CHAPTER V
5. SUMMARY AND CONCLUSION

Importance of Schiff base and its transition metal complexes in biological processes has been well documented. The donor behaviour of Schiff base ligands towards metal ions has been extensively investigated. Recent findings indicate that the Schiff base transition metal coordination complexes are one of the interesting class of materials which are considered to have biological significance and are used as antibacterial and antifungal agents. Hence, attempts have been made in the present work to synthesise and investigate the physiochemical and antimicrobial properties of some promising organometallic complexes. The present study deals with transition metal complexes of Schiff base ligands derived from glutaraldehyde and aminoacids such as L-Leucine (leu), L-Valine (val), L-Alanine (ala), L-Histidine (his) and L-Glutamine (gln). The present work was undertaken with a view to study the donor properties of Schiff base ligand and its application as antimicrobial agent. The complexes of divalent metal ions Copper (II), Nickel (II) and Cobalt (II) with counter anions nitrate and perchlorate were synthesized. The structural and chemical characterizations were made by elemental analysis, conductance measurement, infrared, UV/Visible and $^1$H-NMR spectral studies, Powder XRD, thermal study, magnetic moment measurements and antimicrobial studies.

Cu(II), Ni(II) and Co(II) complexes of glu-leu Schiff base ligand were synthesized and the conductance data revealed that the complexes were non-electrolytes. The chemical composition is confirmed by elemental analysis. The IR spectra confirmed the presence of various functional groups in the complexes and, in particular, the coordination of metals with Schiff base ligand. The electronic spectra of the complexes in DMSO were recorded in the range of 200 -1000 nm. The absorption region, band maxima and their probable assignments were in good agreement with the octahedral geometry of the complexes.
The band around 600 nm, and 390 nm for Cu(II) complex was attributed to $^2\text{E}_g \rightarrow ^2\text{T}_{2g}$ and charge transfer transitions. The magnetic moment value 1.76 BM offered possibility of an octahedral geometry. Ni(II) complex that exhibited bands at 859 nm, 670 nm and 390 nm, attributed to $^3\text{A}_{2g} \rightarrow ^3\text{T}_{2g}(\nu_1)$, $^3\text{A}_{2g} \rightarrow ^3\text{T}_{1g}(\text{F})(\nu_2)$ and $^3\text{A}_{2g} \rightarrow ^3\text{T}_{1g}(\text{P})(\nu_3)$ transitions respectively, indicating the octahedral geometry around Ni(II) ion which was further confirmed by the magnetic moment value of 3.28 BM. The electronic spectra of Co(II) complex exhibited absorption bands in the region 630 nm and 390 nm attributed to $^4\text{T}_{1g}(\text{F}) \rightarrow ^4\text{T}_{2g}(\text{F})(\nu_1)$ and $^4\text{T}_{1g}(\text{F}) \rightarrow ^4\text{T}_{1g}(\text{P})(\nu_2)$ transitions respectively. The magnetic moment value of 4.76 BM further confirmed the octahedral geometry. The $^1\text{H}$-NMR spectrum of the complexes confirmed the presence of azomethine band and the metal coordination of the Schiff base ligand. The characterization by Powder XRD confirmed the complexes were microcrystalline in nature. TG/DTA analyses revealed that the decomposition took place at various steps for the Cu(II) and Ni(II) complexes, which revealed the presence of two coordinated water molecules attached to the central metal atom. The ligand and their metal complexes were screened for antimicrobial activity against various bacterial and fungal species which revealed that the complexes were more active than the corresponding ligand.

