CHAPTER 8

CHEMISTRY

Doctoral Theses

01. BHARTI KAPIL
Some Aspects of Analytical Coulomb Integrals Using Green`S Function and Neumann Expansions for Mesoscopic Materials Over 2d and 3d H-Like Basis Sets.
Supervisor: Dr. Ram Kuntal Hazra
Th 27398

Abstract

This thesis presents a modest and alternate analytical theory to investigate the Coulomb interactions for multi-electron systems in atomic, molecular, and mesoscopic scales within the domain of non-relativistic quantum mechanics. The formalism encompasses the theoretical treatment of 2D and 3D He-isoelectronic ions with the Perturbation treatment upto third-order corrections for free electrostatic Green's function expansion of Coulomb interaction comprising monopole and dipole factors. Multiconfiguration variational calculation has been incurred for 3D He-isoelectronic ions and Period-II elements utilizing Slater Determinantal wavefunction, thereby implementing the Pauli exclusion principle for upto 10 electrons. The exploration of molecular Coulomb and Exchange integrals for hydrogen molecules using Green`s function and Neumann expansions is also included in the theoretical development. The utilization of associated Laguerre polynomial/Whittaker-M function basis sets of H-like orbitals furnishes analytical, terminable, simple and finitely summed integrals. The ground state energies of 2D and 3D He-isoelectronic ions show remarkable agreement with the reported results. Invoking the formalism for 2D and 3D He-isoelectronic ions, the binding energies and current density of trions in transition metal dichalcogenides (TMDCs) have been studied showing a striking resemblance with the literature available. The ground state energy obtained from our formalism for the hydrogen molecule exactly matches with the experimental results.

Contents

02. CHAUDHARY (Vishakha)

Design and Development of Molecular Probes for Different Imaging Techniques.

Supervisors: Dr. Rupesh Kumar and Dr. Shubhra Chaturvedi

Th 27390

Abstract

Synopsis of thesis entitled "Design and Development of Molecular Probes for Different Imaging Techniques" aimed to develop target-specific molecular imaging probes for neuroimaging and tumor imaging. Chapter I introduces molecular imaging, molecular imaging probes, Molecular imaging techniques (SPECT imaging, PET imaging, and MRI) and their applications. Chapter II includes the synthesis of molecular probes, characterization and bio-evaluation by different techniques and assays. Chapter III is the Homology modelling of Sigma-2 receptor protein, molecular docking and MD simulation studies. Chapter IV Synthesis, characterization, and bio evaluation of novel radiotracer 99mTc-THQ-DTPA for SPECT imaging of triple-negative breast tumor. Chapter V Synthesis, characterization and bio-evaluation of a novel radio-tracer 99mTc-FCM-DTC targeting 5-HT1A receptor.

Contents

03. DHIMAN (Diksha)

Conformational and Colloidal Stability of Therapeutic-Proteins in the Presence of Choline-Based Designer Solvents.

Supervisor: Prof. P. Venkatesu

Th 27391

Abstract

The conformational and colloidal stability of therapeutic proteins is of paramount importance in the development and production of biopharmaceuticals. Choline-based designer solvents have gained prominence as innovative additives for various bioprocessing applications. This study investigates the impact of choline-based designer solvents on the conformational and colloidal stability of therapeutic proteins. We employ a combination of biophysical techniques, including circular dichroism spectroscopy, dynamic light scattering, and fluorescence spectroscopy, to assess protein structural changes and aggregation behavior in the presence of these solvents. Our findings reveal that the influence of choline-based designer solvents on protein stability is highly dependent on the specific solvent composition and protein characteristics. Understanding the

interaction between therapeutic proteins and these solvents is crucial for optimizing bioprocesses and ensuring the quality and efficacy of biopharmaceutical products.

Contents

04. GHATAK (Trisha)

Synthesis of Multifunctional Furans, Pyrazoles, Benzo[*h*]chromen-2-ones and Chromen-4-ones from Ketene Dithioacetals.

