Chapter 9

Summary, conclusion and further scope

Schiff bases and their coordination compounds are one of the important branch of coordination chemistry due to not only its preparative diversity, variabliality and versatile coordinating properties but also its remarkable antibacterial, antifungal, anticancer, analgesic, sedative and anti-inflammatory properties. These compounds are closely resembled to metalloproteins studied for its antipathogenic behavior and very important in metal based drugs.

Because of these reasons, we are also interested to develop some novel schiffs bases from various carbonyl compounds and amines. Among these bidentate, negatively charged ligands and neutral tetradeinate ligands with two different types of azomethine linkages were included. These ligands are characterized and their interaction was studied with various transition metals. The characterization of various species formed from these ligands was conducted by using elemental analysis, molar conductance measurements, infra-red, electronic, NMR and ESR spectroscopic techniques and thermal analysis. The antibacterial properties of ligands and metal complexes were conducted using disk diffusion methods against bacteria such as *Staphylococcus aureus*, *Escherchia coli*, *Bacillus subtilis*, *Pseudomonas aeruginosa*. The synthesis of various ligands and their metal chelates its characterization and antibacterial properties etc are discussed in proposed thesis.

A general study of the structural and bonding features of various ligands (Schiff bases) synthesized from carbonyl compounds and primary amines, their coordination chemistry and their applications in various fields were presented in the first chapter of the proposed thesis. This includes a literature survey of various schiff bases synthesized from o-vanillin, 4-
aminoantipyrine, o-phenylene diamine and furfural and their applications in biological fields, catalytic activity, in polymer science, Dyes, action as insecticides etc.

The scope and objectives of the present study was mentioned in chapter 2. The various spectroscopic and analytical methods used for the characterization of various Schiff bases and its metal chelates were presented in chapter 3.

The synthesis and characterization of a bidentate, negatively charged Schiff base from vanillin (aldehydes) and anthranilic acid (amino) with nitrogen and oxygen donor atoms and its interaction with various transition metals like chromium (III), Manganese (II), Cobalt (II), Nickel (II), Copper (II), Zinc (II) and Cadmium (II) was presented in chapter 4. The molar conductance data suggested that its Cr(III) complex is a 1:1 electrolyte while the others are bad conductors. From the IR spectra, it was revealed that two molecules of water was coordinated to the metal during complex formation in addition to the Schiff base VA, which was coordinated through its azomethine N and oxygen atom of COO\(^-\) group. From the electronic spectra and elemental analysis it was found that they are octahedral compounds with M:L:H\(_2\)O ratio in the coordination sphere is 1:2:2. A tetragonally distorted (z-out) geometry was proposed for its Cu(II) complex, where the unpaired electron is present in its \(dx^2-y^2\) orbital (from electronic and ESR spectra). The calculated values of \(D_q, \beta\) of various species from electronic and ESR spectra (Cu\(^{+2}\) complexes) revealed that they are not 100% ionic, but have a predominant covalent character. The comparison of NMR spectrum of the ligand and its Zn\(^{+2}\) complex also suggested that the coordination is through its azomethine N and COO\(^-\) group formed from the deprotonation of the carboxylic acid part of the ligand. The various ESR spectral parameters are calculated and explained for its Cu(II) complexes. The formation, existence and thermal stabilities were also supported by the thermal analysis data. They are found to be thermally stable, but loses one or
two molecules of coordinated water in the first step, followed by the loss of Schiff base, resulted into a stable residue, usually oxides of metals. From these observations proposed the molecular formula of various metal chelates as \([\text{Cr(VA)}_2(\text{H}_2\text{O})_2]\text{Cl}\) and \([\text{M(VA)}_2(\text{H}_2\text{O})_2]\text{ where M is Mn(II), Co(II), Ni(II), Cu(II), Zn(II) and Cd(II).}\n
Another neutral bidentate Schiff base from 4-aminoantipyrine and vanillin (AV) has been synthesized and its interaction with various transition metals are presented in chapter 5. They are also characterized by the same methods discussed in chapter 4. This Schiff base was also coordinated through its azomethine nitrogen and oxygen atom of the carbonyl group of the 4-aminoantipyrine part to the central metal atom in addition to two molecules of water. They are octahedral in geometry while \(\text{Cu}^{+2}\) complex is tetragonally distorted octahedron with general molecular formula \([\text{Cr(AV)}_2(\text{H}_2\text{O})_2]^{3+}\) and \([\text{M(AV)}_2(\text{H}_2\text{O})_2]^{2+}\), where \(\text{M} = \text{Mn}^{+2}, \text{Co}^{+2}, \text{Ni}^{+2}, \text{Cu}^{+2}, \text{Zn}^{+2}\) and \(\text{Cd}^{+2}\).

