

CHAPTER 4

CONCLUSION

The study of the complex formation of copper(II) acetate with selected pyrimidine based ligands derived from the condensation reaction between 2-chloropyrimidine with selected amine series was carried out. The compounds were found to have fluorescence characteristics. A total of ten compounds comprised of six ligands and four copper complexes were successfully synthesized. It was shown that the pyrimidine based ligand could behave as a monodentate ligand and form a binuclear complex.

The x-ray structural study has been carried out for selected ligands and all copper complexes; tetra- μ -acetato- $\kappa^8 O:O'$ -bis{[*N*-ethylpyrimidin-2-amine]copper(II)}(**CuL1**), tetra- μ -acetato- $\kappa^8 O:O'$ -bis{[*N*-(pyrimidin-2-yl)aniline- κN]copper(II)}(**CuL2**), tetra- μ -acetato- $\kappa^8 O:O'$ -bis{[*N*-(pyrimidin-2-yl)4-methylaniline- κN]copper(II)}(**CuL3**) and tetra- μ -acetato- $\kappa^8 O:O'$ -bis{[*N*-(pyrimidin-2-yl)3-methylaniline- κN]copper(II)}(**CuL4**).

The coordination of the metal atoms is distorted octahedral, with the bonding O atoms comprising a square basal plane and is completed by an N atom derived from the ligand and the second Cu atom. Intramolecular N-H...O hydrogen bonding is present between the imino and carboxy groups in all complexes. Each of the ligand molecules (**L1 – L4**) acts in a monodentate manner coordinating through the pyrimidyl nitrogen and is a binuclear complex. In the crystal structure of all complexes, the four acetate groups each bridge a pair of Cu(II) atoms.

Fluorescence characteristics of compounds studied showed that the nature of the substituents played an important role. The presence of an electron donating group in the pyrimidine ring system enhanced the mobility of electrons in the systems, thus high fluorescence intensity was observed.

The effect of solvents on the fluorescence characteristics of pyrimidine derivatives showed that a change in the nature of the emission can occur with the change of solvents. DMSO is a polar aprotic solvent with higher dielectric constant compared to methanol, which is a polar protic solvent with lower dielectric constant value and thus increasing the fluorescence intensity.

Quenching by oxygen and metal ion in the fluorescence intensity was observed. The study shows that the fluorescence intensity of capped samples is higher than the uncapped samples. On prolonged exposure of the solution to the atmosphere, may result in large quantity of oxygen diffusing into solution, thus lower fluorescence intensity observed. The same phenomenon was observed in the presence of metal ion. The study shows that all complexes showed a decrease in fluorescence intensity compared to its ligands, except for tetra- μ -acetato- $\kappa^8 O:O'$ -bis{[*N*-(pyrimidin-2-yl)aniline- κN] copper(II)} (**CuL2**). The increase in fluorescence intensity can be explained by metal to ligand charge transfer when ligand complexes with the metal.