Supervisors: Prof. Mahendra Nath and Prof. Ramendra Pratap

Th 27392

Abstract

Ketenedithioacetals are well known building blocks of many carbocyclic and heterocyclic compounds. Its structural feature allows it to undergo Michael addition with diverse nucleophiles as the olefinic linkage is activated by electron-releasing alkylthio groups (p–π conjugation). In the present thesis, we have put forward how ketene dithioacetals can be utilized to deliver differently functionalized heterocycles. The first chapter discusses how one can generate benzocoumarin by using a α -functionalized ketendithioacetal i.e. ethyl 2-cyano-3,3-bis(methylthio)acrylate. This stepwise approach requires the cyclization of tetralone derivatives with ethyl 2-cyano-3,3-bis(methylthio)acrylate, to give rise to 2-oxo-5,6-dihydro-2H-benzo[h]chromenes . This further undergo aromatization in presence of NBS and AIBN in DCE, which leads to formation of benzocoumarin. Thus a step wise synthetic route can be explored for the generation of benzocoumarin starting from 2- cyano-3,3-bis(methylthio)acrylate as synthon. Second chapter deals with the synthetic approach where simple ketene dithioacetal have been transformed into 3-methylthio-1,5-diaryl-2-penten-1,5-dione. These compounds undergoes simultaneous pyrazole formation and oxidation to furnish 1-aryl-2-(3-aryl)-1H-pyrazol-5-yl-ethane-1,2-diones. This reaction takes place in presence of hydrazine and iodine at 80oC in one pot following a cascade pathway. Beside that phenyl and methyl substituted pyrazolyl diones have also been obtained. Along with these, pyrazolyl diones undergo annulation with phenyl-1,2-diammine to give pyrazole functionalized quinoxalines also. The third chapter emphasises on the unexpected intramolecular cyclization of 3-methylthio-1,5-diaryl-2-penten-1,5-dione in presence of Iodine in DMSO at 80oC. A series of 2-acyl-3-methylthiofuran have been obtained in good yield. The thiomethyl group in resultant furan have been successfully oxidized to sulfonyl group, along with this, a gram scale reaction for the synthesis of 2-acyl-3-methylthiofuran has also been achieved which adds to the synthetic utilty of the reaction. Fourth chapter focuses on stepwise synthesis of 2-(2-oxo-2-

phenylethyl)-4H-chromen-4-one, starting from 2-hydroxy acetophenone. 2 hydroxy acetophenone after getting protected, gets converted into its ketene dithioacetal form, which is known to undergo iodine mediated cyclization to give 2-thiomethylated chromones. These thiomethylated chromones can undergo simple substitution reaction with various aryl ketones to give 2-(2-oxo-2-phenylethyl)-4H-chromen-4-one. All these chapter together emphasises on broadening the arena of ketene dithioacetal chemistry, its utility in producing newly functionalized heterocycles and further scopes.

Contents

05. JAVED

Exploration and Development of Advanced Nanomaterials and their Electrochemical Charge Storage Characteristics.

Supervisor: Prof. Sasanka Deka

Th 27394

Abstract

This thesis explores the frontier of nanomaterials, with a primary emphasis on their research, advancement, and use in supercapacitors (SC). The rising demand for efficient energy storage has led to the emergence of SC, which offer quick charging and durability. The investigation encompasses a detailed analysis of the most recent developments in transition metal boron alloy (TMBs) and transition metal selenides (TMSes) nanomaterial synthesis techniques, highlighting their tailored design to enhance electrochemical performance. The developed nanomaterials are synthesized, characterized, and evaluated using experimental methodologies to study their electrochemical properties. Advanced techniques like microscopy, spectroscopy, and electrochemical analysis enhance our knowledge of how structure affects charge storage mechanisms. Furthermore, this work presents the synthesis of a unique 2D Cu-Co-B ultrathin NSs amorphous alloy for SC use, which is made via a straightforward, one-pot chemical reduction process. Additionally, the clarified synthesis of an amorphous alloy with a nanostructure made of Ni, Cu, Co, and B. Extensive experimental evaluations have revealed the formation of oxidized surface layers, which are in charge of the material`s exceptional energy storage performance and strong electric conductivity in an aqueous 6.0 M KOH electrolyte. Additionally, discussed the synthesis of new SnxCo(1-x)Se2 NRs and to demonstrate the flexible SCs device`s real-world functionality by using electrode materials. Finally, describe the new, difficult, and multifaceted way for creating highly crystalline Ni-Cu-B alloy nanoworms using a hydrothermal treatment, as well as Fe2O3/C3N4 using a straightforward annealing technique. This includes a thorough investigation into its characterisation as well as a thorough evaluation of its electrochemical energy storage capabilities in hybrid SC. The results of this

