DESIGN, SYNTHESIS AND STRUCTURAL ASPECTS OF STERICALLY ENCUMBERED ORGANOSELENIUM DERIVATIVES AND THEIR POTENTIAL APPLICATION AS CHEMICAL SENSORS

By

SHABANA KHAN

Department of Chemistry

Submitted

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to the

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Dedicated to my family and teachers,

Whose support and guidance has helped me

throughout...

Certificate

This is to certify that the thesis entitled, ***'Design, Synthesis and Structural aspects of sterically encumbered Organoselenium Derivatives and Their Potential Application as Chemical sensors',*** *being submitted by* ***Ms. Shabana Khan****, 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. Shabana Khan 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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Dr. Jai Deo Singh

Professor

Department of Chemistry

Indian Institute of Technology, Delhi

New Delhi-110016

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Shabana Khan

ABSTRACT

The thesis entitled '**Design, synthesis and structural aspects of sterically encumbered organoselenium derivatives and their potential application as chemical sensors**' deals with the design and synthesis of new polyfunctional organoselenium compounds and their potential applications as chemical sensor.

Chapter I presents a brief overview on recent developments in the field of organoselenium chemistry and describes applications of selenium species in various fields of chemistry including supramolecular, coordination chemistry, asymmetric synthesis, catalysis and biological chemistry.

Chapter II describes the synthetic strategies and experimental details involved in the preparation of starting materials. This chapter also contains the source of various chemicals used for this work and the physicochemical techniques for e.g. elemental analysis, spectral (IR, ^{1}H NMR, ^{13}C NMR, ^{77}Se NMR, ES-MS) and single crystal X-ray diffraction studies used throughout the investigation.

Chapter III deals with the design and synthesis of bi-, tri-, and tetra functionalized organoselenium species with the view to examine the new reactivity patterns associated with these molecules and could be compared to those known for structurally related O or S analogues.

Chapter IV describes the development of synthetic methodology and applications of sterically encumbered hexasubstituted selenium derivatives, which are based on 1, 3, 5 vs 2, 4, 6 conformational analogy. The synthesis of highly elusive hexa-substituted selenium derivatives has been ably demonstrated in a straightforward manner by the reaction of

RSe^- anion with hexakis(bromomethyl)benzene. Structural aspects of these hexa-host system were also established crystallographically.

Chapter V deals with the detailed reactivity pattern and applications of hexa-host compounds isolated in chapter V. The receptivity of Hg^{2+} and discrimination of other metal ions such as Cd^{2+}, Co^{2+}, Zn^{2+}, Pb^{2+}, Cr^{3+}, Ni^{2+}, Cu^{2+}, and Mn^{2+} was the prime achievement of present system. The exclusive recognition of Hg^{2+} in presence of first row transition and heavy metal ions and further fabrication of ion selective electrodes based on the ionophores for Hg^{2+} ions may have the technological significance.

CHAPTER VI presents the synthesis of sterically encumbering and pressurized selenium containing aza[3]calixarenes and their application towards sensing UO_2^{2+} ions. A reliable synthetic methodology for the synthesis of these molecular species in high yield under non-catalytic conditions has been developed. Fabrication of ion selective electrodes based on ionophores for UO_2^{2+} ions may have technological relevance.

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