

CHAPTER 9

CHEMISTRY

Doctoral Theses

01. AGGARWAL (Priyanka)
Some Aspects of 2-D N-e ($N \geq 2$) Quantum Dots in Arbitrary Magnetic Field Via Exact Formalism of Multipole Expansion.
Supervisor: Dr. Ram Kuntal Hazra
Th 23277

Abstract
(Not Verified)

The thesis portrays a novel methodology to handle coulomb (exchange) correlations of 2-D N-e ($N \geq 2$) harmonically confined quantum dot systems in a perpendicular magnetic field (symmetric gauge) using variational method. Chapter 1 provides a glimpse of important aspects of 2-D N-e systems like quantum dots, mathematical tools, approximate methods and numerical methods. Chapter 2 constructs the formalism to evaluate coulomb (exchange) correlations for 2-D 2-e into an absolutely finite summed Lauricella function and single-summed form via Chu-Vandermonde identity. Chapter 3 focuses on the synergic effect of e-e interaction, role of confinement strength (ω), magnetic field (ω), mass of the carrier (m) and dielectric constant (ϵ) of the medium on energy level spectra, level-spacing statistics of interacting and non-interactive systems. Chapter 4 examines specific heat capacity (C) and magnetization (M) of 2-D 2-e quantum dot against ω at $T \sim 1K$ for various systems. e-e correlation causes peak structure in C and sharp discontinuity in magnetization near crossing points. Chapter 5 build up a formalism to solve N-e ($N \geq 2$) systems by coordinate expansion of individual particle in neighborhood of other coordinates resulting into fascinating multipole (order of pole P) expansion with dipole- and coulomb-type of integrals into finitely single-summed form of Lauricella functions via Chu-Vandermonde identity. Chapter 6 analyzes the impact and interplay of e-e interaction, ω , ω , m and ϵ on electronic structures and statistics of different materials (He, Li, Be, GaAs and BN) for $N \geq 2$ with ω . The order of the pole up to $P=2$ (quadrupole) suffices the convergence of the bound states. Chapter 7 assays C_v and M of $N \geq 2$ quantum dot with ω at $T \sim 1K$ for various systems. Chapters 8 constitutes the study of chemical potential with ω and addition spectra against number of electrons for N-e quantum dot systems. Further, characterize into strongly and weakly degenerate fermions.

Contents

1. Introduction 2. Formalism of 2-D 2-e quantum dot 3. Energy level diagram and statistics of 2-D 2-e quantum dot 4. Specific heat (C_v) and magnetization (M) of 2-D 2-e 5. Formalism of 2-D N-e ($N > 2$) quantum dots 6. Energy level diagram and statistics of 2-D N-e quantum dot 7. Specific heat (C_v) magnetization (M) of 2-D N-e 8. Chemical potential of 2-D N-e quantum dot 8. Chemical potential of 2-D N-e quantum dot.

02. AKSHAY KUMAR
Corrosion Inhibition of Mild Steel in Acidic Media by Using Schiff Bases Derived from 4-Amino Antipyrine.
Supervisor: Prof. Gurmeet Singh

Th 23308

Abstract
(Not Verified)

Corrosion has been a very important field of science, if not taken proper care, can result in extensive damage to the extent that a country loses about 6-8% of its G.D.P. It has been a focus of scientific research for over two centuries. It is a spontaneous process commonly referred to the deterioration of a particular material (usually a metal) or its characteristics by its interaction with the environment. There are number of methods to protect this or minimize this though this science of corrosion prevention and its control is very complex, compounded by the fact that corrosion takes many different forms and is affected by numerous outside factors. Mild steel is an extensively used alloy in construction industries and is severely affected by corrosion. There are numerous methods of protection of this but out of all the methods known in literature, use of corrosion inhibitors is one of the best, most economic, effective and easy to use methods. Therefore in this research work number of Schiff bases have been synthesized and characterized for use as corrosion inhibition in Sulphuric acid medium by a variety of techniques namely: Galvanostatic polarization studies, electrochemical impedance spectroscopy, temperature kinetic studies, quantum chemical calculations, scanning electron microscopy, atomic force microscopy and the inhibitors so synthesized were 1,5-Dimethyl-4-((4-methylbenzylidene)amino)-2-phenyl-1H-pyrazol-3(2H)-one (L1), 1,5-Dimethyl-2-phenyl-4-[(3, 4, 5-trimethoxybenzylidene)-amino]-1, 2-dihydro-pyrazol-3-one (L2), 4-[(4-Methoxy-benzylidene)-amino]-1, 5- dimethyl-2-phenyl-1,2-dihydro-pyrazol-3-one (L3), 4-[(3, 5-Dimethoxybenzylidene)-amino]-1, 5- dimethyl-2-phenyl-1,2-dihydro-pyrazol-3-one (L4), 1,5-Dimethyl-2-phenyl-4-[(2-prop-2-ynyloxy-benzylidene)-amino]-1, 2-dihydro-pyrazol-3-one (L5), 1,5-Dimethyl-2-phenyl-4-[(thiophen-3-ylmethylene)-amino]-1, 2-dihydropyrazol-3-one (L6).

