CHAPTER 17

CHEMISTRY

Doctoral Theses

01. ABHIJEET
Development of Synthetic Strategies for Novel Heterocycle-Appended Porphyrin Macrocycles.
Supervisor: Prof. Mahendra Nath
Th 28200

Abstract

Porphyrin macrocycles are tetrapyrrolic chromophores that play critical roles in diverse biological processes including oxygen transport in humans, and photosynthesis in plants. Recent investigations have demonstrated that extending π-conjugation through structural modifications on the porphyrin periphery significantly alters the electronic and redox properties of porphyrins. These periphery modified porphyrin demonstrated promising applications in various fields including photosensitizers in photodynamic therapy and solar cells, molecular sensing, and optoelectronic devices. By considering these facts, the present research focuses on developing convenient and efficient synthetic strategies for constructing novel heterocycle-appended porphyrins through peripheral functionalization of readily accessible meso-tetraarylporphyrins for the study of their photophysical characteristics. The work presented in the thesis is divided into four chapters. The first chapter describes the synthesis of β-isothiazole-fused porphyrins through the intramolecular cascade nitrogen-sulfur radical coupling reaction which involves the reaction of 2-benzoylamino-3-formyl-meso-tetraarylporphyrins with the Lawesson's reagent in refluxing toluene. The second chapter discusses about the new synthetic route to synthesize the β-pyrimidine-fused porphyrins. These compounds were prepared by an intramolecular condensation cyclisation reaction of 2-aroylamino-3-formyl-meso-tetrakis(4-chlorophenyl) porphyrins with ammonia under mild conditions. The third chapter deals with the La (OTf)3-catalysed synthesis of 3-(4-hydroxy-2-oxo-2H-chromen-3-yl)-5,10,15-triaryloxonaphthoporphyrins from 2-formyl-meso-tetraarylporphyrins. Lastly, the fourth chapter presents a new cascade three-component sequential one-pot synthesis of N-arylpyridone-fused porphyrins by reacting 4-hydroxycoumarin, anilines and 2-formyl-meso-tetraarylporphyrins in refluxing N,N-dimethylformamide. After chromatographic purification, the structures of synthesized compounds have been established based on spectral and single crystal X-ray analysis. On photophysical investigation, these new porphyrins have shown interesting optical properties with a modest to significant bathochromic shift in their electronic absorption and emission spectra as compared to the meso-tetraarylporphyrins. Therefore, the findings presented in this thesis provide valuable insights for the future design of diverse π-extended aromatic scaffolds, offering significant potential as efficient light-harvesting materials and as photosensitizers for photodynamic therapy applications.

Contents

02. ANAND PRAKASH

Designing of Porous Organic Nanoframeworks as Potential Candidates for Environmental Remediation and Antibacterial Activities.

Supervisor: Prof. Rakesh Kumar Sharma

Th 28671

Abstract

The rising life pressure, industrialization, and pollution in the environment lead to severe diseases in human beings and animals. There are no satisfactory treatment methods available to date. Traditional materials, such as silica, polymeric adsorbents, and activated carbon, have drawbacks such poor adsorption effectiveness, restricted selectivity for pollutants, and challenges with regeneration or reusability. The discharge of toxic organic dyes such as Congo Red and Toluidine Blue into water bodies by industries poses a significant threat to aquatic ecosystems and human health due to their carcinogenic and mutagenic properties. Similarly, heavy metal ions like Pb^{2+}, Cr^{3+}, and Cd^{2+} are non-biodegradable and persist in the environment, leading to bioaccumulation and toxicity in humans and animals. There is an urgent need for materials that can rapidly and selectively capture these pollutants from water. In addition to environmental applications, the emergence of antibiotic-resistant pathogens calls for the development of alternative antibacterial strategies that do not rely on traditional antibiotics. The work discussed in this thesis relates to the synthesis of Zr-MOF and M-HOF for adsorption of harmful dye molecules, toxic metal ions and for antibacterial activities. After synthesis, and purification, these particles were characterized for their physicochemical properties using different characterization techniques. The Zr-MOF showed high dye removal efficiency through electrostatic attraction and π–π interactions, while the M-HOF demonstrated highly selective and sensitive detection of Pb^{2+} ions through fluorescence quenching and surface complexation, confirming the suitability of these frameworks for water purification and sensing applications. In addition, the M-HOF exhibits strong antibacterial activity against Gram-negative bacteria like Pseudomonas aeruginosa, which is attributed to the controlled release of melamine and subsequent generation of reactive oxygen species (ROS) that damage bacterial membranes.

Contents

03. ARORA (Aditi)

Synthesis of C-5 Modified Pyrimidine Nucleoside Fluorophores & Pyrano[3,2-c]quinolones and Furo[3,2-c]coumarin C-Glycosides as Topoisomerase-II Inhibitors.

Supervisor: Prof. Brajendra K. Singh

Th 28202

Abstract

The thesis entitled "Synthesis of C-5 Modified Pyrimidine Nucleoside Fluorophores & Pyrano[3,2-c]quinolones and Furo[3,2-c]coumarin C-Glycosides as Topoisomerase-II Inhibitors" presents a multi-faceted approach to synthesizing novel fluorescent nucleoside analogues and bioactive heterocycles with potential anticancer applications. Divided into four chapters, the work explores diverse synthetic strategies and evaluates photophysical and biological properties. Chapter 1 details the synthesis of sugar-coumarin-based 1,2,3-triazole nucleoside analogues using copper(I)-catalyzed Huisgen cycloaddition. These dual-emissive compounds exhibit excellent fluorescence with large Stokes shifts and quantum yields, validated through DFT studies. Their sensitivity to environmental changes marks them as promising ratiometric probes for nucleic acid sensing and bioimaging. Chapter 2 focuses on the green synthesis of 1,4-dihydropyridine nucleoside analogues via solvent-free Hantzsch condensation under microwave irradiation. These fluorescent pyrimidine derivatives demonstrate high yields and enhanced emission properties, especially in solvatochromic environments, positioning them as strong candidates for bioanalytical applications. Chapter 3 introduces a stereoselective synthesis of sugar-derived pyrano[3,2-c]quinolones catalyzed by L-proline. The method achieved 100% stereoselectivity and high yields at room temperature. Molecular docking studies confirmed strong topoisomerase-II binding, surpassing standard drugs like doxorubicin. Chapter 4 presents a one-pot, catalyst-free synthesis of furo[3,2-c]coumarin C-glycosides via isocyanide-based multicomponent reaction, employing β-C-glycopyranosyl aldehydes as key intermediates. Comprehensive characterization of the synthesized compounds using spectroscopic analysis confirmed their structural integrity and purity. To explore their biological relevance, molecular docking studies were performed, which displayed their superior docking affinities towards topoisomerase-II, reinforcing their potential as anticancer agents.

Contents

04. CHAHAR (Deepak)

Structural and Functional Impacts of Nanoparticles on Proteins: Stability and Activity Studies.

Supervisor: Prof. P. Venkatesu

Th 28672

Abstract

We have studied four different proteins: cytochrome c (Cyt c), α-chymotrypsin (α-CT), stem bromelain (SB), and Immunoglobulin G (IgG). We have studied different NPs: Fe3O4 nanoparticles, Fe3O4 supported choline hydroxide NPs, Polydopamine NPs, DES modified Fe3O4 NPs (MNPs-DESs), Silver nanoclusters Agn(SG)m and $Ag_n(NALC)_m$.