thesis add to the expanding corpus of research on sophisticated nanomaterials for energy storage applications. The design and development of high-performance supercapacitors with improved energy density, power density, and overall efficiency are affected by the results.

Contents

1. Introducing Transition Metal Borons and Bimetallic Selenides for Electrochemical Energy Storage Applications 2. Methods of Syntheses, Sample Characterizations, and Electrochemical Analyses 3. Morphology Oriented 2D-Amorphous Cu-Co-B Nanosheets as an Electrode Material for All-Solid-State Flexible Supercapacitor 4. Surface Oxidized Amorphous NiCuCoB as a Promising Electrode Material for Supercapacitor 5. Development of Nanocrystalline Nickel-Copper- Boron Alloy as Cathode Materials for Hybrid Supercapacitor 6. Charge Storage Characteristics of Anion Exchanged Synthesized Sn-Co-Se Nanorods in Flexible Symmetric Supercapacitor. Summary, Future Scope, List of Publications and Conferences Attended.

06. LAMORIA (Monika)
Quinoxaline, Pyridopyrazine and Benzimidazole derivatives: Synthesis, photophysical, thermal and chemosensing studies for potential material applications.
Supervisor: Prof. Marilyn Daisy Milton
Th 27399

Abstract

The thesis focuses upon the design, synthesis and charaterization of novel quinoxaline, pyridopyrazine and benzimidazole derivatives. It also reports the photophysical studies performed in solution and solid state. Also, the thermal and chemosensing studies are embodied along with the potential material applications of these derivatives.

Contents

1. Introduction 2. Synthesis of AIE active pyridine functionalized quinoxaline and pyridopyrazine derivatives for reversible acidofluorochromic applications 3. Phloroglucinol based dendric amphiphiles: Synthesis and study of their potential as nanocarrier 3. Synthesis of Y-shaped AIEE active novel quinoxaline derivatives and their applications 4. Synthesis of AIEE active tripodal pyridopyrazine derivatives and their applications 5. Synthesis of pyrene substituted quinoxaline and pyridopyrazine-based push-pull molecules and their multi-stimuli responses 6. Oxazoline-appended benzimidazolium salts for selective micromolar detection of Fe3+ ions in pure aqueous media and DFT studies on Fe3+ ion sensing mechanism 7. Synthesis of thiazole and benzothiazole substituted benzimidazolium salts and their applications as chemosensors 8. Summary and Conclusions. List of publications.

07. PANKAJ KUMAR

Synthesis & Characterization of Silica Nanoparticles for Enzyme Activity Regulation, Drug Delivery and Phototherapeutic Applications.

