

“New transition metal complexes with N, O-donor ligands and their properties”

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The Thesis consists of six chapters which are summarized as follows:

Chapter 1 gives a concise introduction on coordination chemistry followed by brief and recent literature survey on (a) Schiff bases derived from 2-Hydroxy-1-naphthaldehyde, Salicylaldehyde, 4-Methyl-2,6-diformylphenol, (b) Schiff base transition metal complexes, (c) Applications of Schiff base metal complexes in various fields of research. A brief overview of the present work is also highlighted.

Chapter 2 describes a Cu(II)-Based Metal-Organic Framework whose response has been explored towards toxic pesticides by density functional theory (DFT) analysis.

Chapter 3 represents synthesis and characterization of a mononuclear nickel(II) complex with N,O-donor ligand, which can play a significant role in DNA/HSA protein binding and exhibits selective cytotoxicity towards cancer cell.

Chapter 4 deals with synthesis and characterization of two dinuclear copper(II) complexes with partially hydrolyzed DFP based ligands. Both of these complexes have been used as effective catalysts for the oxidation of some benzyl alcohols in the presence of tert-butyl hydroperoxide (TBHP) as the oxidant.

Chapter 5 presents synthesis and characterization of three mononuclear nickel(II) complexes which act as the electrocatalyst for hydrogen evolution reaction (HER) using acetic acid (AA) and trifluoroacetic acid (TFA) as the proton source in DMF. Some theoretical calculations have also been performed with insight in hydrogen evolution mechanism and effect of chain lengths of the ligands on the catalytic activity.

Chapter 6 deals with electrocatalytic proton reduction reaction (or HER) by two neutral, monomeric transition metal complexes, where Ni(II) and Cu(II) have been chosen as the metal centres. Both of them have been synthesized by conventional method and characterized by several standard methods. The effect of change of metal centre on the generation of hydrogen evolution reaction has been examined.

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