Contents

05. CHAUDHARY (Harish Kumar)
Microcrystalline Cellulose Based Biodegradable Hydrogels for Oral Delivery of Insulin.
Supervisor: Prof. Amita Malik
Th 28203

Abstract

The oral delivery of insulin remains a significant challenge due to its sensitivity to enzymatic degradation and poor absorption in the gastrointestinal tract. This study explores developing and optimizing pH-sensitive hydrogels based on microcrystalline cellulose (MCC) for oral insulin delivery. Three formulations were synthesized: (i) a semi-interpenetrating network (semi-IPN) of MCC and methacrylic acid, (ii) a semi-IPN of MCC and itaconic acid, and (iii) a hybrid network of MCC, methacrylic acid, and itaconic acid. The hydrogels were designed to respond to pH variations along the gastrointestinal tract, ensuring insulin protection in an acidic environment and controlled release under neutral pH conditions. Structural characterization confirmed successful polymerization and crosslinking. Swelling studies demonstrated significant pH-dependent expansion, with maximum swelling observed at intestinal pH, facilitating insulin release. In vitro insulin release studies revealed that the hydrogels effectively shield insulin in gastric conditions (pH 1.2) and enable sustained release at intestinal pH (pH 6.8). Cytotoxicity assays indicated the biocompatibility of the hydrogel matrices, while enzymatic degradation studies confirmed their biodegradability. In vivo studies in diabetic rat models showed a significant reduction in blood glucose levels, validating the hydrogels` potential to deliver insulin effectively via the oral route. These findings highlight the versatility and effectiveness of MCC-based pH-sensitive hydrogels as novel carriers for oral insulin delivery. The combined use of methacrylic acid and itaconic acid enhances the tunability of hydrogel properties, offering promising prospects for non-invasive diabetes management. Further research will focus on optimizing the hydrogel formulation and scaling up production for clinical applications.

Contents

06. KHURANA (Mehak)
Design and Development of Multifunctional Metal-Organic Frameworks as Versatile Heterogeneous Catalysts for Sustainable Organic Transformations.
Supervisor: Prof. Satish Kumar Awasthi
Th 28673

Abstract

The design and development of metal–organic frameworks (MOFs) as heterogeneous catalysts represent a promising approach for advancing sustainable organic synthesis. This thesis explores the synthesis, characterisation, and catalytic performance of innovative MOF-based systems for green transformations. Chapter 1 provides an introduction to MOFs, emphasising their high surface area, tunable porosity, and structural versatility, which make them ideal candidates for environmentally benign catalysis. In Chapter 2, a metal oxide–MOF composite was developed and applied for the sustainable acetylation of benzyl alcohols and amines using acetic acid, achieving excellent selectivity, recyclability, and efficiency under mild, eco-friendly conditions. Chapter 3 focuses on the synthesis of a novel mixed-ligand copper MOF employed to catalyze the preparation of N-acylhydrazones, specifically 2-furoic acid hydrazones and 2-thiophene carboxylic acid hydrazones, which were obtained in high yields under green reaction conditions. Chapter 4 examines the photophysical and biological properties of the synthesized N-acylhydrazones, which exhibited intrinsic fluorescence and strong binding affinity toward human serum albumin (HSA) as confirmed by fluorescence spectroscopy. Molecular docking studies further elucidated their binding modes, while antioxidant activity assays revealed their potential bioactivity. In Chapter 5, a ruthenium-based MOF was developed and used as a robust and versatile catalyst for the synthesis of sulfonamides, including primary sulfonamides, under sustainable conditions. All synthesized MOFs and omposites were thoroughly characterized using PXRD, SEM, TEM, BET surface area analysis, EDAX, TGA, FTIR, ICPMS, UV-VIS NIR and Raman to confirm their structural, morphological, elemental properties and thermal stability while the organic compounds were confirmed using nuclear magnetic resonance NMR and MASS spectroscopy. Overall, this work demonstrates the efficiency, reusability, and environmental compatibility of MOF-based catalysts, bridging materials chemistry with bioorganic and photophysical studies and contributing significantly to the advancement of green and sustainable methodologies in heterogeneous catalysis.

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Mixed-Ligand Copper-based MOF (CuBPY) for Sustainable N-Acylhydrazones Formation 4. Design and Evaluation of Fluorescent N-Acylhydrazones: Spectroscopy, Molecular Docking and Antioxidant Potential 5. Constructing a Ruthenium–NDC MOF for Efficient and Sustainable Synthesis of Primary Sulfonamides. List of Publications, Conferences and Seminars.

07. KRITIKA

Metal and Metal Oxide-Based Nanomaterials for Anticancer and Bone Regenerative Applications.

Supervisor: Prof. Indrajit Roy

Th 28204

Abstract

This thesis explores the potency of metal and metal oxide-based nanomaterials in the treatment of breast cancer and bone regeneration. Chapter I lays the groundwork by providing an in-depth overview of the fundamental properties and healthcare applications of metal and metal oxide nanomaterials. It emphasizes on their evaluation as innovative tools for advancing breast cancer therapies and enhancing bone regeneration strategies. Chapter II provides a literature review of these nanomaterials, focusing on their role in inducing cytotoxic effects in breast cancer cells and their potential in magnetic hyperthermia, photothermal, and photodynamic therapy. It also explores their regenerative properties in bone healing, which is the key for developing advanced orthopaedic biomaterials. Chapter III outlines the synthesis, characterizations and in vitro studies of iron oxide, cobalt ferrite nanoparticles and Molybdenum disulfide nanosheets involved in the thesis. Additionally, anticancer potential was tested on MCF-7 breast cancer cells, and bone healing on MC3T3 osteoblast precursor cells using various assays. Chapter IV presents a comparative analysis of cobalt ferrite and iron oxide nanoparticles as magnetic hyperthermia and photothermal agents. It also explores their interaction with human hemoglobin, focusing on the significance their interaction with blood plasma in drug delivery and targeting. Chapter V explores the biochemical mechanisms triggered by methylene blue loaded cobalt ferrite nanoparticles in magnetically targeted photodynamic therapy (MT-PDT). Chapter VI involves the development of 2D multilayer Molybdenum disulfide nanosheets for NIR activated photothermal therapy. Moreover, their mechanistic interaction with human hemoglobin was also investigated. Chapter VII emphasizes on exploring the bone regenerative properties of TREK loaded iron oxide and cobalt ferrite nanoparticles using Magnetic Ion Channel Activation (MICA) technology. Chapter VIII concludes the thesis, summarizing the experimental findings and discussing their current and future significance in breast cancer and bone regeneration applications.

Contents

08. LALITA KUMARI

Design and Synthesis of Diversified Cobalt Based MOFs and Their Derived Materials for Various Organic Transformations.