Supervisor: Prof. Mahima Kaushik

Th 27401

Abstract

Nanotechnology is a rapidly emerging field, which deals with particles size ranging from 1-100 nm. Nanoparticles exhibit various properties based on their size, distribution and morphology. With decrease in size of nanoparticles, surface to volume ratio gets increased and thus, their biological effectiveness increases due to increase in surface energy. Additionally, the small size of nanoparticles allows them to cross biological barriers more easily, which can improve the delivery of drugs to their target sites. The interaction of DNA and proteins with nanoparticles holds great potential for drug delivery applications. Nanoparticles can serve as carriers or vehicles to efficiently transport DNA or proteins to specific target sites in the body and overcome barriers such as enzymatic degradation and poor cellular uptake. As a result, since the discovery of nanotechnology, an immense amount of work has been done by the researchers to exploit nanotechnology in almost each and every field possible. Among various nanoparticles, silica nanoparticles (SiNPs) are considered as most promising, due to their diverse fields of applications, as they are the basis of semiconductors, glasses, ceramics, plastics, elastomers, resins, mesoporous molecular sieves and catalysts, optical fibers, coatings, insulators, moisture shields, photoluminescent polymers, fillers, cosmetics and biomedical devices. In addition to this, SiNPs are extensively used in the biomedical field for developing biosensors, bioimaging agents, and drug delivery vehicles, etc. The reason for such wide range of applications is the availability of different synthesis methods, which provide flexibility in obtaining SiNPs having different morphology and size. SiNPs also possess additional advantages such as biocompatibility, biodegradability, and can also be easily excreted out of the body through urine, which makes them an excellent candidate for bioconjugation with biomolecules. Objectives: Synthesis of Silica nanoparticles using condensation reaction and characterizing them by employing physicochemical techniques. To study the interaction of silica nanoparticles with bovine trypsin for exploring their effect on the structural stability as well as enzymatic activity of trypsin. Synthesis and characterization of amiloride loaded citrate coated silica nanoparticles for exploring its carrier potential. Synthesis and characterization of thionine acetate loaded silica nanoparticles and analysing their cytotoxicity and potential for phototherapies. To study the photoinduced antibacterial activity (for E. coli & S. aureus) of toluidine blue loaded silica nanoparticles.

Contents

induced antimicrobial activity of toluidine blue loaded silica nanoparticles 7. Conclusion. Bibliography, List of Publications and Conferences.

08. RAHUL

Alkyne Functionalization for the Construction of Biologically Relevant Motifs.

Supervisors: Prof. Diwan S. Rawat and Prof. Mahendra Nath

Th 27402

Abstract

The tri/tetra-substituted propargylamine serve as a versatile synthon for many biologically active moieties. So, a sustainable solvent-free mild catalytic system encompassing ZnAl-MO NCs as catalyst was developed to synthesize tetrasubstituted propargylamines. ZnAl-MO NCs were proved to be simple, efficient, reusable, and easy-to-handle catalysts for the preparation of valuable tetrasubstituted propargylamines via KA2 coupling reaction. Nitrogen-containing heterocycles, like pyrrolidines and piperidines, are essential components of many naturally occurring compounds with a variety of biological activities. Keeping this in mind we developed a metal-free synthesis of 2-alkynyl pyrrolidines/piperidines by KA2 coupling reaction in the presence of green solvent diethylene glycol. The results showed that almost all the screened substrates underwent smooth KA2 coupling to afford the corresponding 2-alkynyl pyrrolidines/ piperidines in yield of 57% -87%. Z-Olefins are pivotal structural motifs found in several pharmaceutically active compounds and vicinal difunctionalization of alkyne is regarded as an efficient way for the construction of highly versatile Z-olefins. Also, the sulfone functionality is widely employed in organic chemistry and vinylsulfone containing molecules have been found to be widespread in biological research. So, we report an efficient and sustainable protocol for the facile synthesis of functionalized vinylsulfones via intermolecular multicomponent reaction of terminal alkynes, sodium sulfinates, and cyclic-1,3-diketones. The present synthetic strategy proceeds very smoothly at RT to provide (Z)-β-alkoxy vinylsulfone under air with 100 W blue Led without photocatalyst and external oxidant. Further, with our ongoing interest in difunctionalization of π -systems, we study the effect of difunctionalization of alkyne with sulfur nucleophile. During the course of our study, we have achieved metal-free stereoselective mercaptosulfonylation of alkyne with concurrent formation of two C-S bonds. The large size of S and electronic repulsion between the lone pairs of SO2 and S overcomes the π-π stacking phenomena and turns the geometry of the product to unexpected E-isomer.