Contents

1. Introduction 2. Literature review 3. Experimental procedure 4. Gravimetric polarization studies 5. Electrochemical impedance spectroscopy 6. Temperature kinetics study 7. Quantum chemical analysis 8(a). Surface morphological study-I: scanning electron microscopy 8(b). Surface morphological studies-II: atomic force microscopy 9. Conclusions and publications.

03. ARORA (Smriti)
Chemical Reactions of Selected Porphyrinoids and Polyaromatic Hydrocarbons.

Supervisor: Prof. Ramesh Chandra and Prof. S.M.S. Chauhan
Th 23285

Abstract
(Not Verified)

A photoactive mimic incorporating an electron donor, an electron acceptor, and 1,2,3-triazole moiety has been developed using clicked triazole porphyrin ligands, inverse and regular, with their corresponding heteroleptic Ru(II) conjugates. The energies of the orbital in the conjugates depend on ligand/linker, connecting pattern of linker, and the metal ion in the porphyrin core. The structural changes in porphodimethene, bearing 3,5-di-*tert*-butyl-4-hydroxyphenyl, on tautomeric conversion from the phenolic to oxo state have been studied. Oxoporphyrinogen formation takes place in presence of polar solvents or TBAOH, while, fluoride interacts with the inner core of oxoporphyrinogen only in presence of DMSO. The fused PAH system have been incorporated in the conformationally flexible porphodimethene ring and a conformational change from the usual rooftop or cone shaped with increase in PAH units is observed. The diprotonated form of PAH porphodimethene shows a bathochromic shift in UV visible, accompanied by colour change from yellow to dark pink as a result of increase in conjugation, a result of non planarity. The PAH substituted porphyrin system and

the accompanied structural changes depending on their states of protonation and relative susceptibilities to oxidation have been studied. Such systems show hyperporphyrin effect upon protonation and oxidation followed by colour changes from purple to green. Moreover, cyclodehydrogenation in trans-HPB substituted porphyrins have been studied. The sulfonation of largest sp hybridized polyaromatic graphene sheet and its adsorption properties for organic cationic dyes have been studied and found to be dependent on adsorbent dosage, dye concentration, contact time, and pH. The adsorption is found to be maximum for methylene blue being cationic in nature and while rhodamine B is adsorbed to a lesser extent.

Contents

1. Synthesis of triazole linked ruthenium (II) porphyrins their photophysical and electrochemical studies 2. Synthesis of solvatochromogenic 5,15-porphodimethenes and their application in anion binding 3. Synthesis of polyaromatic substituted porphodimethene and their conformational changes upon acid binding 4. Synthesis of polyaromatic linked porphyrin as model for functional grapheme in the development of newer materials 5. Synthesis of sulphated graphene and their application as an effective adsorbent towards cationic dyes.

04. ARVIND KUMAR

Design, Synthesis and Characterization of Newer Antimalarial Tetraoxanes, Modified Peptide Nucleic Acids and Catalytic Activity of SnCl₂-nano-SiO₂ Catalyst.