Supervisor: Prof. Satish Kumar Awasthi

Th 28674

Abstract

The development of efficient, sustainable, and multifunctional catalysts is a major pursuit in modern synthetic chemistry. Metal–organic frameworks (MOFs), owing to their high surface area, tunable porosity, and versatile structures, have emerged as promising candidates for diverse organic transformations. In this thesis, we focus on the design and synthesis of diversified cobalt-based MOFs and their derived materials as effective catalytic systems for various organic reactions. The introductory chapter provides an overview of cobalt-based MOFs and their derived composites, highlighting their structural diversity, physicochemical properties, and catalytic potential in organic synthesis. In the second chapter, a ZIF-9/GO composite was synthesized and well characterized, demonstrating excellent catalytic performance in the Knoevenagel condensation and N-formylation reactions, signifying the role of graphene oxide in enhancing stability and activity. The third chapter describes the synthesis of a Co-MOF-derived $Co_3O_4/C/SiO_2$ nanocomposite, obtained from $ZnO/ZIF\text{-}9/SiO_2$, which functions as a multifunctional heterogeneous catalyst for the hydrogenation of nitroarenes and the reduction of organic dyes, thereby exhibiting both environmental and synthetic utility. In the fourth chapter, a novel N-doped porous carbon (NPC)-supported single cobalt catalyst (Co@NC) derived from a new Co-MOF was developed. This material showed outstanding activity and selectivity in the ammoxidation of alcohols, showcasing the synergistic effect of nitrogen-doping and cobalt dispersion. Finally, the fifth chapter reports the design and synthesis of a new cobalt-based MOF from BDC and TIB as organic ligand tailored for the Paal–Knorr pyrrole synthesis, underlining the scope of MOFs in heterocyclic chemistry. Overall, this work establishes diversified Co-MOFs and their derivatives as versatile catalytic platforms, bridging structural design with practical applications. The findings not only expand the catalytic horizon of MOFs but also provide insights into their transformation into functional materials for sustainable organic synthesis.

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09. MEENA (Hari Mohan)

Isolation and Characterization of Heavy Metals and Organic Impurities from Waste Water.

Supervisors: Prof. Shrikant Kukreti and Prof. P. S. Jassal

Th 28675

Abstract

The substantial increase in using of heavy metals in recent decades has therefore resulted in a higher concentration of metallic compounds in aquatic ecosystems. Industrial wastewater contains high levels of heavy metals, which can result in water pollution upon its discharge into the environment. The management of industrial wastewater must address the presence of hazardous heavy metals, such as arsenic, mercury, chromium, aluminum,and copper. Heavy metals are characterized as elements possessing a density above five times that of water. Heavy metals contribute to water contamination. At least 20 metals are categorized as hazardous, with around half of these being discharged into the environment in quantities that pose a threat to both ecological systems and human health.Water is a vital and crucial resource for the life of living organisms, allowing sustainable existence. Securing access to clean and safe drinking water has emerged as a critical issue, especially in developing and emerging nations, due to fast industrialization, excessive urbanization, climate change, and water pollution resulting from industrial effluents and domestic sewage. The 2018-19 edition of the UN World Water Development Report indicates that between 47-50% of the global population lacks access to a reliable and uncontaminated drinking water source. The percentage is anticipated to increase to 57% by 2050, aligning with an expected population of 9.4 to 10.2 billion, predominantly situated in Africa and South Asia. Nonetheless, this inherent talent faced considerable challenges due to the Industrial Revolution in the late 18th century, evidenced by water pollution that caused enduring and fatal diseases, frequently resulting in death. Contamination of water by heavy metals and chemical dyes is a substantial and complex issue that has persistently attracted global attention. Even at minimum doses, these contaminants impact human health and tend to bioaccumulate in organisms.

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10. MEENA (Shivam Abhineet)

Novel Strategies for the Construction of Pharmaceutically Relevant Succinimides, Aza-bicyclo[4.1.0]heptanes and Oxindoles from Enynes and Acrylamides.

Supervisor: Prof. Akhilesh Kumar Verma

Th 28676

Abstract

The development of efficient and selective synthetic methodologies for constructing pharmaceutically relevant molecular scaffolds remains a central challenge in modern organic and medicinal chemistry. Among these, succinimides, aza-bicyclo[4.1.0]heptanes, and oxindoles are prominent nitrogen-containing heterocyclic motifs frequently found in a variety of biologically active compounds and therapeutic agents. This study presents novel strategies for the synthesis of these valuable frameworks from readily available enynes and acrylamides, leveraging innovative catalytic and reaction design approaches. By employing metal-catalyzed cyclization, tandem addition–cyclization, and radical-mediated transformations, the proposed methods enable the efficient formation of complex heterocycles with high chemo-, regio-, and stereoselectivity under mild reaction conditions. Our strategy utilizes the unique reactivity of enynes—compounds containing conjugated alkene and alkyne functionalities—and acrylamides as versatile substrates to access structurally diverse products through carefully optimized reaction pathways. The construction of succinimide derivatives is achieved via intramolecular cyclization of activated intermediates, offering streamlined access to five-membered lactams with potential biological applications. The synthesis of aza-bicyclo[4.1.0]heptane structures is accomplished through strain-driven cycloaddition or radical cyclization routes, leading to compact and conformationally constrained bicyclic systems with utility in CNS drug development. Additionally, the oxindole core, a privileged scaffold in drug discovery, is efficiently synthesized through oxidative annulation of acrylamides with enynes, forming the spirocyclic or fused indole architectures. This work not only provides modular and scalable synthetic pathways for these heterocycles but also broadens the scope of accessible molecular diversity for pharmaceutical research. The operational simplicity, functional group tolerance, and compatibility with complex molecular architectures make these strategies particularly attractive for drug discovery and development.

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11. MISHRA (Neeraj)

Synthesis of Metal Oxide/Multi-Walled Carbon Nanotube Composites Using Herbal Extracts and Their Photocatalytic Application.

Supervisor: Prof. Sanjay Kumar

Th 28205

Abstract

The study explores the synthesis, characterization, and application of advanced nanomaterials for environmental remediation, with particular focus on photocatalytic dye degradation. Rapid industrialization has led to widespread release of harmful organic dyes such as Methylene Blue (MB) and Methyl orange (MO) into water bodies, causing severe ecological and health risks. To address this, the research emphasizes the development of biogenic nanocomposites as cost-effective and sustainable photocatalysts. By leveraging green synthesis approaches using natural extracts, such as Aloe vera leaf and pineapple peel, the study successfully synthesized Cu 2 O, ZnO nanoparticles (NPs), and their hybrid composites, such as ZnO/MWCNT, Cu 2 O/MWCNT, Cu 2 O/ZnO and Cu 2 O/ZnO/rGO with MWCNTs and rGO. These materials were systematically characterized using advanced techniques to validate their structural, morphological, and optical properties, including XRD, FT-IR, XPS, SEM, PL, TEM, Raman spectroscopy, UV-Vis spectroscopy, and BET analysis. The nanocomposites with different ZnO/MWCNT ratios (1:1, 2:1, and 3:1) were carefully examined under visible light. The observed optimum circumstances (catalyst dose of 0.2 g, dye concentration of 10 ppm) result in outstanding removal efficiency, with 99.42% and 91.30% elimination for MB and MO, respectively. The synthesized Cu 2 O/MWCNT composites demonstrated exceptional photocatalytic efficiency under visible light irradiation, achieving dye degradation rates of 99.74% for MB and 94.26% for MO. The composites exhibited enhanced performance due to their high surface area, efficient charge carrier separation, and extended light absorption range. The photodegradation efficiency of Cu 2 O/ZnO/rGO onto MB and MO is achieved under the observed ideal conditions (0.1 g of Cu 2 O/ZnO/rGO, pH 7, a 300 mL concentration of 10 ppm dye solution, and a 400 W tungsten bulb for visible light; the time of irradiation is 75 minutes), as established by UV-visible spectral studies at 99.51% and 92.48%, respectively.

Contents

12. MITTAL (Ashi)

Photosensitizer-Loaded Hybrid Nanomaterials for In Vitro Anti-Cancer Applications.