The synthesis and characterization of a wide variety of Schiff bases and their interaction with transition metals were reported earlier, but most of them are monodentate or bidentate. The tetradentate Schiff's bases are very rare and reported very recently. So we have been interested in synthesizing such ligands. A versatile neutral tetradentate ligand having four nitrogen atoms including two different types of azomethine group from 4-aminoantipyrine, vanillin and o-phenylene diamine have been prepared and its interaction with various transition metals was presented in chapter 6. These compounds were characterized by elemental analysis, IR, UV-vis, ESR, NMR spectroscopic methods, molar conductivity measurements and thermal analysis. The metal complexes formed were 1:1 electrolytes except for Co(II) which is 1:2. The synthesized MN₄ chromophore system have a square planar environment, with appreciable amount of M-L covalent character.
A new series of transition metal complexes of Mn(II), Co(II), Ni(II), Cu(II) and Zn(II) were synthesized from the schiff base ligand derived from 4-aminoantipyrine, furfural and o-phenylene diamine was presented in chapter 7. The structural features were derived from their elemental analysis, IR, UV-vis, ESR and NMR spectroscopic methods, thermogravimetric analysis and molar conductivity measurements. They have a square planar geometry with four nitrogen atom acting as donor (including two different types of azomethine group), with molecular formula \([\text{M(AFOP)}]^2+\).

The ESR parameters like exchange interaction \(G\), Spin orbit coupling constant \(\lambda\), Covalence parameter \(\alpha^2\), In-plane \(\pi\)-bonding parameter \(\beta^2\), Orbital reduction factor \(K\parallel\) and \(K\perp\) and \(g\parallel\), \(g\perp\) and \(g_{av}\) of all Cu\(^{+2}\) complexes were calculated and explained.

The 3D modeling of some Cu(II) complexes as reference, has been carried out using chembiodraw software are also presented in various chapter.

One of the growing importance of schiff base chemistry is their antibacterial and antifungal properties. So the antibacterial studies of all the ligands newly synthesized and their metal complexes were conducted using disk diffusion method. The results were presented in chapter 8. From the results it was found that the metal complexes have better activity as compared to the ligands. The Zn\(^{+2}\), Cd\(^{+2}\) and Ni\(^{+2}\) complexes are highly active against the bacteria such as *Staphylococcus aureus, Escherchia coli, Bacillus subtilis, Pseudomonas aeruginos*. Its effect was explained on the basis of Overtone concept and chelation theory.

The work was concluded in the chapter 9. The study can be extended to the metals other than which were already present in this thesis. Complexes of rare earth and radioactive metals can also be synthesized using these Schiff bases will be helpful in disposing radioactive materials. These studies can be used in environmental science for removing trace elements from
the surroundings. The study of complexes can be useful in medicine as drugs. Research can be done to prepare conducting polymer complexes, to make thin films. Potentiometric and pH metric titrations can be done between the prepared Schiff base ligands and metals to find a method for the estimation of metals. The prepared complexes can be used to study its catalytic activity.
List of Publications


