The thesis entitled, “Synthesis and characterization of coordination polymers using conjugated ligand having nitrogen and oxygen donors” is divided into six chapters. The introductory chapter 1 describes about significance of coordination polymers in general and multifunctional coordination polymers in particular and significance of π–conjugated ligand in coordination polymers and as multifunctional materials. On the basis of available literature the criteria for good conducting materials with magnetic properties have been outlined and a design for multifunctional coordination polymers based on π–conjugated ligand having good conducting and magnetic properties has been proposed. In light of our proposed design a review of the previous work on π–conjugated ligand 2,5–dichloro–3,6–bis(ethylamino)–1,4–benzoquinone and the deficiencies of the available literature have been outlined. The application of 2,5–diamino–1,4–benzoquinone derivatives in general have been presented. Finally, the aims and objectives of undertaking the present investigation have been presented in the introduction chapter.

The second chapter deals with the specifications of the commercially available starting materials, purification of the solvents, synthesis of the ligand, its monometallic and heterobimetallic coordination polymers, analytical procedures and equipments used for the various physico–chemical measurements.

In the chapter 3, mechanism / basis of modifying the procedure for the synthesis of the ligand H₂dedb and its single crystal x-ray structure has been discussed. The ligand H₂dedb has been characterized by elemental analysis, FAB mass, ^{1}H and ^{13}C NMR spectra, electronic spectra spectroscopic techniques, cyclic voltammmogram. IR and Raman vibrational assignment using potential energy distribution (PED) have been done. The DFT level calculations of optimized structure and APT charges have been discussed. Finally, the solid state DC electrical conductivity of H₂dedb has been presented.

The chapter 4, describes the synthesis of the coordination polymers of the type [Cu,Zn_{1-x}(dedb).yH₂O]n {where dedb = dianion of 2,5 dichloro –3,6–bis(ethylamino)–1,4–benzoquinone; x = 1, 0.5, 0.25, 0.125, 0.0625 and 0; y = 0 – 2} and their characterization with elemental analyses, metal estimation, powder X–ray diffraction, TEM, thermal, spectroscopic (IR, UV–visible and ESR) techniques. The
solid state electrical conductivity measurements by the conventional two probe method have been presented.

Chapter 5 deals with the synthesis and characterization of coordination polymers of the type \([\text{Cu}_x\text{Ni}_{1-x}(\text{dedb}).y\text{H}_2\text{O}]_n\) \(\{x = 1, 0.5, 0.25, 0.125, 0.0625 \text{ and } 0; y = 0 - 2\}\). Field dependent, temperature dependent magnetic susceptibility and solid state electrical conductivity of monometallic and heterobimetallic polymers have been presented.

Chapter 6 deals with the synthesis of polymers of the type \([\text{Cu}_x\text{Fe}_y(\text{dedb}).2\text{H}_2\text{O}]_n\) \(\{x = 0, y = 0.67; 0.5, 0.33; 0.25, 0.5; 0.125, 0.583; 0.0625, 0.625\}\). Characterizations of these polymers have been done by elemental analyses, metal estimation, powder X–ray diffraction, thermal, IR, Mössbauer and ESR spectroscopic techniques. Temperature dependent magnetic and solid state electrical properties of these polymers have been investigated.

Some of the important findings of the present investigations are:

(i) Single crystal X–ray of ligand \(\text{H}_2\text{dedb}\) and the optimized structure shows presence of two parallel \(\pi\)–conjugated strands and presence of 1–D short contacts. Solid state DC conductivity measurements show it is a semiconductor.

(ii) Powder X–ray diffraction lines of the heterobimetallic coordination polymers clearly indicates that they exhibit characteristic lines at different positions as compared to those of the corresponding monometallic polymers and equimolar mixture of resoective monometallic polymers. This indicates the formation of heterobimetallic polymers as a new compound rather than a mixture of monometallic polymers in appropriate mole ratio.

(iii) Thermal studies (TGA, DTG, and DTA of the heterobimetallic polymers indicate that their thermal degradation are different from those of monometallic polymers.

(iv) ESR spectral studies concluded that the heterobimetallic polymers exhibit electronic communications between two different metal ions bridged by \(\pi\)–conjugated ligand \(\text{H}_2\text{dedb}\).
(v) Variable temperature magnetic susceptibility measurement studies reveal the presence of ferromagnetic interactions affected by the amount of copper ion present in the heterobimetallic polymer.

(vi) All the heterobimetallic polymers of the \([\text{Cu}_x\text{Zn}_{1-x}(\text{dedb}).y\text{H}_2\text{O}]_n\) and \([\text{Cu}_x\text{Fe}_y(\text{dedb}).2\text{H}_2\text{O}]_n\) exhibit semiconductor behavior and the conductivity of heterobimetallic polymers are higher than monometallic polymers. Heterobimetallic polymers of types 10, 11 and 12, exhibit semiconductor as well as metallic conductivity.

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