Supervisor: Prof. Indrajit Roy

Th 28206

Abstract

We prepared photosensitizer-loaded ZIF-8 and zinc alendronate hybrid nanoparticles for in vitro anti-cancer phototherapies. Light-based therapies or phototherapies leverage light and light-activated substances to target and destroy cancer cells with precision. Photodynamic therapy (PDT) and photothermal therapy (PTT) are minimally invasive and promising anti-cancer therapies. In PDT, reactive oxygen species (mainly singlet oxygen) are formed by energy/electron transfer reaction between light-activated photosensitizer and molecular oxygen. On the other hand, in PTT the light-activated photosensitizer releases heat by non-radiative relaxation process to kill cancer cells. These phototherapies can be combined with other anti-cancer therapies such as chemodynamic therapy (CDT) and immunotherapy to obtain synergistic therapeutic effects. Biological macromolecules, particularly serum proteins are inevitably adsorbed on the nanoparticle's surface upon entering biological systems resulting in the formation of a protein corona. This layer can significantly alter the nanoparticle's behaviour, including its stability, circulation time, and ultimately its biological fate. Serum albumins constitute a major portion of serum proteins found in blood plasma. Thus, understanding the dynamics of protein corona formation by analyzing the interaction of nanoparticles with serum albumins is essential before employing these nanoparticles for other purposes such as drug delivery. We studied the interaction of ZIF-8 nanoparticles with bovine serum albumin (BSA), a model serum protein analogous to human serum albumin.

Contents

13. NIDHI

Physicochemical and Spectroscopic Studies of Molecular Interactions in Industrially Important Multi-Component Systems.

Supervisor: Prof. Anil Kumar Nain

Th 28207

Abstract

Understanding the physicochemical and spectroscopic properties of binary liquid mixtures is crucial for optimizing industrial processes and developing novel materials. This study is aimed to investigate the molecular interactions in binary systems consisting of polyethylene glycols and ionic liquids through a comprehensive thermodynamic, acoustic, and spectroscopic approach. This work comprises the detailed analysis of the obtained data of binary liquid mixtures to enhance our understanding of

how composition, temperature, and molecular structure influence physicochemical properties, aiding in the understanding of molecular interactions and formulation of predictive models. Liquid mixtures offer significant advantages over pure solvents, as mixing induces interactions among unlike components and provide solvents with wide-ranging properties. Various parameter such as density, viscosity and speed of sound of the chosen binary systems were recorded as functions of composition and temperature. These data have been used to calculate various thermodynamic and acoustical parameters, including excess properties, viz., excess molar volume, excess isentropic compressibility, excess intermolecular free length, excess speed of sound, excess molar isentropic compressibility and excess acoustic impedance. These excess properties were correlated with the Redlich-Kister equation. In addition, the partial molar volume and compressibility; excess partial molar volume and compressibility of the components over the entire composition range; and partial molar volume and compressibility and excess partial molar volume and compressibility of the components at infinite dilution have also been calculated. These evaluated parameters have been interpreted in terms of prevailing intermolecular interactions in these mixtures. The scaled particle theory has been employed to estimate the speeds of sound in the studied binary systems, and the results were compared with experimental findings to evaluate their accuracy and applicability. Additionally, spectroscopic methods like FTIR spectroscopy were utilized to probe molecular-level interactions and identify specific functional group interactions.

Contents

14. POOJA

Synthesis and Characterization of Some Potential Adsorbents and Exploring Their Pesticide Detoxification Efficiency in Wastewater.

Supervisor: Prof. Rakesh Kumar Sharma

Th 28208

Abstract

Pesticides are widely used in agriculture, which has greatly increased agricultural output. However, their careless usage has created serious environmental problems. Because residual pesticides in wastewater are toxic and persistent, they pose a serious risk to human health as well as aquatic ecosystems. To lessen the harmful impacts of these toxins, effective remediation techniques are essential. Adsorption`s ease of use, affordability, and high efficiency make it one of the most promising methods for treating wastewater. Advanced adsorbents with certain physicochemical characteristics—like high surface area, porosity, and selective adsorption capabilities—are crucial to handle the complexity of pesticide detoxification. Chlorpyrifos (CPy) and Captan (CA) are widely used pesticides with significant environmental and health implications. The selective recognition and removal of these pesticides are crucial for mitigating their adverse effects. Diquat is a widely used non-selective contact herbicide and desiccant, primarily employed in agriculture to manage weeds and to dry crops before harvest. Atrazine is a selective herbicide extensively used to control broadleaf weeds such as corn and sugarcane. Activated charcoal (AC) and graphene oxide (GO) are two intriguing options that have drawn a lot of interest due to their distinct physicochemical characteristics and potent adsorption capabilities. These attributes enable GO to interact with various pollutants. AC being a traditional and widely used adsorbent, is known for its porous structure, and excellent adsorption capabilities for a wide range of contaminants. By systematically comparing the adsorption efficiencies of GO and AC for specific pesticides, this study aims to elucidate their strengths and limitations. Calix[4]pyrrole has attracted significant attention due to its unique structural properties and ability to form non-covalent interactions with guest molecules. Among its derivatives, octamethylcalix[4]pyrrole (CP) stands out for its potential in molecular recognition and catalysis. The study of calix[4]pyrrole is essential to understanding and enhancing their applications in diverse fields such as environmental remediation and sensing. The functionalization of calix[4]pyrroles, has opened new avenues in molecular recognition and environmental remediation. Azo-functionalization of CP introduces electron-donating azo groups, creating additional H-bonding and π-π interaction sites. These modifications make azo-functionalized CP derivatives promising candidates for the selective detection and binding of pesticides. The work presented in this thesis mainly focuses on the synthesis, characterization, and efficacy of possible adsorbents in the removal of pesticides from wastewater. The results are intended to aid in creating environmentally friendly wastewater treatment methods and offer guidance on how to design adsorbents for environmental remediation applications best.

Contents

15. PRERNA

Theoretical Models for Diffusion, Migration and Ohmic Couplings with Electron Transfer Kinetics on Rough Electrodes.

Supervisor: Prof. Rama Kant

Th 28210

Abstract

This thesis primarily contains the theoretical formalisms developed emphasizing the influence of diffusion-migration coupling with electron transfer kinetics and electrode surface roughness. The specific focus of each chapter is as follows: The chapter 1 provides a comprehensive review of the ionic screening in the electrolytes; the electrolyte conductivity; structure and dynamics of the electric double layer (EDL); contributions from diffusion and migration in mass transport; surface kinetics and boundary constraints; electrode roughness and heterogeneity; mathematical approaches for electrochemical response at rough electrodes; determining the electrode roughness using CV-SEM and electrochemical impedance spectroscopy root mean square roughness (EIS-RMS). In Chapter 2 a novel soft ionic atmosphere model is developed which allows us to estimate the molar conductivities for concentrated symmetric and asymmetric electrolytes. The elegant sets of equations developed in chapters 3 to 6 accredit us to study the effect of diffusion-migration coupling on reversible and quasi-reversible charge transfer kinetics. The temporal and frequency domain analyses are performed using chronoamperometry and EIS techniques. The concentration and potential dependent anomalies due to migration-diffusion coupling conclude that migration effects are significant at critical ionic strength which ranges from 0.1M to 2M. Beyond this concentration range, migration effects become weak, and potential dependent migration is substantial for the window RT/F to 3RT/F. Theoretical results are in good accord with experimental results for reversible as well as quasi-reversible processes. The developed theoretical models have strong implications and importance in studying the electrochemical response in realistic experimental conditions including electrode roughness. This theoretical work has significance in modeling the challenging problem of DC-biased EIS response in the presence of faradic and non-faradic contributions. Our theoretical results are useful for the understanding and applications of complex energy storage devices.

