

## Abstract

Synthesis of bimetallic model compounds and thereby stabilization of coordination aggregates of *3d* metals are of particular interest because of their catalytic applications in organic transformation, bio-mimicking functional abilities to that of natural metalloproteins and enzymes, and as magnetic materials. Both terminal mono-metal centric and or central phenol based binucleating Schiff bases with various rigid, semi-rigid and flexible chelating arms play pivotal role for the synthesis of newer multimetallic architectures through self-assembly. Organic ligands with specific metal binding pockets can selectively chelate the bioactive and hazardous metal ions and therefore their quantification and selective detection through fluorescence spectroscopic technique is another important application. In the present thesis, we have explored the coordination potential of terminal phenol bearing ONO, *bis*-bidentate NO, *bis*-tridentate O<sub>2</sub>N and central phenol based *bis*-ONO and NNO towards V<sup>IV</sup>, Co<sup>II</sup>, Ni<sup>II</sup>, Cu<sup>II</sup> and Zn<sup>II</sup> ions. By changing reaction conditions and solvent of crystallization, several solution based synthetic strategies have been employed to explore the generation and isolation of simplest mononuclear to dodecanuclear *3d* metal complexes. To the use of primary chelating ligands and externally added anionic bridging units (e.g., O<sup>2-</sup>, HO<sup>-</sup>, MeO<sup>-</sup>, OCN<sup>-</sup>, SCN<sup>-</sup>, N<sub>3</sub><sup>-</sup>, RCO<sub>2</sub><sup>-</sup>), predetermined and serendipitous metal complexes of varying nuclearity have been structurally characterized. Mechanochemical grinding of multi-components is applied in solid state ligand exchange and core conversion. Torsional angle mediated weak ferromagnetic and phenoxido/methoxido bridging angle dependent antiferromagnetic exchange interactions with theoretical support based on DFT calculations of a new family of diazine ligand bound complexes have been explored. Anion coordination induced photophysical properties have been explained with TD-DFT calculations for zinc based fluorescence chemosensor. Development of paramagnetic metal ion chemosensor and stabilization of novel 1D zig-zag chain is uncommon and interesting observation. Several cobalt, copper and zinc based bimetallic synthetic model compounds have been structurally characterized and some of these duplicate the catalytic function of the catechol oxidase.

**Keywords:** Multinuclear aggregate; Ancillary bridge; Schiff base; Self-assembly; X-ray structure; Chemosensor; Anion recognition; Magnetism; TD-DFT analysis; Catechol oxidation.