Supervisor: Prof. Satish K. Awasthi

Th 23316

Abstract
(Not Verified)

The thesis entitled “*Design, Synthesis and Characterization of Newer Antimalarial Tetraoxanes, Modified Peptide Nucleic Acids and Catalytic Activity of SnCl₂-nano-SiO₂ Catalyst*” are presented in four chapters: Chapter I focuses on the selection of an appropriate catalyst for one-pot synthesis of newer *N*-Benzoylpiperidine 1,2,4,5-tetraoxane analogs. Three Mo(VI) catalysts were tested. The synthesized 1,2,4,5-tetraoxane analogs were tested for their antimalarial activity *in vitro*. The results of the optimized catalyst and antimalarial activities against *Plasmodium falciparum* are included. Chapter II describes the one-pot synthesis of five series of piperidine tethered triazinetetraoxane hybrids using MoO catalyst, which was optimized in chapter I. The five series of synthesized piperidine tethered triazine-tetraoxane hybrids were tested for their antimalarial activity *in vitro*. The results of antimalarial activities against *Plasmodium falciparum* are included. Chapter III discusses about the design and synthesis of β-D-Thioglycosylated, 1,2,3- Triazole linked acetylated glycoside and lactoside, and Triazolylphosphonate PNA monomers. The use of these PNA monomers in future for solid-phase peptide synthesis of sequence-specific PNA oligomers for antisense inhibition of their respective genes is also discussed. Chapter IV compares the catalytic activities of heterogeneous SnCl₂-nano-SiO₂ catalyst with homogeneous SnCl₂ catalyst for the synthesis of 5-substituted-1H-tetrazoles. The results regarding the better catalyst for tetrazole synthesis have been included.

Contents

1. Molybdenum trioxide catalyzed one-pot synthesis of newer mixed *N*-benzoylpiperidine 1,2,4,5-tetraoxane analogs and their *in vitro* anti-malarial activity 2. Molybdenum trioxide catalyzed one-pot synthesis of piperidine tethered triazine-tetraoxane hybrids and their *in vitro* antimalarial activity 3. Design and synthesis of

β -D- thioglycosylated, 1,2,3-triazole linked acetylated glycoside and lactoside and triazolylphosphonate PNA monomer 4. Heterogeneous stannous chloride supported silica nanoparticles as catalyst in the synthesis of 5-substituted -1H-tetrazole 5. Summary and list of publications.

05. ASTHANA (Sonal)
Development of Catalyst and Process Studies for Direct Synthesis of Dimethyl Ether from Syngas.
 Supervisor: Prof. R. K. Sharma, Dr. Basudeb and Dr. Ravi Kumar Vollapalli
Th 23779

Abstract
 (Not verified)

The thesis entitled "Development of catalysts and processes for direct synthesis of Dimethyl Ether from syn-gas" has been divided into five Chapters. Chapter-I: This chapter describes introduction and background information on the synthesis of dimethyl ether (DME). DMF can be synthesized from syn-gas via (1) a two-step process in which syn-gas is converted to methanol and then methanol is dehydration and (2) one-step direct synthesis in which the two sequential reactions take place in the same reactor. Both the processes employ Cu-based catalysts consisting of different promoters. Details of these processes are included in the chapter. Chapter-II: In this chapter we have listed the general methods used for the preparation of catalysts. A brief description about the characterization techniques of the catalyst has been given. The reactor details and general experimental procedures for studying direct conversion of syn-gas to DME have been discussed. Chapter-III: In this chapter, the role of MgO as a promoter in Cu based catalysts for direct DME synthesis from syngas has been discussed along with identifying a suitable methanol dehydration agent. Chapter-IV: This chapter discloses the effect of different Cu:Zn ratio in the catalyst on the conversion of syngas to DME. A relation between physicochemical characteristics and activity of the catalyst has been established. Chapter-V: This chapter presents the synthesis of a novel Cu based catalyst prepared through glucose assisted precipitation using Fehling's solution for direct synthesis of DME from syngas. A study related to the effect of aging temperature and using sub-stoichiometric amount of precipitating agents for catalyst preparation is also presented.

Contents

1. Introduction and background 2. General methods and techniques for catalyst synthesis, characterization and activity evaluation 3. Promoting DME synthesis: Elucidating the role of MgO as a promoter in Cu/ZnO catalyst 4. The effect of varying Cu:Zn ratio on direct conversion of syngas to DME 5. Synthesis of a novel Cu₂O-ZnO/MgO catalyst using glucose assisted precipitation route with Fehling's solution for direct conversion of syngas to DME. Final summary and conclusion.