Contents

16. RAM KUMAR

Development of Colorimetric and Fluorometric Chemosensors for the Selective Recognition of Metal Ions and their In Silico Docking Studies.

Supervisor: Prof. Balaram Pani

Th 28211

Abstract

The thesis explores the investigation, design, and development of colorimetric and fluorometric chemosensors for the detection of analytes. The work is organised into six detailed chapters, each focussing on significant developments of chemosensor technology. Chapter I: Colorimetric and fluorometric chemosensors provide rapid, sensitive, and selective detection of metal ions, with signals visible to the naked eye. These sensors play a crucial role in catalysis, analytical applications, and environmental chemistry. Chapter II: A novel Schiff base ligand was synthesized and characterized using analytical techniques. It selectively detected Cu^{2+} ions with a 1:1 binding stoichiometry and a detection limit of 42.09 nM. DFT and docking studies confirmed its structural and biological interactions. Chapter III: A new Schiff base sensor was synthesized and exhibited high selectivity for Cu^{2+} with a 1:1 binding stoichiometry and a detection limit of 32.2 nM. Potential biological applications, with practical utility demonstrated in real water samples. Chapter IV: This study reports a novel rhodamine-based Schiff base chemosensor that selectively detects Pb^{2+} with a distinct colorimetric and fluorescence response. The sensor exhibits high sensitivity (LOD = 1.97 nM), a 1:1 binding stoichiometry, and reversible detection with EDTA. Chapter V: A novel chemosensor was synthesized for selective and sensitive Pb^{2+} detection. It exhibited distinct colorimetric and fluorescence responses, with a 1:1 binding ratio and a binding constant of 0.954×10^4. Low detection limit (3.77 nM) and practical applicability in real water samples. Chapter VI: A chemosensor was synthesized for Cd^{2+} detection. It exhibited a distinct turn-on fluorescence response, a 1:1 binding stoichiometry, and a low detection limit of 2.01 nM. The thesis integrates synthetic organic chemistry, molecular docking, and theoretical investigations to tackle current issues in environmental monitoring. The results are expected to make substantial contributions to analytical sensing, facilitating future advancements in these areas.

Contents

17. RAVEENA

Synthesis of Organic-Based Hybrid Materials for Applications in Water Remediation and Value-Added Product Formation.

Supervisor: Dr. Pratibha Kumari

Th 28212

Abstract

Organic hybrid materials have emerged as pivotal components in material science due to their advantageous properties, such as high surface area, porosity, tunability, and robustness. The present thesis deals with synthesizing various organic hybrid materials using bio-based organic linkers, including gallic acid, caffeic acid, quercetin, and porphyrin. These materials are versatile in nature, making them suitable for applications in water remediation through adsorption and photodegradation, as well as in forming value-added products such as cyclic carbonates and food packaging materials. The contamination of water bodies by heavy metal ions, pesticides, and dyes presents a critical environmental challenge, necessitating efficient remediation strategies such as adsorption and photodegradation. Chapter 1 deals with the synthesis of a copper-quercetin polymeric hybrid material, which demonstrated over 95% adsorption efficiency for mercury, cadmium, and chromium ions under neutral and acidic conditions from water. In Chapter 2, a copper-caffeic acid hybrid material was prepared, which revealed high surface area and mesoporosity. This hybrid framework exhibited high adsorption capacity for pesticides such as dichloran pesticide. Chapter 3 includes the synthesis of a hybrid material by covalently attaching photoactive porphyrin to graphene oxide. This material exhibited efficient photocatalytic activity for the degradation of crystal violet dye under visible light in water. Excessive concentrations of carbon dioxide levels also contribute to water contamination by forming carbonic acid, which is responsible for ocean acidification. To address this, carbon dioxide can be utilized to produce value-added products by a catalytic cycloaddition reaction. Chapter 4 is related to developing a titanium oxide-functionalized cobalt-porphyrin covalent framework and its utilization in the cycloaddition reaction of carbon dioxide with epoxide. It produces industrially important cyclic carbonates with a yield of>99%. Chapter 5 deals with forming chitosan, nanocellulose, and copper-gallic acid hybrid frameworks in the form of films, which exhibited excellent barrier properties, low water solubility, reduced moisture content, and prolonged antioxidant activity, effectively extending the shelf life of foodstuff. The present research underscores the versatility and effectiveness of organic hybrid materials in water remediation and forming value-added products.

Contents

18. RUVUBU (Sylvanus Bisaba)
Nanoparticle Technology in Environmental Remediation and Biomedical Applications.
Supervisor: Prof. Indrajit Roy
Th 28786

Abstract

In our work we have presented an integrated approach to environmental remediation and biomedical applications using advanced and green-synthesized nanoparticles. Magnetic chitosan nanoparticles modified with triglycine (Gly-Gly-Gly) and 2-mercaptoethylamine (2-MEA) achieved up to 99.9% Malachite green removal under optimized conditions. Similarly, sodium diphosphate cross-linked chitosan magnetic nanoparticles demonstrated strong adsorption and excellent reusability due to their superparamagnetic properties. A green synthesis approach using Pueraria montana root extract produced ZnO nanoparticles, which, when modified with trisodium pyrophosphate, showed enhanced catalytic degradation of Malachite green and Aniline blue. Additionally, polyaniline-coated chitosan nanocomposites exhibited high adsorption efficiency for Rhodamine B and nonsteroidal anti-inflammatory drugs (NSAIDs) through chemisorption, with effective reuse cycles. Further studies targeted ibuprofen removal using chitosan–Emeraldine salt magnetic nanohybrids, demonstrating broad-spectrum adsorption and high reusability. The biomedical potential of green-synthesized nanoparticles from Pueraria montana, Vernonia amygdalina, and Tephrosia vogelii extracts was also evaluated. These nanoparticles displayed significant antibacterial activity, including against multidrug-resistant strains, and insecticidal efficacy against Periplaneta americana. Their bioactivity is attributed to phytochemical capping, highlighting eco-friendly and multifunctional applications. Complementing pollutant removal, the study also reviewed advanced detection technologies for heavy metals using chromogenic reagents, nanomaterials, perovskites, and nanozymes. These platforms enable sensitive, selective, and real-time monitoring of toxic metals such as lead, mercury, cadmium, and arsenic, offering portable and sustainable sensing solutions for environmental protection. Overall, this work underscores the transformative potential of nanotechnology in wastewater treatment, pollutant adsorption, catalytic degradation, and environmental monitoring. By integrating eco-friendly synthesis, high-performance adsorption, and innovative sensing strategies, the study provides scalable, reusable, and sustainable solutions to mitigate global water pollution and support public health protection.
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Underexplored Tanzanian Medicinal Plants: A Comparative Study using Pueraria montana, Vernonia amygdalina, and Tephrosia vogelii 9. General Conclusion and Recommendations. List of Publications and Conferences. Posters. Workshops.