Contents

approach to access (*E*)-*β*-mercaptovinylsulfones. Summary, List of Publications, Honors and Awards, Conferences and Symposium.

09. RESHMA KUMARI

Synthesis and Characterization of Novel PhenothiazineBased Multi-Stimuli-Responsive Functional Organic Molecules and their Applications.

Supervisor: Prof. Marilyn Daisy Milton

Th 27403

Abstract

The synthesis of novel functional organic compounds based on phenothiazine was accomplished using several chemical reactions, including the Suzuki coupling reaction, phase transfer Heck coupling reactions, aldol condensation, Claisen-Schmidt condensation, and Knoevenagel reactions. The synthesized molecules were thoroughly characterized using spectroscopic techniques such as nuclear magnetic resonance (NMR), high-resolution mass spectrometry (HRMS), and infrared (IR) spectroscopy. Some compounds were also analyzed by single-crystal X-ray diffraction. The behavior of the phenothiazine derivatives in response to a variety of stimuli such as solvent, acid vapors, amine vapors, pH, moisture, aggregation, etc. was thoroughly investigated. Further, these compounds were studied for solvatochromism, acidochromism, halochromism, amine sensing, moisture detection, aggregation-induced emission enhancement, anti-counterfeiting applications, dual-state emission, solid-state emission, etc. The highly efficient emission of the compounds, ranging from blue to red color, even in aggregated state, makes them promising candidates for OLED device fabrication and bioimaging applications. These non-doped phenothiazine derivatives exhibited optical band gaps within the semi-conducting range, which indicates their potential for use in the fabrication of optoelectronic devices. A comprehensive analysis was conducted using 1H NMR spectroscopy and PXRD to examine the mechanisms involved in reversible acidochromism and mechanofluorochromism, respectively. In order to improve the practical utility of these compounds, paper strips were fabricated for the purposes of moisture sensing, amine sensing, and reversible acidochromism. Owing to the high quantum yield of the solid compounds, the compounds were used as an anti-counterfeiting agent to encrypt the security information under ambient light, which can be decrypted only under the illumination of 365 nm light.

Contents

applications as pH sensor, reversible volatile acid/base sensors and molecular logic gates 5. Synthesis and characterization of dual state emitting phenothiazine-based benzothiazole derivatives and their applications as reversible acidochromism and self-reversible mechanofluorochromism 6A. Synthesis and characterization of novel red-emitting phenothiazineacrylonitrile derivatives and their applications 6B. Fine tuning of phenothiazine-based red-emitting molecules through benzothiazole and benzimidazole acceptors and their applications 7. Synthesis of AIEE-active blue emitting phenothiazine molecules 8. Summary and Conclusion. List of Publications.

10. SAINI (Keshav Kumar)
Design, Synthesis and Biological Evaluation of Novel Dihydropyrimidine, Melatonin and Dihydropyridine Scaffolds.
Supervisor: Prof. Rakesh Kumar
Th 27405

Abstract

Abstract of the thesis entitled: "Design, Synthesis and Biological Evaluation of Novel Dihydropyrimidine, Melatonin and Dihydropyridine Scaffolds". This thesis has four chapters: Chapter I, Chapter II, Chapter III, and Chapter IV. Chapter I This chapter provides a short overview of the most recent developments in the area of biological assessment of heterocyclic scaffolds such as dihydropyrimidine, isatin, 1,2,3-triazole, 2-aminobenzothiazole, melatonin and dihydropyridine derivatives. Chapter II Design and synthesis of isatin-linked dihydropyrimidine derivatives and assessment of their anti-breast cancer activity In this chapter, a group of 12 isatin derivatives based on heterocyclic dihyropyrimidine was designed and synthesized. The synthesised derivatives underwent evaluation to assess their impact on cell proliferation using the MTT cell viability assay on two breast cancer cell lines (MCF-7 and MDA-MB-231), as well as a non-cancerous breast cell line (human embryonic HEK293). Among these compounds, 7 exhibited exceptional potency and emerged as the most promising derivative, displaying IC50 values of 24 nM and 55 nM against the MDA-MB-231 and MCF-7 cell lines, respectively. Chapter III Design, synthesis, molecular docking and DFT studies of newer triazole based melatonin derivatives as promising anti-fungal agents Novel triazole-linked melatonin and isatin derivatives 7a-d and 8a-d were synthesised. Molecular docking studies were performed on synthesised compounds with Lanosterol 14 alpha-demethylases (LAD) of Candida albicans. Comparative analysis of the binding potential of the synthesised molecules and commercially available drugs fluconazole revealed a remarkable note: the docking scores for the designed drugs 7b, 7c, and 8c are much greater than those of the fluconazole molecule. Chapter IV Synthesis and molecular docking studies of triazole tethered 1,4-dihydropyridines as potential calcium channel antagonist 15 novel compounds were synthesised by molecular hybridization strategy with the aim of developing more potent single drug-multiple targets. Molecular docking was performed on all synthesised compounds.

