ppy)_2(L)]PF_6$ with a ligand bearing azo (N=N) linkage. Molecular structures of both the ligand and complex were confirmed by single-crystal X-ray diffraction. The ground and excited-state geometries, absorption, and emission properties of the iridium(III) complex were further examined by DFT and TD-DFT methods.

Chapter-III deals with the synthesis and characterization of an N, N donating iridium(III) complex of composition $[Ir(2\text{-}ppy)_2(L)]PF_6$. The ligand and complex are characterized by various spectroscopic techniques. DFT studies were also performed to support the experimental aspects of the complex. Further, in vitro analysis of the anticancer activity of the complex was studied mainly with the MCF - 7 cell line.

Chapter-IV describes synthesis and characterization of a copper(II) complex of composition $[(L)_2Cu]$. The complex was characterized by spectroscopic studies. X-Ray structures of $[(L)_2Cu]$ was determined to confirm the molecular species unequivocally. The photoluminescence properties of the ligand and complex were studied. Oxidation of benzyl alcohol using the newly synthesized complex as catalyst has been studied.

Chapter-V deals with the synthesis and characterization of a copper(II) complex with 2-hydroxy-5-methyl-3-(((4-((E)-phenyldiazenyl)phenyl)imino)methyl) ligand (HL_1). The complexes were characterized by analytical and spectroscopic studies. X-ray structures of $[(L_1)_2Cu]$ was determined to confirm the molecular species unequivocally

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