ABSTRACT

Synthesis of single crystals of metal-organic hybrid complexes is an emergent field of research in material science, chemistry, *etc.* The vast interest in this field has stemmed from their fascinating features (like magnetic and electronic properties, high porosity, *etc.*). These properties lead to their wide range of applications as gas storage, gas adsorption, catalysis, *etc.* Hydrothermal synthesis is an environmentally benign, cheap and efficient method for the synthesis of single crystals of hybrid complexes. Compounds with interesting structure and riveting properties are often obtained using this technique.

Chapter I is an introductory one that describes metal-organic hybrid complexes and their applications in various fields as well as single crystals, their classification and methods of growth. Object and application of the present research work has also been outlined in this chapter. A brief description of the advantages of hydrothermal technique of crystal growth was described.

Chapter II includes the experimental section. This chapter includes the chemicals and materials used in this research work. A brief description of the organic ligands used in different works was given. This chapter also contains details of the physico-chemical and spectroscopic techniques, *viz.,* single crystal and powder X-ray diffraction, FTIR spectroscopy, TGA, EPR, SQUID and FESEM, *etc.*, used for the physicochemical characterization of the synthesized complexes. This chapter also describes the theoretical characterization (DFT, etc) of the hybrid complexes.

Chapter III includes synthesis, structural characterization and magnetic studies of deep green crystals of Poly[diaquo(1,10-phenanthroline-$\kappa^2N^1:N^{10}$)(μ_2-sulphato-$\kappa^2O:O'$)copper(II)] using hydrothermal technique. The study of single crystal X-ray diffraction revealed the three-dimensional monoclinic system with space group I2/c of the complex. The unit cell dimensions are a = 7.0081(3), 13.8198(7) and c = 14.2897(8) Å; α = 90°, β = 99.282(5)° and γ = 90°. In the complex, the successive pairs of Cu(II) ions are held together by SO_4 bridges with each Cu(II) ion coordinated 1,10-phenanthroline and two H_2O molecules leading to distorted octahedral geometry. with zigzag channels within its three dimensional architecture.

Chapter IV includes the hydrothermal synthesis, structural characterization and magnetic studies of blue crystals of a Cu(II) hybrid complex, [{Diaquo(3,5-

dinitrobenzoato-κ^1O^1)(1,10-phenanthroline-κ^2N^1:N^{10})}copper(II)]3,5-dinitrobenzoate. The physico-chemical characterization of the synthesized complex was performed using single crystal X-ray diffraction, FTIR spectroscopy, EPR, SQUID, TGA and FESEM. Single crystal X-ray diffraction study revealed that the complex crystallizes in a monoclinic form with the space group $P12_11$. The unit cell dimensions are a = 9.3085(5), b = 5.9069(2) and c = 25.0995(12) Å; the axial angles are α = 90°, β = 96.790(4)° and γ = 90°. The assymetric unit contains a penta-coordinated Cu(II) ion coordinated to two H_2O molecules, two N-atoms of 1,10-phenanthroline and O-atom of the carboxylic group of 3,5-dinitrobenzoic acid in a distorted square pyramidal geometry. TGA, EPR and SQUID studies revealed it to be a stable and weakly antiferromagnetic material.

Chapter V includes the hydrothermal synthesis structural characterization and magnetic studies and DFT study of blue crystals of a new metal-organic hybrid complex [Bis(picolinate-κ^2N:O)Copper(II)] di(benzene-1,3,5- tricarboxylic acid). Single crystal X-ray diffraction study revealed that the complex crystallizes in a monoclinic form with space group P1 21/c 1. The unit cell dimensions are a = 4.9853 (4), b = 13.1082 (5), c = 21.6616 (8) Å; the axial angles are α = 90°, β = 91.230° (6) and γ = 90°. The asymmetric unit of the title complex is composed of a Cu(II) ion and two 2-picolinic acid anions in a slightly distorted square planar coordination environment. EPR and SQUID studies revealed it to be a stable paramagnetic material.

Chapter VI includes the synthesis, structural characterization, Hirschfeld surface analiysis, catalytic activity and DFT study of the complex [Diaquo{bis(*p*-hydroxybenzoato-κ^1O^1)}(1-methylimidazole- κ^1N^1)}copper(II)] using conventional method. The synthesized complex acts as good catalyst in benzimidazole synthesis with good recyclabilty as catalyst up to 5th run.

Finally chapter VII contains the concluding remarks of the research works embodied in this thesis