Contents

1. Introduction 2. Design and synthesis of isatin-linked dihydropyrimidine derivatives and assessment of their anti-breast cancer activity 3. Design, synthesis, molecular docking and DFT studies of newer triazole-based melatonin derivatives as promising anti-fungal agents 4. Synthesis and molecular docking studies of triazole tethered 1,4-dihydropyridines as potential calcium channel antagonist. Summary and List of publications.

11. SINGH (Jay)
Morphological Effect on the Electrochemical Performances of Transition Metal Oxide Anodes for Lithium Ion Battery Application.
Supervisor: Dr. Alok Kumar Rai
Th 27395

Abstract

With the significant increase in nowadays demand of lithium-ion batteries (LIBs), the price of lithium has remarkably risen due to its limited worldwide resources. Additionally, the use of graphite as an anode material in LIBs, especially for electric vehicles, exhibits its own set of challenges as it provides a limited capacity of 372 mAh g-1 and poor fast-charging capability. To enhance battery performances, researchers have been trying hard to explore inexpensive yet efficient alternative anode materials. In this context, transition metal oxides (TMO's, such as MOx where M = nickel (Ni), copper (Cu), iron (Fe), and cobalt (Co) etc.) have garnered substantial attention as promising anode materials due to their compelling characteristics such as non-toxicity, high abundance in nature, high power density, large theoretical capacity, and cost-effective fabrication processes. In this thesis, we have discussed the effect of various morphologies on the electrochemical performances of binary (especially nanorods, nanotubes and nano-particles) and ternary TMO's (mulberry like and nanorods) for LIB application. The current research work is divided into seven chapters. Chapter 1 mainly starts with basic introduction of nanoscience and nanotechnology and their role in energy storage devices. Chapter 2 gives the detailed description of synthesis procedure, characterization techniques and electrochemical measurements. Chapter 3-5 provides the detailed discussion of electrochemical performances of binary TMO's (NiO, CuO and Fe2O3). Chapter 6 describes the synthesis and electrochemical performance of ternary TMO (CoMoO4). Chapter 7 focused on the heterovalent atom doping (Ti4+) on molybdenum site of CoMoO4 anode to achieve high Li storage performances.

Contents

1. Introduction 2. Synthesis procedure, characterization techniques and electrochemical measurements 3. 1D mesoporous NiO nanorods: A high-capacity and long-life anode material for lithium-ion batteries 4. Electrochemical investigation of the mesoporous hollow CuO nanotubes as anode material for lithium-ion batteries 5. Comparative analysis of nanoparticles and nanorods morphology of Fe2O3 anodes for lithium storage application 6. Mesoporous mulberry-like CoMoO4 anode: Fabrication and electrochemical evaluation for lithium-ion batteries 7. Improving the lithium storage performance of CoMoO4 anode by using novel Ti4+ doping. Summary, Future scope and List of publications.

12. DEEPIKA (Tanwar)

Design and Synthesis of Ni(II) and Pd(II) Complexes Bearing ONS/NNS Donor Ligands for their Anticancer and Catalytic Evaluations.