19. SAURAV SHANKAR
Development of Nanomaterials Based Biosensors for Lung Cancer Detection.
Supervisor: Prof. Neera Sharma
Th 28213

Abstract

Lung cancer is the leading mortality among other cancer around worldwide. The early detection of lung cancer plays a critical role in diagnosis and subsequent treatment. However, conventional techniques like chest X-ray, magnetic resonance imaging, computerized tomography screening etc. limit the applications due to low sensitivity, expensive with invasive procedure and unable to detect lung cancer in early stage. To overcome these limitations, detection of lung cancer via quantification of biomarker through electrochemical biosensors, remarks a significant potential for quick, minimal invasive and sensitive approach for early diagnosis of lung cancer. First two works of this thesis present development of nanomaterials i.e. MgO@MWCNT and nZrS3 modified ITO based biosensors for lung cancer biomarker (cytoskeleton associated protein; CKAP4) detection. The EDC-NHS chemistry has been used to covalently immobilize anti-CKAP4 over fabricated electrodes, and drop-cast method has been utilized to immobilize BSA to block non-specific sites. However, their rigidity, brittleness, and high cost restrict their utility for developing wearable, cost-effective and disposable point-of care devices. To overcome such limitations, other chapters of this thesis focusses on the development of flexible and environment friendly thread-based biosensors integrated with conducting polymer (PEDOT:PSS) [poly(3,4-ethylenedioxythiophene):poly (styrenesulfonate)] and nanomaterials (ZrS3@rGO and ZrS3@PC) for detection of CKAP4. Various spectroscopies and electrochemical techniques have been used to characterize the synthesized as well as functionalized nanomaterial and fabricated electrodes. The concentration of CKAP4 in serum sample has been measured by ELISA technique and the developed biosensors have been validated through electrochemical techniques. The obtained results demonstrated strong correlation with that of standard samples. Among the fabricated biosensors, nZrS3@PC based biosensing platform surpasses other platform in terms of broader linear detection range as well as lower limit of detection. This developed biosensor also demonstrate significant potential to distinguish healthy subjects from the lung cancer patients.

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20. SEWARIYA (Shubham)

Discovery and Development of Secondary Metabolites as Anticancer Drugs: Noscapinoids and Coumarins.

Supervisors: Prof. Shrikant Kukreti and Prof. Ramesh Chandra

Th 28214

Abstract

This thesis investigates the development of noscapine-based derivatives (noscapinoids), and the discovery of coumarins as potential anticancer agents. Through a multidisciplinary approach integrating synthetic modifications, computational modeling, biophysical and bioactivity studies, the research aims to address the existing challenges in cancer therapy such as drug resistance, poor solubility, and inefficient delivery. The study begins with an overview of cancer, its increasing global burden, and the limitations of conventional therapies. Emphasis is placed on the role of secondary metabolites from natural products in drug discovery and development, particularly noscapine and coumarin derived from the shikimate pathway. Following this, the synthesis and characterization of 9-bromo noscapine ionic liquid ([9-Br-Nos]IBr2) and 9'-substituted Suzuki-coupled noscapine derivatives are detailed. These compounds demonstrated enhanced tubulin-binding affinity and superior anticancer activity, as confirmed through molecular docking, molecular dynamics simulations, and cytotoxicity assays. Additionally, a dual-drug delivery system using solid lipid nanoparticles (SLNs) loaded with 9-hydroxymethyl noscapine and telmisartan was developed. Characterization and binding studies confirmed their stability and controlled release properties, with in vitro cytotoxicity assays revealing greater anticancer efficacy than the individual drugs. Lastly, a novel mass defect (MD) filtering approach was applied to prioritize natural product fractions for anticancer screening. LC-MS and bioactivity-guided isolation led to the identification of five bioactive coumarins from the Micromelum minutum plant extract. Overall, this research highlights the potential of noscapine-derived ionic liquids, noscapine based dual-drug nanoparticles, and coumarins in developing next-generation cancer therapeutics. While the findings provide promising leads, further in vivo pharmacokinetics, toxicity assessments, and mechanism-based studies are recommended to facilitate their translation into clinical applications.

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21. SONI (Prakshi)

Understanding the Role of Doping Induced Synergy in Perovskite Oxide@2D Nanomaterials in Charge Storage.

Supervisor: Prof. Raj Kishore Sharma

Th 28209

Abstract

The urgent need for efficient, sustainable energy storage systems has directed significant research focus toward electrochemical technologies, particularly supercapacitors. Supercapacitors offer advantages such as high-power density, rapid charge-discharge capability, and long cycle life, making them suitable for applications ranging from portable electronics to electric vehicles. However, their relatively low energy density compared to conventional batteries poses a major limitation. To overcome this, the design of advanced electrode materials with enhanced electrochemical properties is critical. Among various materials, perovskite oxides (ABO3-type) have emerged as promising materials due to their tunable structure, rich redox activity, and mixed ionic-electronic conductivity. The thesis work systematically investigates doping-induced synergy and heterostructure engineering in perovskite oxide@2D nanomaterials for improved charge storage. Chapter 1 describes the motivation behind this work. Chapter 2 comprehensively overviews the structural, morphological, and electrochemical characterization techniques employed to analyze perovskite-based materials. Chapter 3 focuses on the hybridization of oxygen-deficient SrFeO3-δ with reduced graphene oxide nanoribbons. This integration enhances electrical conductivity, ion diffusion, and active surface area, leading to superior charge storage in both symmetric and asymmetric configurations. Chapter 4 explores the formation of a heterostructure between LaCo0.95Mo0.05O3-δ and amorphous CoMnB nanosheets. Mo doping generates abundant oxygen vacancies, which promote efficient anion intercalation. The engineered heterointerface significantly improves electrochemical kinetics, structural integrity, and cycling stability. Chapter 5 describes the findings of tungsten doping at the Co-site in double perovskite La2CoMnO6 and forming Ohmic heterojunction/contacts with metallic vanadium nitride nanosheets. This dual approach maximizes charge transfer and stabilizes the redox-active framework. Finally, Chapter 6 summarizes the collective insights, emphasizing the role of defect modulation, conductive matrix integration, and heterostructure design in unlocking the full electrochemical potential of perovskite-based nanomaterials for next-generation supercapacitor applications.

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22. SUMIT KUMAR

Design and Synthesis of C-5 Modified 2`-Deoxyuridine, Carbohydrate-Conjugated Pyrano[3,2-c]quinolones and Bis-coumarin Derivatives.

Supervisor: Prof. Brajendra K. Singh

Th 28215

Abstract

The thesis is divided into two sections; Section-A and Section-B, each having two chapters, i.e., Chapter 1, Chapter 2. Section-A Design and Synthesis of C-5 Modified 2`-Deoxyuridine The work presented in Chapter 1 entitled "Synthesis and Fluorescence Studies of Base-Modified Furo[3,2-c]coumarin Nucleosides" describes the synthesis of novel 5-furo[3,2-c]coumarin-2`-deoxyuridine nucleoside analogues from diacetylated 5-formyl-2`-deoxyuridine via a one-pot multi-component reaction. Comprehensive fluorescence and photophysical analyses were subsequently conducted on the synthesized derivatives. Additionally, their electronic structures were extensively examined using DFT. The work presented in Chapter 2 entitled "Microwave-Assisted Synthesis and Fluorescence Studies of Base Modified Furo[3,2-c]quinolone Nucleosides" describe the synthesis of novel 5-furo[3,2-c]quinolone-2`-deoxyuridine nucleoside analogues using microwave-assisted, catalyst-free conditions in a greener solvent (2-Me-THF). The detailed photophysical studies of the synthesized compounds further underscores their potential as fluorescent probes. DFT calculations provided insights into the electronic structures, supporting the observed fluorescence properties. Section-B Design and Synthesis of Carbohydrate-Conjugated Pyrano[3,2-c]quinolones and Bis-Coumarin Derivatives The work presented in Chapter 1 entitled "Diastereoselective Synthesis of Carbohydrate-Conjugated Pyrano[3,2-c]quinolones" describes the synthesis of two distinct series of pyrano[3,2-c]quinolones, inspired by natural products. Unlike prior methods, which resulted in low yields and poor selectivity, this study achieves remarkable diastereoselectivity (dr 97:3) and yields (87-95%) under mild conditions, utilizing ethyl acetate as the solvent at room temperature. The work presented in Chapter 2 entitled "Design, Synthesis and In-silico Studies of Carbohydrate-Conjugated Bis-Coumarin Derivatives as Anticoagulant Agents" describes the synthesis of two distinct series of bis-coumarin derivatives conjugated with carbohydrate. We have utilized an efficient synthetic methodology starting from glucose and galactose to synthesize twenty-four novel carbohydrate-conjugated bis-coumarin analogues. Furthermore, the in-silico studies have also been conducted on the thus synthesized molecules for their potential application as anticoagulants using Swissdock.