In view of the importance of Schiff base chelates, Cu(II), Ni(II) and Co(II) metal complexes of glu-val Schiff base were synthesized and characterized. The synthesized complexes were found to be non-electrolytes, which were confirmed by conductance studies. Elemental analysis confirmed the chemical composition of the complexes. The presence of important functional groups, azomethine linkage and metal coordination in the sample was confirmed using IR spectral studies. The electronic spectra recorded in DMSO showed band at 670 nm and 515 nm in Cu(II) complex revealed the possibility of octahedral geometry.
The electronic spectra of Ni(II) complex exhibited bands at 830 nm, 600 nm and 380 nm attributed to $^3A_{2g} \rightarrow ^3T_{2g}(v_1)$, $^3A_{2g} \rightarrow ^3T_{1g}(F)(v_2)$ and $^3A_{2g} \rightarrow ^3T_{1g}(P)(v_3)$ transitions respectively indicating octahedral geometry. The magnetic moment value 3.22 BM obtained further confirmed the geometry. The electronic spectra of Co(II) complex exhibited bands in the region 785 nm and 500 nm indicating the transition supported $^4T_{1g}(F) \rightarrow ^4T_{2g}(F)(v_1)$ and $^4T_{1g}(F) \rightarrow ^4T_{1g}(P)(v_2)$. The $^1$H-NMR spectrum of the complexes the i.r. inferences and exhibited signal in the range of 7.3 - 8.4 ppm which was assigned for the –CH=N proton and multisignals within 1.3 - 3.5 ppm attributed to –CH, –CH$_2$ and –CH$_3$ protons in the complex. Powder XRD study of the complexes revealed that the complexes were microcrystalline in nature. Thermal study of the complexes revealed the decomposition at various stages leading to the information of the corresponding metal oxide. Biological studies of these complexes revealed that these complexes show better activity compared to their respective ligands.

An attempt was made to synthesize Cu(II), Ni(II) and Co(II) metal complexes of glu-alac Schiff base complexes and was characterized successfully. The conductance measurement of the complexes showed that they were non-electrolytes. The chemical compositions were confirmed by elemental analysis. The presence of various functional groups, alkyl groups, azomethine group and metal coordination were confirmed by IR spectral studies. The electronic spectrum of Cu(II) complex showed the d-d transitions nearly at 670 nm, attributed to $^2E_g \rightarrow ^2T_{2g}$ transition which revealed the possibility of octahedral geometry. It is further confirmed by the magnetic moment value of 1.8 BM. The electronic spectrum of Ni(II) complex displayed bands in the region of 820 nm, 620 nm and 380 nm characteristic of octahedral geometry corresponding to $^3A_{2g} \rightarrow ^3T_{2g}(v_1)$, $^3A_{2g} \rightarrow ^3T_{1g}(F)(v_2)$ and $^3A_{2g} \rightarrow ^3T_{1g}(P)(v_3)$ transitions respectively.
The magnetic moment value of 3.25 BM was in consistency with the octahedral environment. The Co(II) complex showed the aband in the region of 380 nm assigned to \( ^4T_{1g}(F) \rightarrow ^4A_{2g}(F) \) suggesting octahedral geometry around the cobalt ion. The \( \mu_{\text{eff}} \) value of 4.85 BM at room temperature suggested the octahedral geometry. The \( ^1H\)-NMR spectrum showed the signal as singlet at 7.8, 8.1 and 8.71 ppm for Cu(II), Ni(II) and Co(II) complexes attributed the presence of azomethine protons. The n.m.r results obtained further supported i.r inferences. Results of powder XRD studies of the complexes indicated that the crystals were microcrystalline in nature. Thermal analysis of the synthesized complexes revealed the stability of the complexes and their decomposition at various stages leading to the formation of the corresponding metal oxide. The results of the biological activity of the metal complexes against various microbial species indicated that the metal chelates exhibited higher antimicrobial activity than that of the free ligand.