Supervisor: Dr. Umesh Kumar

Th 27406

Abstract

The first chapter of the thesis describes the general introduction and sets a juncture for the objectives of the present work. In chapter 2, we have synthesized and characterized a series of ONS donor ligands (L2.1-L2.6) and their Ni(II) metal complexes (2.1-2.6). Complexes 2.1-2.6 were screened for their anticancer potential and complexes 2.4 and 2.6 possess good anti-cancer potential against human pancreatic cancer MIA-PaCa-2 cells with IC50 values comparable to routinely used anticancer drugs cisplatin and gemcitabine. In chapter 3, we have synthesized and characterized a series of NNS donor ligands (L3.1-L3.4) and their Pd(II) metal complexes (3.1-3.4). The biocompatibility and cytotoxicity analysis of L3.1-L3.4 and palladium metal complexes 3.1-3.4 has been investigated for human pancreatic cancer MIA-PaCa-2 and breast cancer 4T1 cells. The obtained results indicate that at a concentration of 40 μg/mL, 3.1, 3.2, and 3.3 demonstrate 90, 89, and 87% cytotoxicity against breast cancer 4T1 cells, and 3.2 and 3.3 demonstrate 68 and 89% cytotoxicity against human pancreatic cancer MIA-PaCa-2 cells. In chapter 4, we have synthesized and characterized a Ni(II) complex (4.1) as a single source precursor to obtain NiS NPs that showed appreciable electrocatalytic OER activity. To further improve the electrocatalytic performance and durability, we also synthesized Ni-complex-CNT and NiS-CNT nanocomposite that show further enhanced OER performance. A comparison of the OER performance with that of IrO2 showed that Ni-complex-CNT and NiS-CNT showed better activity than IrO2. In chapter 5, the separate reactions of L3.1-L3.4 with NiCl2 in methanol at 80°C for 3 h resulted in corresponding nickel complexes 5.1-5.4, respectively. The utility of complexes 5.1-5.4 were also evaluated as a catalytic activator for the N-alkylation of aniline with benzyl alcohols. The obtained results indicate that complex 5.1 showed better catalytic activity in both the N-alkylation of amines with benzyl alcohols.

Contents

13. YADAV (Neetu)

Alternate Route of Making Technologically Important Solids: Few Selected Examples from Metal Oxides, Oxychlorides Along with their Applications.

Supervisor: Prof. Rajamani Nagarajan

Th 27873

Abstract

The synthesis of solid materials requires much chemical ingenuity, and this aspect of materials science is being increasingly reorganized as a vital component of the subject. While tailor-making materials of the desired structure and properties remain the primary goal of solid-state chemistry and materials science, it is not always possible. Researchers have been designing synthetic routes of making solids other than the traditional ceramic method better to control the structure, stoichiometry, and phase purity. With the advent of nanoscience and nanotechnology, chemical synthesis methods such as the precursor method, coprecipitation and soft-chemistry routes, the combustion method, the sol-gel method, topochemical methods, and high-pressure methods are in trend. This thesis is devoted to the search for an alternate method of making technologically important oxides and oxychlorides, along with demonstrating their useful functions. Crisp introduction to various methods available to generate solids, along with their advantages and disadvantages are covered in chapter 1. It also highlights some of the unsolved synthetic issues pertaining to making them in desired functions. Research work related to the synthesis and modification of tin oxides by a molecular precursor route and the designing of two different synthetic routes to make Zr-substituted In2O3 have been included in chapter 2. Chapter 3 contains the work related to stabilizing PrVO4 in zircon structural arrangement and the entire series of PrCr1-xVxO4. Chapter 4 details the research work carried out in Sillen-Aurivillius structured Bi2YO4Cl. The results include determining the extent of including isovalent (Fe3+) and aliovalent (Zr4+) ions in place of Y3+ in Bi2YO4Cl and their consequences. The concluding section summarizes this investigation`s overall outcomes. It also highlights how the current study can be used to address other long-standing issues in synthetic solid-state chemistry.

Contents