ABSTRACT OF THE THESIS
ENTITLED

“STUDIES ON TRANSITION METAL COMPLEXES
OF SOME OXYGEN, NITROGEN/SULPHER DONOR
LIGANDS”

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Transition metal complexes have a prominent role in modern coordination chemistry because of their role in catalytic processes, biological systems and medical science. They have paramount applications in the field of food and dye industries, analytical chemistry, biology, and agriculture, polymer science, in liquid crystal devices and as myocardial perfusion imaging agents.

Studies in coordination behaviour of potentially important ligands containing various functional groups with transition metal ions is one of the subjects of interest. The development of numerous newer organic chelating agents that can coordinate with transition metal ions has opened up a broad scope to research scientist in this field. The transition metal complexes of bidentate, tridentate, tetradentate organic ligands/Schiff bases containing oxygen-nitrogen, oxygen-sulphur, oxygen-nitrogen-sulphur as a potential sites have been reported.

Schiff bases (imines) are an important class of ligands in coordination chemistry and have many applications in various fields. Schiff bases have notable contribution in the development of coordination chemistry. The fact is supported by number of publications in this field. The Schiff base is a compound containing azomethine group which are also referred as azomethines, imines and anils. The chemistry of Schiff base
(imines) complexes have been reported with wide applications in food industries, dye industries, analytical chemistry, catalysis, fungicidal and agrochemical activity. The transition metal complexes of various Schiff bases derived from salicylaldehyde, 2-hydroxy-1-naphthaldehyde, 2-hydroxy acetophenone, dehydroacetic acid and different amines have been reported from this laboratory due to their novel chemical, electronic and magnetic properties.

From earlier reported study, it is planned to undertake a detailed and comprehensive investigation of metal complexes of Schiff bases using various modern techniques. The proposed work includes synthesis and characterisation of Schiff bases (ligands) and study of their coordination behaviour towards transition metal ions. The results obtained from various physicochemical experimental techniques are used for determine the structure of complexes.
The work to be presented in the thesis is divided into six chapters

CHAPTER 1

INTRODUCTION:-

Schiff bases, their metal complexes along with applications, importance have been discussed briefly, followed by the general introduction to coordination chemistry and its theories. A brief survey of literature on previous studies on metal chelates of salicylaldimines, 2-hydroxy acetophenoneimines, ketoimines, Schiff bases of DHA and some other metal complexes have been discussed.

CHAPTER 2

SYNTHESIS AND CHARACTERISATION OF SCHIFF BASES AND THEIR METAL COMPLEXES:-

The experimental procedures followed in the synthesis of Schiff base ligands have been given. The characterisation of ligands by elemental analysis, electronic absorption, and PMR spectroscopy has been included. General methods of synthesis of Cu (II), Ni (II), Co (II), Fe (III) and Mn (II) complexes with Schiff bases have been described.

CHAPTER 3

EXPERIMENTAL TECHNIQUES:-

A brief account of various experimental techniques used for the study of coordination complexes is given. The experimental details of measurement of magnetic susceptibility, solution conductivity, electronic absorption spectra, infrared spectra, X-ray powder diffraction and thermal analysis of complexes are given.
CHAPTER 4
RESULTS AND DISCUSSION OF MAGNETIC SUSCEPTIBILITIES, ELECTRONIC ABSORPTION SPECTRA, THERMOANALYTICAL AND X-RAY POWDER DIFFRACTION STUDIES OF METAL COMPLEXES:-

The experimental data on conductivity, magnetic susceptibility, electronic absorption spectra, thermoanalytical and X-ray powder diffraction measurements of Cu (II), Ni (II), Co (II), Fe (III), and Mn (II) complexes of Schiff bases are presented and discussed in this chapter.

The discussion is mainly concerned with magnetic susceptibilities, electronic absorption spectra and ligand field parameters of metal complexes, in relation to their probable stereochemistry in the light of ligand field theory and information available in the literature on similar compounds. It also includes discussion on conductivity and elemental analysis.

The discussion on thermal decomposition behaviour of metal complexes on the basis of simultaneous TG-DTA curves is confined and thermal kinetic parameters are calculated.

The unit cell data and crystal lattice parameters of metal complexes calculated from strong refluxes in the XRD pattern by using computer program are presented and discussed with respect to lattice parameter, density, porosity percentage, crystal system and probable space group.

CHAPTER 5
RESULTS AND DISCUSSION OF INFRARED SPECTRAL STUDIES OF LIGANDS AND THEIR METAL COMPLEXES:-
The infrared spectral data of ligands and their metal complexes are discussed with respect to frequencies of different groups involved in complex formation. The assignments of absorption frequencies for different groups are empirical and tentative and are based on information cited in literature on similar transition metal complexes.

The chapter also devote for presenting conclusions of present investigation drawn on the basis of various physicochemical and spectral analytical technique employed in characterization of metal complexes.

CHAPTER 6

STUDIES OF ANTIFUNGAL ACTIVITY:-

The brief biology of fungi is discussed with fungal growth, biotechnological, industrial, economic importance and harmful effects.

The experimental procedure of screening of antifungal activity of Schiff bases and their metal complexes is described. The experimental data in terms of yield of MDW and percentage inhibition of fungal growth are presented and discussed from the point of view of comparative fungal toxicity of ligand and their metal complexes.
The physicochemical study of Schiff bases and their transition metal complexes is used to study the structure of complexes, nature of bonding involve and the effect of substituents on the complexes. The comparative study of Schiff bases and their metal complexes towards biological activity is also studied in the present work.

With this aim in view, the present study deals with the synthesis of solid complexes of Cu(II), Co(II), Ni(II), Mn(II) and Fe(III) with Schiff bases derived from dehydroacetic acid and aromatic amine-

- 3-chloro aniline
- 3-bromo aniline
- 3-amino phenol
- 3-amino benzoic acid
- 3-methoxy aniline
- 3-methyl aniline
- 3, 4-dichloro aniline
- 2-ethoxy aniline

The characterization of Schiff bases is carried out by elemental analysis, PMR, IR and electronic absorption spectra. The characterization of complexes is done by elemental analysis, electronic absorption spectra, conductometry, thermal analysis, IR spectroscopy and X-ray powder diffraction techniques.

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