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23. TAKKAR (Priya)

Design and Synthesis of Novel 1,4-Dihydropyridine and Rhodamine Based Scaffolds Possessing Promising Biological and Chemosensing Properties.

Supervisor: Prof. Rakesh Kumar

Th 28216

Abstract

The thesis explores the investigation, design, and development of sophisticated molecular structures with notable medicinal and diagnostic applications. The work is organised into six detailed chapters, each focussing on significant developments in medicinal chemistry and chemosensor technology. Chapter I offers a comprehensive examination of 1,4-dihydropyridine (1,4-DHP) scaffolds, clarifying their therapeutic adaptability. 1,4-DHPs, as preferred structures in medicinal chemistry, are essential to numerous authorised medications, having extensive uses in cardiovascular and anticancer therapies. This chapter establishes the groundwork for future research, offering insights into their structural, functional, and pharmacological significance. Chapter II concentrates on the design, synthesis, and in-silico assessment of innovative 1,4-DHP-derived amlodipine bioisosteres. These compounds are evaluated as possible antihypertensive medicines, with computational docking and ADMET profiling demonstrating their enhanced pharmacokinetic properties and molecular interactions with target receptors. This research offers a viable avenue for the advancement of next-generation antihypertensive medications. Chapter III examines the therapeutic potential of 1,4-DHP-tethered isatin scaffolds for the treatment of liver and stomach malignancies. This chapter identifies effective candidates with significant anticancer activity through the integration of synthetic and computational techniques. Molecular docking studies targeting essential cancer-related enzymes underscore their potential as effective therapeutic agents, fulfilling a critical need in oncology. Chapter IV shifts focus to chemosensors, providing a comprehensive analysis of rhodamine-based probes for the selective detection of metal ions. The chapter elucidates the design concepts and mechanisms that govern their sensitivity and selectivity. This thorough evaluation highlights the usefulness of rhodamine derivatives in environmental and analytical contexts. Chapter V presents a dual-function fluorescent and colorimetric chemosensor utilising pyranopyrazole-substituted rhodamine for the detection of lead ions (Pb^{2+}). This sensor exhibits exceptional selectivity, rapid response, and practical applicability in aqueous and real-world sample analysis. The results demonstrate considerable potential for tackling environmental and industrial lead pollution issues. Chapter VI involves the creation of a rhodamine-based turn-on chemosensor for the selective detection of nickel ions (Ni^{2+}). Practical applications, such as the examination of environmental water and food samples, are supported by theoretical investigations that validate a 1:1 binding stoichiometry. This dual-mode sensor exhibits the amalgamation of experimental and computational methodologies in the advancement of chemosensor technology.

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antihypertensive agents 3. Development of newer 1,4-dihydropyridine tethered isatin scaffolds as potential therapeutics for liver and gastric cancer Treatment 4. A comprehensive assessment of rhodamine based chemosensors: advancing selective detection of metal ions 5. A dual turn-on fluorescent and colorimetric chemosensor based on pyranopyrazole appended rhodamine for the detection of lead ions 6. Rhodamine based turn-on dual mode chemosensor for the selective recognition of nickel ions: practical and theoretical applications. Summary. Published Papers and Conference Attended.

24. THAKUR (Deepika)
Synthesis of Biologically Relevant Naphthyridines, Isoquinolines, Chromenes and Indoles from *o*-Alkynylaldehydes, Anilines and Vinyl Benzotriazoles by Phosphonylation, Carbene Insertion and Tosylation.
Supervisor: Prof. Akhilesh Kumar Verma
Th 28677

Abstract

The efficient synthesis of biologically significant heterocyclic scaffolds remains a key area of research in organic and medicinal chemistry. This thesis outlines a divergent synthetic strategy for the construction of various heterocycles—namely naphthyridines, isoquinolines, chromenes, and indole derivatives—starting from o-alkynylaldehydes and vinyl benzotriazoles, using phosphonylation, cyclization, N-functionalization, 1,3-migration, and tosylation as key transformations. Naphthyridines, isoquinolines, and chromenes were synthesized via phosphonylation of o-alkynylaldehydes, followed by cyclization. The nature of the substituents and reaction conditions played a crucial role in determining the outcome of the cyclization, allowing access to a variety of heterocyclic frameworks with high efficiency and selectivity. Indole derivatives were synthesized via a distinct pathway involving N-functionalization of o-alkynylaldehydes, followed by 1,3-migration to construct the indole core. This route offers a modular and flexible approach to access functionalized indole frameworks. Furthermore, an alternative method was employed to generate indole derivatives through the tosylation of vinyl benzotriazoles, followed by a denitrogenative ring-opening reaction. This process enabled the efficient generation of indoles with structural diversity, demonstrating the utility of vinyl benzotriazoles as versatile precursors in heterocyclic synthesis. All synthesized compounds were characterized by standard spectroscopic techniques, including NMR (^{1}H, ^{13}C), IR, and HRMS. Selected compounds were further confirmed by single-crystal X-ray diffraction analysis. Overall, this work introduces a robust and flexible synthetic platform for accessing a wide array of biologically relevant heterocycles from o-alkynylaldehydes and vinyl benzotriazoles, contributing significantly to the advancement of heterocyclic and medicinal chemistry.

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Sulfonylated Indoles 4. Harnessing the Reactivity of *ortho*-Alkynylaldehydes: Silver Triflate Catalyzed Regioselective Synthesis of Phosphonylated Fluorescent Molecules. Summary of the work and Publications.

25. YADAV (Pooja)
Palladium(0) Catalyzed Aminocarbonylation and Ruthenium(II) Catalyzed N-Methylation and Aldehyde-Water Shift Reactions.
Supervisor: Prof. Natesan Thirupathi
Th 28217

