

Table of Contents

Content	Pages
Acknowledgement	i-v
Abbreviations	vi-viii
Table caption	ix-x
Figure caption	xi-xix
Abstract	xx-xxiii
Chapter 1: Introduction	1-19
1.1 General	
1.2 Molecular properties	
1.2.1 Magnetic properties	
1.2.2 Interactions with serum albumins	
1.2.3 Interaction with DNA	
1.3 Scope	
Chapter 2: Structural and Magnetic Characterization of three Tetranuclear Cu(II) complexes with Face-sharing-dicubane / Double-open-cubane like core Framework	20-48
2.1 Introduction	
2.2 Experimental	
2.2.1 Materials and methods	
2.2.2 Synthesis of ligands	
2.2.3 Synthesis of complexes	
2.2.4 Crystallographic data collection and refinement	
2.3 Results and discussion	
2.3.1 Synthetic aspects	
2.3.2 Crystal structure description	
2.3.3 Electronic absorption spectra of complexes	
2.3.4 Magnetic properties of complexes	
2.4 Conclusion	

Chapter 3: Synthesis, crystal structure and DNA/protein binding of **49-81**
Tetranuclear Cu(II) complexes with Double-open-cubane like core Framework

3.1 Introduction

3.2 Experimental

3.2.1 Materials

3.2.2 Physical measurements

3.2.3 X-ray crystallography

3.2.4 Synthesis of ligand and the complexes

3.2.5 Albumin binding studies

3.2.6 DNA binding studies

3.3 Results and discussion

3.3.1 Synthetic aspect

3.3.2 Crystal structures

3.3.3 Electronic absorption and fluorescence spectra of complexes

3.3.4 ESI mass spectroscopy

3.3.5 Protein binding studies

3.3.6 Interaction with Calf-Thymus DNA

3.3.7 Redox properties of the complexes

3.4 Conclusion

Chapter 4: Schiff base coordinated two tetranuclear Cu(II) complexes with **82-120**
double-open-cubane like core framework: DNA/protein binding and molecular
docking

4.1 Introduction

4.2 Experimental

4.2.1 Materials and physical measurements

4.2.2 X-ray crystallography

4.2.3 Synthesis of ligand

4.2.4 Synthesis of complexes

- 4.2.5 Albumin binding studies
- 4.2.6 DNA binding studies
- 4.2.7 Molecular docking
- 4.3 Results and discussion
 - 4.3.1 Synthetic aspect
 - 4.3.2 Crystal structure description
 - 4.3.3 IR, electronic absorption and fluorescence spectra of complexes
 - 4.3.4 Protein binding studies
 - 4.3.5 Interaction with Calf-Thymus DNA
 - 4.3.6 Molecular docking
- 4.4 Conclusion

Chapter 5: DNA / protein binding and magnetic properties of a 1D Cu(II) 121-155
complexes containing fumarate/terephthalate and Schiff base ligands

- 5.1 Introduction
- 5.2 Experimental
 - 5.2.1 Materials and physical measurements
 - 5.2.2 Synthesis of ligands
 - 5.2.3 Crystallographic data collection and refinement
 - 5.2.4 Albumin binding studies
 - 5.2.5 DNA binding studies
- 5.3 Results and discussion
 - 5.3.1 Synthetic aspects
 - 5.3.2 Molecular structure
 - 5.3.3 Electronic absorption and emission spectra of complexes
 - 5.3.4 Protein binding studies
 - 5.3.5 DNA binding studies
 - 5.3.6 Magnetic properties
- 5.4 Conclusion

Chapter 6: Tetranuclear copper(II) complexes with close and double-open cubane core: magnetic properties, DNA/protein binding and molecular docking **156-195**

6.1 Introduction

6.2 Experimental

6.2.1 Materials and measurements

6.2.2 Synthesis of the ligands

6.2.3 Synthesis of complexes

6.2.4 Crystallographic data collection and refinement

6.2.5 Protein binding studies

6.2.6 DNA binding studies

6.2.7 Molecular docking

6.3 Results and discussion

6.3.1 Synthesis aspects

6.3.2 Crystal structure description

6.3.3 Electronic absorption and emission spectra of complexes

6.3.4 Magnetic properties of complexes

6.3.5 Protein binding studies

6.3.6 Interaction with Calf-thymus DNA

6.3.7 Molecular docking

6.4 Conclusion

Conclusion **196-197**

Summary **198-200**

References **201-240**