Summary

The thesis entitled *“Synthesis, characterization and molecular properties of coordination polymers with homo- and/or hetero- donor ligands”* has been divided into six chapters.

Chapter 1

This chapter gives a brief account of the subjects, which are of significance in this thesis, *viz.* coordination polymers (CPs), their synthesis, and applications. The recent developments in this area were also discussed in this chapter. The synthesis and characterization of infinite 1, 2, and 3-D networks has been an area of rapid growth. Construction of 3D and multi-functional molecular architecture can be of great significance as they are likely to afford new materials for potential applications in several areas like gas adsorption, molecular storage, catalysis, photochemistry, magnetism and so on. Dynamic structural transformation based on flexible frameworks is one of the most interesting and most probably characteristic phenomena of CPs.

Chapter 2

Chapter 2 accounts for the structural description and luminescence property of two new coordination polymers of lead(II) synthesized with dicarboxylic acids (iminodiacetic and naphthalene-2,6-dicarboxylic acids) and for one of these also 1,10-phenanthroline which acts as ancillaryligand limiting the coordination sites at the metal. The PbII -idiac-phen complex comprises a trinuclear discrete molecular complex and the overall dimensionality is 3D, where the architecture shows strong π–π interactions between the phen moieties. The PbII–ndc complex has a 3D network structure and the network is reinforced by C-H...π-ring interactions between the ndc rings. The intraligand π* – π charge transfer transition is responsible for the emission behavior observed for both the complexes.

Chapter 3

In this chapter we discussed three polymeric networks obtained through hydrothermal reaction of zinc(II) and cadmium(II) ions with aromatic hetero N-/O-donor ligands. Structural study reveals that in case of Zn(bipy) and Cd(bipy) units with 5-nitro-isophthalate dianions a 1D zigzag polymeric arrangement and a linear double chain was obtained. On the other hand 1,4-benzenediacrylate and nitrate anions alternatively connect $Cd(bipy)_2$ fragments to form another zig-zag polymeric ribbon. π-π interactions among bipy rings and H-bonds are responsible of the supramolecular networks observed in each crystal. Solid state luminescence study of the complexes as well as of ligands are ascribed to intraligand π–π* CT transition.

Chapter 4

Chapter 4 is focussed on the crystal structures of three Mn(II) coordination polymers synthesized by using hetero donor (N, O) ligands. Different dimensionalities for the complexes were detected by single crystal X-ray structural analysis. The supramolecular packing was governed by non-covalent interactions. The results indicated that organic species with rigid –COOH and flexible $–CH_2COOH$ carboxyl groups were useful synthons for the synthesis of coordination polymers, the topology of which can be modulated by ancillary ligands such as chelating phen or 2,2’-bipy. Metal perturbed intra ligand transition was responsible for the emissions observed in **6** and **8**.

Chapter 5

The single crystal X-ray structure of two Ag(I) coordination polymers was determined and some important structural features regarding the role of weak forces in the crystal lattices were emphasized in this chapter. Both the structures exhibited two-dimensional layer architectures. The overall self-assembled structures of these frameworks were the outcome of the competitiveness as well as cooperativity of weak C-H···π and unique metal···π interactions in the organization of metal nodes with flexible auxiliary ligands.

Chapter 6

Ligands containing carboxylate groups were useful tools for the construction of coordination polymers. In this chapter two interesting 1D polymers with lead(II) were discussed. The detailed x-ray single crystal structure analysis revealed that $Pb_2(dbsf)_2$ rings were connected thorough bipy ligands which evolve in a rare example of a polyrotaxane 1D→1D interpenetrated coordination mode, a topology clearly favoured by the electron configuration of Pb(II) that involved the $6s^2$ lone pair.