Name of the Scholar: Abdul Kareem
Name of Supervisor: Prof. Nahid Nishat
Name of the Department: Chemistry
Ph.D. thesis title: "Synthesis and characterization of ligand systems containing N, O and S donors, their metal complexes & biological studies"

Abstract

The primary objectives of the present research were: (I) To design and synthesis of various biologically active compounds (Schiff base ligands and dithiocarbamates) such as curcumin, nicotinamide, ninhydrin, oxalyldihydrazide etc. (II) To obtain biologically active, stable transition metal complexes starting from synthesized ligands and (III) To study the structure and property in terms of solubility, nature, crystallinity, morphology, thermal stability, structure and biological and catalytic activities of the newly synthesized metal complexes.

Five different hetroatomic ligands and complexes were synthesized starting fromcommercially available raw materials in several steps. All the synthesized ligands, metal complexes were confirmed by different analytical techniques. All the complexes are stable up to 600°C showing good thermal stability. Slight shifting of chemical shift values in ^{1}H NMR and ^{13}C NMR spectral graphs indicates formation of metal complexes. From the FT-IR spectra the confirmations of groups involve in the formation of metal complexes were achieved and the additional peaks for metal coordination with heteroatoms such as nitrogen, oxygen and sulfur, further stems the formation of metal complexes. Wide angle X-ray diffraction analysis and SEM images disclose that all the newly synthesized metal complexes crystallinity and surface morphology and the results revealed that the morphology change after complexation in all the cases. Using Brags equation, calculation of structural geometry determination was carried out and crystalline size were also calculated. All the newly synthesized compounds were screened for their catalytic and biological activity. From obtained data, it could be concluded that, these metal complexes may

serve as a candidates for the treatment of diseases caused by various gram positive and gram negative bacterial strains, the result of last chapter the antimicrobial activity is most promising in the case of Zn(II) complex.

The present work on synthesis of new ligands starting from commercially available raw materials have expanded the range of heterocyclic ligands available for preparation of a host of biologically significant transition metal complexes. Transition metal complexes have a pronounced structural variety and have far more diverse stereochemistry than organic compounds and by rational ligand design, provide control over key kinetic properties. Furthermore, they are kinetically stable, usually uncharged and relatively lipophilic and their metal atom is in a low oxidation state. Different types of ligand systems which contain N, O or S donor atoms were synthesized in the present work could easily be used to synthesize such type of complexes which by themselves represent valuable compounds in pharmacological field of chemistry. Synthetic coordination complexes or coordination polymers are materials which exhibit a large range of interesting electronicandoptical properties, including electronic conductivityelectrochromism and electroluminescence. Many efforts have been devoted towards synthesizing new coordination complexes in an effort to enhance their applicability, optimize the desirable properties and explore new properties. In particular, attaching metal group’s results in hybrid materials, where the properties of both metal complex and polymer may be coupled. In the past two to three decades a number of monomer-containing ligands have been introduced for the formation of metal complexes with many of the benefits of monomers retained. It would be interesting to design and prepare a novel series of curcuminic dithiocarbamates and biologically significant molecules based monomers for synthesis of metal complexes.