

## ABSTRACT

Title of the thesis: **Synthetic, spectral and supramolecular exploration of some metal complexes with nitrogen-based heterocycles**

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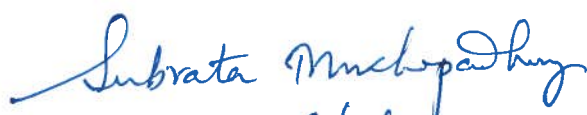
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The thesis includes synthesis, characterization and exploration of supramolecular features of some metal complexes with nitrogen-based heterocyclic ligands. The nitrogen-based heterocycles were synthesized through one-pot condensation reaction using various aromatic amines and aldehydes or ketones. The metal complexes were synthesized at room temperature in aqueous medium by mixing metal salts, heterocyclic ligands along with various auxiliary ligands in their stoichiometric ratios.

Coordination complexes of metals with those typical nitrogen-based heterocycles, when crystallized, show esthetic beauty in their structures having hydrogen bonding,  $\pi \cdots \pi$ , lone pair  $\cdots \pi$ , C—H  $\cdots \pi$  and anion  $\cdots \pi$  types' non-covalent interactions. The associative interactions of non-covalent forces to form extended networks and their supramolecular consequences in the solid state are of primary importance in this study.


The possible cooperativity effects for weak non-covalent interactions have been explored in detail by theoretical (DFT) calculations including MEP surface, AIM and NCI plot analysis, which conclude energetically favorable associations. Fluorescence emission spectral studies recognized the “turn on” chemosensor property of a pyridine based compound for  $Al^{3+}$  ion in solution as well as in living cell.

Finally, photo-physical properties and biological properties of some synthesized metal-heterocycles have also been explored.

  
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