Metal complexes of glu-his Schiff base ligand were synthesized and characterized by various studies. The Cu(II), Ni(II) and Co(II) complexes of the ligand were subjected to conductance study which revealed that they were non-electrolytes. The presence of important functional groups, azomethine linkage and the coordination with metal ion was also confirmed by IR spectral study. The chemical composition was studied by elemental analysis. Within the UV spectrum of the Cu(II) complex, there existed absorption bands at 645 and 380 nm due to \( ^2E_g \rightarrow ^2T_{2g} \) transition and charge transfer transition respectively. The magnetic moment value of 1.82 BM further supported the possibility of octahedral geometry. The electronic spectrum of Ni(II) complex displayed bands at 800 nm, 650 nm and 475 nm assigned to \( ^3A_{2g} \rightarrow ^3T_{2g} \), \( ^3A_{2g} \rightarrow ^3T_{1g}(F) \) and \( ^3A_{2g} \rightarrow ^3T_{1g}(p) \) transitions respectively and additional transition at 380 nm was attributed to ligand to metal charge transfer.
The magnetic moment value of 3.32 BM additionally confirmed the octahedral geometry of Ni(II) complex. The electronic spectra of Co(II) complex exhibited bands at 920 nm and 500 nm assigned to $^4T_{1g} (F) \rightarrow ^4T_{1g} (P)$ transitions attributed to octahedral geometry of the complex. The magnetic moment value of 4.9 BM for the Co(II) complex further supported the octahedral geometry of the complex. The $^1$H NMR study further confirmed the azomethine linkage and the coordination with metal ion. Results of Powder X-ray diffraction studies revealed the microcrystalline nature of the complexes. TG/DTA analysis revealed the decomposition of the complexes at various steps that gave the information about the thermal stability. Antimicrobial studies of the Schiff base and its complexes indicated that the complexes showed more antimicrobial activity than its corresponding ligand. The Schiff base ligand glu-gln and their Cu(II), Ni(II) and Co(II) complexes were synthesized and characterized. All the complexes were found to be non-electrolytes which was confirmed by conductance study. Elemental analysis revealed the chemical composition of the synthesized compounds. The IR spectra confirmed the presence of various functional groups in the complexes and, in particular, the coordination of metals with the Schiff base ligand. The electronic spectrum of the Cu(II) complex showed two broad bands at 640 nm and 450 nm attributed to $^2E_g \rightarrow ^2T_{2g}$ and charge transfer transitions. It suggested the distorted octahedral geometry for the complex and was further supported by the magnetic moment value of 1.81 BM. In the electronic spectrum of Ni(II) complex, three bands at 380 nm, 620 nm and 930 nm were observed and assigned to $^3A_{2g} \rightarrow ^3T_{1g}(P)$, $^3A_{2g} \rightarrow ^3T_{1g}(F)$ and $^3A_{2g} \rightarrow ^3T_{2g}$ transitions respectively suggesting the octahedral environment for Ni$^{2+}$ ion and was further confirmed by the magnetic moment value of 3.20 BM. The Co(II) complex exhibited bands in the region 830 nm and 510 nm that corresponded to $^4T_{1g}(F) \rightarrow ^4T_{2g} (F)$ and $^4T_{1g} (F) \rightarrow ^4T_{1g} (P)$ transitions.

It suggested the possibility of octahedral geometry and was further confirmed by the magnetic moment value of 5.1 BM. The $^1$H-NMR study further confirmed the formation of the
complexes and its structure. Powder XRD study confirmed the microcrystalline nature of the complexes. TG/DTA study revealed the decomposition of the complexes at various stages. It confirmed the coordination of two water molecules to the metal ion that led to the formation of octahedral structure and the final residue obtained was the corresponding metal oxide. The study on antimicrobial activity of the synthesized Schiff base and its complexes revealed that the complexes showed higher activity towards the microbial species than its corresponding ligand.

The present investigation confirmed the octahedral geometry for all the synthesized complexes. These studies also showed that the oxygen and nitrogen donor atoms present in the complexes are involved in coordination. The Schiff base complexes showed good antimicrobial activities and so they can be suggested to use as antimicrobial agents against various bacteria and fungi.

In the present study only a few complexes were synthesized by the complexation of the glutraldehyde-amino acid Schiff base ligands with the metal ions such as Cu(II), Ni(II) and Co(II) and characterized using various spectral and physiochemical techniques. In future, attempts can be made to synthesize and characterize complexes with various other transition metal ions. Attempts can be made to investigate the catalytic, biological, anti cancer and anti tumour activity of the synthesized complexes.