ABSTRACT

The present research work is aimed at synthesis of newer multidentate Schiff base ligands and to devise appropriate synthetic strategy to access mononuclear and binuclear VO(IV) and Fe(III) complexes. Spectral characterization and investigation of magnetic, mesogenic, electrochemical, thermal and antimicrobial properties of synthesized compounds is the focal theme of the work undertaken for the present Ph.D. thesis. The structure optimization of few selected compounds by DFT method (Gaussian 03) is also carried out the in present research programme. The content of the thesis is distributed over six chapters followed by conclusions, references, figures and graphs. Each chapter is virtually complete in itself including references.

The Chapter 1 portrays an introductory overview highlighting the significance and explaining the motive of undertaking the present work.

Chapter 2 deals with review of literature. The current status vis-a-vis the historical developments in the field of metal-Schiff base complexes with special reference to iron(III) and vanadyl(IV) complexes have been highlighted in this chapter.

Chapter 3 presents a description of experimental methods, chemicals and materials, and details of equipment used for physical measurements.

Chapter 4 describes the synthetic route to various types of Schiff bases. An account of synthesis various types of Schiff base ligands with different denticity (di, tri and tetra) are included in this chapter. The strategy to functionalise the ligand with long alkoxy chain to create mesogenicity has been demonstrated in select cases. The ligands possessing N / O donor coordinating sites were primarily accessed from the condensation of salicyldehyes, diketones, benzoin, furfuraldehyde with different types of amines.
Chapter 5 describes the complexation of the Schiff base ligands with iron(III) and oxovanadium(IV). Different strategies adopted to devise synthesis of mono- and dinuclear compounds have been reported herein. Ligand exchange reactions with loosely coordinated solvent molecules to access newer mixed-ligand Schiff base complexes have been dealt with in this chapter. The complexes accessed are of the types [Fe(L)₂(NO₃)₂]NO₃ and [VO(L)₂]SO₄.H₂O (L=N, N donor bidentate Schiff bases obtained from condensation of benzil with p-anisidine or p-toludine); [FeLCl]₂ and [VOL]₂ (L=O, N, O donor tridentate Schiff bases obtained from condensation of 4-n-alkoxy salicylaldehyde with 2-aminophenol); [Fe(L)Cl]₂, [Fe(L)ClX], [Fe(L)(H₂O)]₂ and [VOL]₂·H₂O, Na[VO₂L] (L=O, N, O donor tridentate Schiff bases obtained from condensation of acetylacetone with 2-aminophenol and X=Im or PPh₃); [Fe(L)Cl] and [VO(L)(H₂O)].H₂O (L=O, N, O donor tridentate Schiff bases obtained from condensation of acetylacetone with 2-aminobenzoic acid); [FeL(acac)(EtOH)] (L=O, N, O donor tridentate Schiff bases obtained from condensation of 2-hydroxy-1-napthaldehyde with 2-aminophenol or 2-aminobenzoic acid); [Fe(L)(H₂O)]₂[NO₃, [Fe(L)(H₂O)(NO₃)], [Fe(L)₉(H₂O)]₂, A[Fe(L)₉X₃] (A=NH₄, X=F, NCS; A=Na, X=N₃), [Fe(L)X₂]NO₃ (X=Im or Py) and [VO(L)].H₂O (L=N₂O₂ donor tetradentate Schiff bases obtained from condensation of acetylacetone, 2-hydroxy-1-napthaldehyde and benzoin with ethylenediamine or ortho-phenylenediamine); [FeLCl₂]Cl and [VOL]SO₄.H₂O (L=tetraimine macrocyclic Schiff bases obtained from condensation of benzil with ethylenediamine or ortho-phenylenediamine); [Fe(L)(H₂O)]₂[NO₃]₃ and [VOL]SO₄.H₂O (L=N₂O₂ donor neutral tetradentate Schiff bases obtained from condensation of furfuraldehyde with hydrazine).

Chapter 6 of the thesis deals with results and discussion pertaining to the work. Herein, is described the characterization of the synthesized compounds using elemental
analysis, IR, UV-VIS, NMR and Mass spectroscopy. Single crystal XRD analysis of one of the ligands is also discussed in this chapter. Besides structural characterization, the mesogenic, electrochemical, thermal and magnetic behaviour of the compounds is described in this chapter. A description of the results of antimicrobial activity of some select compounds towards some microbial strains is included herein. Structure optimization and computation of geometrical parameters by DFT using GAUSSIAN 03 package is also incorporated in this chapter.

Conclusions provided at the end highlight the salient findings of the research work.

Part of the work described in the thesis has been published or under communication (as detailed below) with the rest being processed for publication.

Published / Accepted


**Communicated**

