

DESIGN, SYNTHESIS AND STRUCTURAL ASPECTS OF STERICALLY ENCUMBERED ALKYLTHIOETHERS AND THEIR POTENTIAL APPLICATIONS

By

N. PRABHU

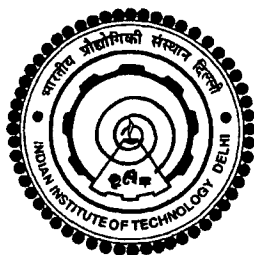
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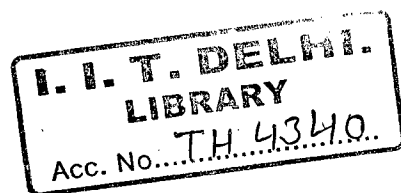
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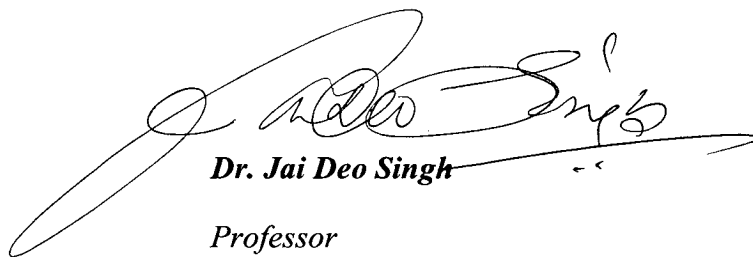


This Thesis has been Respectfully Dedicated
to
my Father Mr. J. Nallamuthu & my Mother Mrs.V.Thanapackiam
For their sacrifices to made my life meaningful

Certificate

This is to certify that the thesis entitled “Design, Synthesis and Structural Aspects of Sterically Encumbered Alkylthioethers and Their Potential Applications” being submitted by Mr. N.Prabhu, to the Indian Institute of Technology Delhi, for the award of degree of ‘Doctor of Philosophy’ in Chemistry is a bonafide research work carried out by him. Mr. N.Prabhu has worked under my guidance and supervision and has fulfilled the requirement for the submission of thesis, which to my knowledge has reached the requisite standard. The results contained in this thesis have not been submitted in part or in full, to any other University or Institute for award of any degree or diploma.

Date: Dec. 20, 2012



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ABSTRACT

The thesis entitled “**Design, Synthesis and Structural Aspects of Sterically Encumbered Alkylthioethers and Their Potential Applications**” deals with the design and synthesis of alkylorganosulfur compounds and their biological applications, coordination behaviour with different metal ions.

Chapter I provides a brief overview on organosulfur compounds in view of various significant results and applications of organosulfur compounds that have been realised in past several decades. This chapter also defines the aims and objectives of the present research work.

Chapter II describes the synthetic strategies and experimental details involved in the preparation of starting materials and a list of chemicals procured from various sources for the current study. It also describes various physicochemical studies used for characterization of newly synthesized compounds.

Chapter III deals with the synthesis of sterically hindered dipodal systems of the type 1,4-bis(alkylthiomethyl)-2,3,5,6-tetramethylbenzene. Interestingly, the silver containing organosulfur compounds were able to work as a potential antimicrobial agent for the dangerous multi drug resistant (MDR) bacteria gram negative *Pseudomonas aeruginosa*. The solution behaviour of these dipodals was studied in detail with various alkali, alkaline earth metal and transition metals through fluorescence studies. The complexation behaviour also studied and identified as these organosulfur molecules are selectively formed complexes with Ag^+ and Hg^{2+} only. The solution studies are revealing that the Ag^+ ions more interactive than other metal ions in solution state.

Chapter IV further elaborates the synthesis of sterically hindered alkyl based sulfur containing dipodal systems of the type 1,3- bis(alkylthiomethyl)-2,4,6-trimethylbenzene with a view to examine the change in design of the ligand and substituent effects on sulfur centre

that can reveal both, similarities and differences in the chemistry with respect to the alkyl dipodal system discussed in the previous chapter. This 1,3-substituted organo sulfur dipodals containing silver showed their potency towards the multi drug resistant (MDR) bacteria gram negative *Pseudomonas aeruginosa* as an antimicrobial agent. In solution studies it has been identified that these dipodals are differing in their reactivity towards the metal ions, which is emphasizing the design of the ligand, and steric factors regulate their interactive properties and results obtained herein have the more interactivity observed with Pb^{2+} metal ion.

Chapter V further describes the synthesis of sterically hindered 1,3,5-tris-(alkylthiomethyl)-2,4,6-trimethylbenzene tripodal systems containing 1,3,5-trimethylbenzene spacer. Interestingly, study about the change of alkyl groups in a tripodal system, which influencing the final structure of the desired molecular structure. The role of steric hindrance created by the alkyl groups around the sulfur atom in the organic tripodal molecule, leading to various structural organization with Ag(I) metal ion has been demonstrated.

Chapter VI further extends the synthesis of sterically encumbered 1,2,3,4,5,6-hexakis(alkylthiomethyl)benzene ‘hexapodal’ molecules in high purity and good yields, followed by their evaluation for host behavior with various metal ions. The limited coordination ability of the species under investigation towards Ag^+ or Hg^{2+} ions offers the possibility to use them as a cation recognition probes. The quantification of Hg^{2+} ion at nanomolar scale (nM) by sulfur derivative and a picomolar scale (pM) by analogous selenium derivative highly rewarding. These hexapodal system may be a leading example for the fluorescence chemical sensor without having any external fluorophores. Another significant application of these organosulfur molecules was identified as an antimicrobial agents for gram positive *Bacillus subtilis* bacterias.

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