06. BADRI PARSHAD
Chemo-Enzymatic Synthesis of Polymeric and Dendritic Architectures for Biomedical Applications & Synthesis of Biologically Potent Heterocyclic Compounds.
 Supervisor: Prof. Sunil K. Sharma
Th 23310

Abstract
 (Verified)

Describes the synthesis, characterization and bio-medical applications of polymeric/dendritic architectures and heterocyclic compounds. The polymeric/dendritic architectures were synthesized by chemo-enzymatic approach using *Candida antarctica* lipase (Novozym 435) and measured for their size and self-assembly behavior in aqueous medium. The size of the resulting nanostructures formed in aqueous solution was studied using dynamic light scattering (DLS) and TEM measurements. They further were investigated for their transport behaviour using

hydrophobic drug/dye in aqueous medium. We also synthesized small heterocyclic compounds, *i.e.* imatinib analogues and coumarin derivatives to study their kinases inhibition potential and antioxidant activity, respectively. In lieu of the remarkable clinical success of the drug imatinib, many different imatinib analogues have been synthesized, wherein, the head portion of imatinib (PPAP scaffold) was coupled with different pharmacophores and screened for their kinase inhibitory potential. In addition, triazole derivatives containing PPAP scaffold were also synthesized by taking into consideration the bioisosteric nature of triazole and amide. Of all the compounds synthesized, five representative compounds were evaluated for their Abl1 and c-Src kinase inhibitory activity. In addition to this, we have synthesized thirteen di- and trihydroxycoumarins and studied the effect of hydroxyl groups on the antioxidant potential. The synthesized derivatives were characterized from their physical and spectroscopic data and were evaluated for their AOA by using three *in vitro* antioxidant assays (DPPH, ABTS, and LPO). The AOA of compounds has been compared with 'Trolox' taken as a standard and the results have been expressed as Trolox Equivalence Antioxidant Capacity (TEAC).

Contents

1. Chemo-enzymatic synthesis of perfluoroalkyl-functionalized dendronized polymers as cyto-compatible nanocarriers for drug delivery applications 2. Dendrimers as cyto-compatible nanocarriers: synthesis and study of their self-assembly and transport behaviour 3. Pyridylpyrimidinylaminophenyl derivatives: synthesis and evaluation of their kinase inhibitory potential 4. Synthesis and SAR study of antioxidant potential of polyhydroxy coumarin derivatives 5. Summary.

07. BATRA (Neha)

Synthesis and Antimalarial Activity of Sulfonamide Based Nitrogen and Oxygen Containing Heterocycles.

Supervisor: Prof. M. Thirumal

Th 23276

Abstract (Not Verified)

The main objectives of this dissertation are to synthesize diversity oriented sulfonamide based nitrogen and oxygen containing heterocycles as antimalarial agents. Sulfonamides are an important class of biologically relevant compounds and occupied a unique place in medicinal chemistry. The drugs containing sulfonamide scaffolds were firstly introduced as antibacterial agents during the era of Second World War. Later, the compounds of this class have shown their ability to act as anti-viral, anti-carbonic anhydrase (CA), diuretics, cyclooxygenase (COX)-2 inhibitors, anticancer, cysteine protease inhibitors and aspartic HIV protease inhibitors. Additionally, they have also been found useful for treating eye infections, influenza, meningitis, actinomycosis and fungal infections. Presently, 22 drugs having sulfonamide framework are either being used or under clinical trials including carbonyl anhydrase inhibitors, COX inhibitors and epileptic drugs. The work presented in this thesis is divided into five chapters. The first chapter presents a brief account on the biological significance of sulfonamides. Chapter 2 discusses about the synthesis and antimalarial activity of sulfonamide tethered [1,2,3]-triazoles. Chapter 3 describes the synthesis of various 7-chloroquinoline tethered sulfonamides and sulfonamidequinoline-[1,2,3]-triazole hybrids and their antimalarial efficacy against malaria parasite *Plasmodium falciparum* (3D7 strain). Chapter 4 deals with the synthesis of a novel series of berberine-sulfonamide-[1,2,3]-triazoles and study of their potential to be used as antimalarial agents. Chapter 5 includes the synthesis, spectroscopic characterization and evaluation of *invitro* antimalarial activity of various sulfonamide-coumarin based [1,2,3]-triazoles. The preliminary *in-vitro* screening results are found to be encouraging and may prove useful for the future development of new antimalarial agents.

