

**DESIGN, SYNTHESIS AND STRUCTURAL ASPECTS OF
CHALCOGEN BEARING MULTIFUNCTIONAL ORGANIC
DONORS AND THEIR APPLICATIONS**

By

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Department of Chemistry

Submitted

In fulfillment of the requirements of the degree of Doctor of Philosophy

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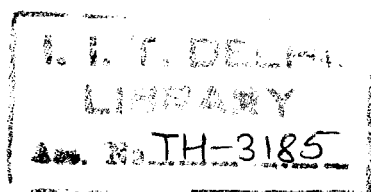


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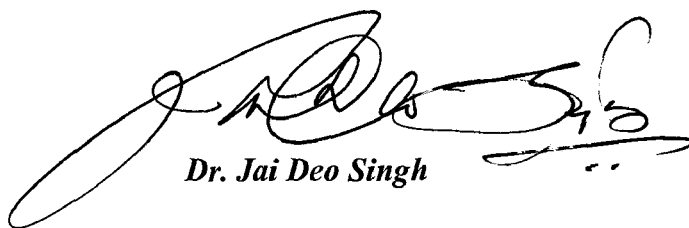


*Dedicated to my family,
whose unabated support and guidance has helped me
throughout...*

Certificate

This is to certify that the thesis entitled, 'Design, Synthesis and Structural Aspects of Chalcogen Bearing Multifunctional Organic Donors and Their Applications', being submitted by Mr. Naveen Kumar, 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. Naveen Kumar has worked under my guidance and supervision and has fulfilled the requirements 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: Feb. 11, 2005



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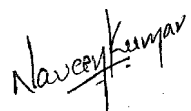
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-Naveen Kumar

ABSTRACT

The thesis entitled '**Design, Synthesis and Structural Aspects of Chalcogen Bearing Multifunctional Organic Donors and Their Applications**' deals with the design and synthesis of chalcogen bearing multifunctional organic species and their potential applications as specific donors or in assembly forming unit. The reactions of some species with d^8 and d^{10} have also been investigated with a view to understand the behavior of selenium in a multifunctional hybrid ligand framework.

Chapter I present a brief overview of recent developments in the field of organoselenium chemistry and describe applications of selenium species in various fields of chemistry including supramolecular chemistry, materials science, catalysis and biological chemistry.

Chapter II deals with the synthetic methodologies involved in the preparation of precursor compounds. It also describes various characterization techniques used in the present investigation.

Chapter III deals with the synthesis and characterization of organochalcogen species based on C_3 symmetric spacers. The chapter highlights a new and efficient method developed for the formation of carbon-heteroatom bond. Organochalcogen species based on C_3 spacers have been easily prepared using this method and structurally investigated for the presence of intermolecular chalcogen...chalcogen interactions. The effect of various intermolecular interactions including intermolecular chalcogen...chalcogen interactions has been described in this chapter. In the solid-state structure of tellurium species, $Te...Te$ intermolecular short contacts have been observed which can be held responsible for the unique crystal packing obtained for these species.

Chapter IV deals with the design and synthesis of pyridine dicarboxamide based multifunctional organoselenium donors possessing N_3Se_2 type donor set. The use of pyridine dicarboxamide moiety as a structure-controlling unit has been successfully exemplified. The reactivity of these species towards some d^8 and d^{10} metal ions has been investigated. The palladium complex obtained for one of these species have been structurally characterized where the ligand exhibit a so-called '*Chair-like*' conformation. Weak interactions of a representative species with Zn^{2+} , Cd^{2+} and Ag^+ ions have been investigated using 1H NMR titrations.

Chapter V describes synthesis and characterization of phenol based 'End-Off' compartmental ligands bearing selenium donor atoms in the appended arms. These species provide N_2OSe_2 type potentially pentadentate donor set. The presence of phenolate oxygen also provides way for the formation of bimetallic complexes. A bimetallic complex of one representative species have been isolated and characterized.

Chapter VI deals with the design and synthesis of selenium bearing Hexa-Host molecules. A series of selenium hexa-host have been synthesized employing new synthetic methodology (Chapter III) in an efficient manner. The appended arms of these molecules orient in a more favorable *ababab* arrangement that is inherent to its rigid design. A representative compound has been structurally characterized using single crystal X-ray diffraction.

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