Abstract

Section 2.1 A family of N,N-diaryl-N″-(pyridine-2-ylmethyl)guanidines (B) were prepared in 70%−92% yields and subjected to palladium(0) catalyzed aminocarbonylation reactions with aryl iodides using CsOH/CHCl3 mixture as CO surrogate to afford the corresponding N-aroylguanidines (C) in 70%−93% yields. A gram scale synthesis was reported for a representative example. When the aforementioned reaction was carried out with 2-iodoaniline as an electrophile, either a mixture of two distinct 2-aminoquinazolinones (D and E) or one of these 2-aminoquinazolinones are formed. The scope of guanidines and aryl iodides were explored for both of the above-mentioned reactions. The role of directing group in the substrates upon the successful aminocarbonylation of guanidines, B is outlined. The reactions of a pair of N-aroylguanidines, C with PhI(OAc)2 afforded 2-aminobenzimidazoles, T with unanticipated core. Plausible mechanisms of formation of C, D, E and T are outlined. Section 2.2 Nine ethylene bridged biguanidines 2.2.1–2.2.9 and one propylene bridged biguanidine 2.2.10 were isolated in 75%–89% yields. The bridge-splitting reaction of [η6-(p-cymene)Ru(μ-Cl)Cl]2 with biguanidines 2.2.1, 2.2.2 and 2.2.4–2.2.8 in toluene at RT afforded cationic half-sandwich ruthenium(II) complexes 2.2.11–2.2.17 in 75%–86% yields. Molecular structures of biguanidines 2.2.1, 2.2.5·MeOH and 2.2.8·MeOH and those of complexes 2.2.11 and 2.2.14·MeOH were determined by single crystal X-ray diffraction. Nine ruthenium(II) complexes were screened as catalysts for N-methylation of p-toluidine at 1 mol% catalyst loading and complex 2.2.14 was found to be the best catalyst for N-methylation of aromatic amines. The scope of 22 aromatic amines were explored. The scope of five aromatic amines with CD3OD as C1 source was also explored. A few control experiments were carried out to gather proofs for the proposed mechanism of N-methylation reaction. Section 2.3 One 8-quinolyl tethered N-arylguanidines [(DG)N(H)(NHAr)C=NAr] (2.3.1) was prepared in 94% yield and fully characterized. The bridge–splitting reaction (bsr) of [η6-(p-cymene)Ru(μ-Cl)Cl]2 with guanidine 2.3.1 and a known guanidine 2.3.2 and the bsr of [(η6-C6Me6)Ru(μ-Cl)Cl]2 with known guanidines 2.3.3 and 2.3.4 afforded cationic complexes [η6-(p-cymene)Ru(NN)Cl]Cl (2.3.13 and 2.3.14) and [(η6-C6Me6)Ru(NN)Cl]Cl (2.3.15 and 2.3.16) in 83%-89% yields. The bsr reaction of [η6-(p-cymene)Ru(μ-Cl)Cl]2 with guanidine 2.3.3 in the presence of NH4PF6 in MeOH at RT afforded [η6-(p-cymene)Ru(NN)Cl]PF6 (2.3.17) in 90% yield. Molecular structures of guanidine 2.3.1 and complexes 2.3.13 and 2.3.15–2.3.17 were determined by SCXRD. Thirteen new complexes were screened as catalysts for Aldehyde-Water Shift (AWS) reaction of p-anisaldehyde at 0.1 mol% catalyst loading and 2.3.9 turned out to be the best catalyst. The scope of 16 substrates was explored and a plausible mechanism of AWS reaction is proposed.

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1. Introduction 2. Results and discussion 3. Supporting information. Synopsis, Abstract and Published work.

26. YADAV (Priya)
δ-MnO_2: A Suitable Cathode for Aqueous zinc-ion Battery.
Supervisor: Dr. Alok Kumar Rai
Th 28678

Abstract

With the increasing global demand for safe, sustainable, and cost-effective energy storage technologies, aqueous zinc-ion batteries (ZIBs) have emerged as a promising alternative to conventional lithium-ion batteries, particularly for grid-scale and stationary applications. Zinc is abundant, inexpensive and exhibits a high theoretical capacity, while aqueous electrolytes offer enhanced safety and environmental benefits. However, the development of efficient and stable cathode materials remains a major bottleneck for the commercial realization of aqueous ZIBs. The current thesis focuses on δ-MnO2, a polymorph of manganese dioxide with a layered structure, as a potential cathode material for aqueous ZIBs. δ-MnO2 is attractive due to its high theoretical capacity, enough layered spacing to accommodate Zn^{2+} ions, and relatively simple and cost-effective synthesis. Despite these advantages, challenges such as structural degradation and poor cycling stability caused by Jahn-Teller distortion due to the in-situ formation of Mn3+, which eventually limits its long-term performances. First the through literature survey was done to study the electrochemical behaviour of δ-MnO2 cathode and explores strategies to overcome its limitations. Therefore, to enhance structural stability and suppress Mn3+-induced distortions, the use of novel dopants and modifying synthesis conditions are majorly focused. Before electrochemical measurements, the systematic characterizations were used to analyse the purity, porosity, morphology, thermal stability etc. of synthesized electrode materials. Electrochemical analysis including cyclic voltammetry, galvanostatic charge-discharge, and electrochemical impedance spectroscopy were used to check the suitability of fabricated δ-MnO2 cathode for aqueous zinc ion battery applications. They provide insights of the material's capacity, reversibility, rate capability and long-term cyclability properties. The obtained findings demonstrate that the used strategies in the current work for δ-MnO2 cathode exhibits excellent cycling performances, enhanced Zn2+ diffusion, and high structural integrity over prolonged operation. This work concludes that the engineered δ-MnO2 has high potential as cathode material for aqueous ZIBs and offers valuable insights for the development of next-generation, sustainable energy storage devices.

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1. Introduction 2. Synthesis procedure, characterization techniques and electrochemical measurements 3. High rate capability of oil bath synthesised δ-MnO_2 cathode for aqueous zinc ion battery 4. Facile hydrothermal approach to fabricate pom-pom flower-like δ-MnO_2 cathode for aqueous zinc ion battery 5. Detailed study to investigate mitigation of Jahn-Teller distortion in δ-MnO_2 cathode using 3d and 4d block elements as dopants to enhance zinc-ion battery performance 6. Selective Mo doping in

δ-MnO2 cathode for ultra-long cycling life and highly reversible insertion/extraction mechanism for aqueous zinc ion battery. Summary of the work, Future scope, List of publications and Conferences attended.

27. YOGESH KUMAR

Development of Nanomaterials Modified Conducting Paper Based Biosensors for Swine Flu Detection.

Supervisors: Prof. S. K. Awasthi and Prof. Suveen Kumar

Th 28218

Abstract

The increasing need for advanced biosensing technologies has led to the development of highly flexible substrates capable of reliable and sensitive detection of biomolecules. In biosensing applications, various conducting substrates like glassy carbon, indium tin oxide (ITO), and gold-coated glass substrates are commonly employed. However, their rigidity, brittleness, and high cost restrict their suitability for developing wearable, flexible, cost-effective, and disposable point-of-care devices. To overcome such limitations, this Ph.D. thesis presents the development of flexible and environment friendly paper-based sensors integrated with conducting polymer (PEDOT:PSS) [poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate)] and various 2D nanomaterials like Borophene and Hydrogen substituted graphdiyne for the detection of Serum Amyloid A (SAA); a promising swine flu biomarker. These nanomaterials display intriguing characteristics, including high surface-to-volume ratio, enhanced surface reactivity, efficient catalytic properties and robust adsorption capabilities, making them promising candidates for biosensor fabrication. The anti-SAA was immobilized via drop cast approach and further bovine serum albumin (BSA) was used to block the non-specific binding sites for the fabrication of efficient biosensing platform. The comprehensive analyses using spectroscopic and electrochemical methods confirm the successful fabrication of these biosensors and their high sensitivity in detecting SAA. The sensors demonstrate significant potential in distinguishing between healthy and infected swine flu patients, showcasing excellent biosensing parameters. Furthermore, the practical applicability of these sensors is validated through electrochemical response tests conducted with spiked serum samples, which exhibit a high correlation with standard sample results. Among these fabricated biosensors, the Phosphorus doped hydrogen substituted graphdiyne (P-HsGDY) based platform surpasses other platform in terms of broader linear detection range, higher sensitivity and lower limit of detection. This thesis work highlights the promising future of flexible conducting paper-based biosensors in the field of medical diagnostics, offering both high sensitivity and practicality for real-world applications.

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