ABSTRACT

Title of the thesis: **Exploration of structural features of some newly synthesized transition metal coordination complexes**

Submitted by: **Pampi Pal** **[Index No. 266/15/Chem./24]**

This thesis contains syntheses of some transition metal (Co, Ni and Cu) complexes with pyridyl based heterocyclic ligands, their characterizations and exploration of supramolecular assemblies in the solid state. Theoretical calculations have been carried out to establish the noncovalent interactions in building of supramolecular self-assemblies. Metal complexes were synthesized at ambient temperature by mixing suitable metal salts in appropriate solvents, heterocyclic bases and ancillary ligands in stoichiometric ratios.

For actual crystal structure interpretation, a precise understanding and complete control over the interplay of noncovalent interactions is necessary. Although crystal engineering deals with the individual potentiality of weak forces, an exciting aspect is still in a state of infancy, that is, the associative interactions of noncovalent forces to form extended networks and their supramolecular consequences in the solid state. Subtle alteration of the factors like reaction conditions and reacting components that can affect the self-assembly processes have been studied. It illustrates the imperative role of classical and non-classical hydrogen bonding, C–H···π, π···π, π···π^+, anti-electrostatic π^+···π^+, anion···π and anion···π^+ interactions in the formation of different dimensional supramolecular networks.

These supramolecular interactions have also been successfully rationalized by various theoretical calculations, such as density functional theory (DFT), Molecular Electrostatic Potential (MEP), Bader's theory of Atoms in Molecules (AIM), Non-Covalent Interaction plot (NCI plot) to characterize and explore the energetic consequences of the noncovalent interactions quantitatively.

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