

## **ABSTRACT**

Design and synthesis of transition metal complexes with polydentate ligands and commercially available ligands is a significant field of research in Chemistry. Coordination compounds in coupling between transition metals and various ligands have drawn a great deal of interest to Chemist and Biologists for their remarkable structural features, biomimicking activities, catalytic activities, optoelectronic applications, magnetic materials, semiconductors, functional composites and different biological activities. Noteworthy, metal complexes that are the synthetic analogs of various metalloenzymes create significant progress in bioinspired chemistry with fascinating mechanistic perception of the catalytic cycles.

**Chapter I:** This introductory chapter describes the design, synthesis and application of transition metal complexes based on Schiff base and commercially available ligands. It also states the catalytic and biological activities of metal complexes and the objectives of the present work.

**Chapter II:** This chapter consists of the synthesis, catecholase, and phosphatase activity of an oxido-and acetate-bridged tetranuclear iron (III) cluster  $[\text{Fe}_4^{\text{III}}(\mu\text{-O})_2(\mu\text{-OAc})_6(\text{phen})_2(\text{H}_2\text{O})_2](\text{NO}_3)_2(\text{H}_2\text{O})_3$  (**1**), [OAc = acetate; phen = 1,10-phenanthroline. X-ray structural analysis of the compound reveals that all the Fe(III) centres in **1** adopt an octahedral coordination geometry and the tetra-iron(III) core exists in an unusual asymmetric conformation. The bond valence sum (BVS) calculation recommends the existence of all iron ions in the +3 oxidation level in the crystalline state. The tetra-iron(III) cluster elegantly catalyzes the oxidation of 3,5-di-*tert*-butylcatechol (DTBC) viz. Catecholase-like activity with a good turnover number,  $k_{\text{cat}} 9.28 \times 10^2 \text{ h}^{-1}$  in acetonitrile medium. Spectrophotometric titration exhibits two distinct isobestic points, which unanimously proves the rarely observed enzyme-substrate binding phenomenon in solution. Electrochemical analysis recommends the production of Fe(II)-semiquinone species in the catalytic oxidation of DTBC. Furthermore, the same iron(III) cluster displays phosphoester cleavage activity towards disodium salt of p-nitrophenylphosphate (PNPP) in an aqueous-methanol medium with a rate of  $7.20 \times 10^{-4} \text{ m}^{-1}$ . ESI-MS measurements of tetra-iron(III) complex in the presence of PNPP recommend the formation of organophosphorous intermediate in solution and solvent aqua molecules probably make a nucleophilic attack to phosphorous centre favouring the generation of organophosphorous intermediate.

**Chapter III:** This chapter demonstrates the synthesis, structural characterization and transesterification activity of a mononuclear zinc(II) complex, [Zn(HL)(H<sub>2</sub>O)]. (H<sub>2</sub>O) (**1**) containing a previously reported Schiff base ligand, H<sub>3</sub>L = *N,N'*-bis(salicylidene)-1,3-diamino-2-propanol]. X-ray structural analysis of **2** reveals that Zn(II)-Schiff base complex crystallizes in hexagonal crystal system with *P6<sub>1</sub>* space group and adopts a distorted tetrapyramidal geometry. Self-assembled molecular units of **2** exhibit a beautiful construction of 3D crystalline architecture through intermolecular hydrogen bond wire. The zinc (II) complex enhances fluorescence intensity compared to HL in a methanol medium. Catalytic behaviour of **2** towards disodium salt of 2,4-dinitrophenylphosphate (PNPP) in aqueous-methanol medium exhibits good transesterification activity with an initial rate constant value of  $1.73 \times 10^{-4} \text{ min}^{-1}$ . Detailed DFT calculations are also employed to cope with the geometrical parameters of **2** and explore the proposed catalytic mechanism of transesterification activity.

**Chapter IV:** This chapter comprises the synthesis, supramolecular architecture and fluorescence properties of a mixed ligand 1D Pb (II) coordination polymer(3). In this work, we prepared a 1D lead(II) coordination polymer consisting of phenanthroline, acetate, nitrate ion and water as ancillary ligands. The physicochemical and structural properties of this Pb(II) compound have been studied through different analytical techniques. Computational modelling on X-ray structure displays a very close structural relationship and strongly recommends forming a 1D octahedral Pb (II) structure in the solid state.

**Chapter V:** In the end, the future scope of the research work has been given in this chapter.