Design and Synthesis of Polynucleating Organochalcogen (Se/Te) Species and Their Structural and Functional Relationship

by

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polynucleating Organochalcogen

Dedicated to my Father whose moral support encouraged me throughout my research..........

Certificate

This is to certify that the thesis entitled, 'Design and Synthesis of Polynucleating Organochalcogen (Se/Te) Species and Their Structural and Functional Relationship', being submitted by ***Ms. Sarika Singh****, 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 her. Ms. Sarika Singh 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.*

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-Sarika Singh

ABSTRACT

The thesis entitled "***Design and Synthesis of Polynucleating Organochalcogen (Se/Te) Species and Their Structural and Functional Relationship***" embodied herein is the design, synthesis and structural aspects of polynucleating organochalcogen species. The presence of various non-bonded interactions due to chalcogen centers as well as chalcogen...heteroatoms, the research work presented herein is in the studies carried out towards the polynucleating organoselenium species. The passivity of the molecular species isolated herein towards various metal centers has been rationalized in terms of non-bonded interactions present within the molecular species. Their existence in both soild and solution states seems to be retainable. Whatsoever, the study elaborates towards the synthesis of polychalcogen centers that can be selective in nature.

Chapter I deals with the concise literature related to the organochalcogen compounds and their applications in various fields from organic synthesis, asymmetric organic synthesis, catalysis, supramolecular organization, co-ordination behavior, organic metals and superconductors and in biological sciences.

Chapter II comprises the known literature procedures used to synthesize precursors throughout the research work. Various physicochemical techniques are also mentioned that have been used in the analyses of the newly synthesized organochalcogen compounds.

Chapter III consists of design and synthesis of organochalcogen species substituted on central cyanuric core and 1,3,5-tribromobenzene. Here highly efficient synthetic procedure for carbon-heteroatom bond formation is described. The various non-bonded interactions present in the molecule gives the preorganized structure in the crystal

packing. The co-ordination behavior of representative species is also investigated towards Pd(II) and Pt(II) ions.

Chapter IV describes the design and synthesis of conformationally rigid polyseleno-substituted organic compounds in a noncatalytic manner. The structural information obtained for these compounds from the crystal structures shows that the Se...Se interactions may be valuable tools in the supramolecular chemistry.

Chapter V describes the reactivities of tetraselenosubstituted compounds synthesized in chapter **IV**. These molecules have shown passive behavior towards various metal ions under normal reaction conditions. The structure-property correlationship has been done to evaluate their reactivity. Sonochemical reactions were found helpful to activate the molecules as various interactions due to chalcogen and heteroatoms were responsible for their passivity. Formation of a helical structure in presence of Ag(I) ions was the major achievement and opens new pathways to understand the fundamentals and design-aspects for new organoselenium donors.

Chapter VI comprises the design and synthesis of polynuclear organochalcogen species with limited flexibility as compared to the rigid species synthesized in the chapters **III** and **IV**. As it has been seen by the molecular structures of these compounds that chalcogen....heteroatom interactions are responsible for the preorganized structures. These molecules are found to be unreactive towards various metal centers. Their reliability in the solution is equally measurable and one can explain the reactivities only after analyzing solid and solution state behaviors of these molecules. Whatsoever, studies of given molecular systems are always essential before one could arrive at conclusions about reactivity and applications of polychalcogen centers.

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