Contents

1. Biological significance of sulfonamides: An overview 2. Synthesis and antimalarial evaluation of novel [1,2,3]- triazole tethered sulfonamides 3. Synthesis and antimalarial efficacy of sulfonamide- quinolone and sulfonamide-quinoline [1,2,3]-triazole conjugates. 4. Synthesis of sulfonamide –berberine-[1,2,3]-triazole conjugates as a new class of antimalarials. 5. Synthesis, characterization and antimalarial activity of sulfonamide based coumarin-[1,2,3]-triazole conjugates 6. Summary and publications.

08. BEIG (Subzar Ahmed)

Convolution and Linear Combinations of Harmonic Mappings.

Supervisor: Prof. V. Ravichandran

Th 23769

*Abstract
(Verified)*

A harmonic mapping in the plane is a complex-valued function whose real as well as the imaginary parts are real harmonic mappings. Earlier these mappings were studied by the differential geometers for the minimal surface. With the paper entitled "Harmonic univalent functions, Ann. Acad. Sci. Fenn. Ser. A I Math. 9 (1984), 3-25" of Clunie and Sheil-Small, wherein they studied these mappings as the natural generalization of analytic mappings for the geometric as well as the analytic mapping properties, these mappings became interest of the function theorists. Finding the univalent harmonic mappings whose convolution or a linear combination carries the univalence or any geometric property, such as convexity, starlikeness, close-to-convexity or directional convexity etc, are important problems in the theory of harmonic mappings. This thesis studies the univalence and the directional convexity of these two combinations of the univalent harmonic mappings normalized suitably in the open unit disk D with centre at the origin. The harmonic mappings considered here are the one whose convolution or the linear combination considered are shears of some directional convex analytic mappings. This, in view of the Clunie and Sheil-Small's method of *shear construction*, gives the directional convexity of these combinations provided they are locally univalent and sense-preserving. Also, it is shown that the dilatation of these combinations lies in D for some of the mappings by direct calculations or by the *Cohn's rule*. This, in view of the Lewy's theorem, shows the local univalence and the sense-preservation of these combinations.

Contents

1. Introduction 2. Directional convexity of the convolution of harmonic mappings 3. Local univalence of the convolution of harmonic mappings 4. Convolution of harmonic mappings with n -starlike mappings 5. Convex combination of harmonic mappings 6. Linear combinations of harmonic mappings. References. Index.

09. BISHT (Meena)

Understanding the behavior of Proteins in the Presence of Ionic Liquids

Supervisor: Dr. P. Venkatesu

Th 23773

Contents

1. Introduction and review of the literature 2. Materials and experimental techniques 3(a). Influence of alkylammonium-based ionic liquids on the stability and activity of lysozyme 3(b). Refolding effects of alkylammonium-based ionic liquids on the urea-induced unfolded lysozyme structure 4(a) Influence of amino acid-based ionic liquid on the stability and activity of stem bromelain: comparative study between [Bmim] and [Bmim][Gly] 4(b). Influence of amino acid-based ionic liquid on the stability and activity of stem bromelain: comparative study between [Ch][Br] and [Ch][Gly] 5. Influence of choline-based ionic liquids on the stability of α -chymotrypsin (CT) 6. Influence of pH seitchable choline-based ILs on the stability and activity of cytochrome C 7. Conclusions.

10. BISHT (Yogita)
Mucrowave Dielectrics: Understanding the Reproducibility Issues in Complex Perovskites.
 Supervisor: Prof. M. Thirumal
Th 23305

*Abstract
(Verified)*

The complex perovskite ceramics, $A(B' B'')O$ where $A=Ba, Ca, Sr$; $B'=Mg, Zn$; $B''=Ta, Nb$; have attracted tremendous attention because they exhibit excellent dielectric properties at microwave frequencies and hence used in wireless communications. Thesis has been divided into four chapters Chapter I discuss general introduction of the thesis with the basic classification of materials, structure, synthesis and tools used to characterize the materials and their properties. Chapter II discuss Ba-Mg-Ta complex perovskites. This chapter has been further divided into four parts: The first part discuss solid solution and composite range for $(1-x)Ba(MgTa)O - (x)Ba(MgTa)O$ ($0 < x < 1.0$) by solid state method. The second part discuss the synthesis of a new hexagonal twinned 8-layer phase $BaMgTaO$ using $BaZnTaO$ topotaxy. The third part of this chapter discuss synthesis and characterization of $(1-x)Ba(MgTa)O - (x)[Ba(MgTa)O$ with $Ba(ZnTa)O]$ ($0 < x < 0.05$) by topotaxy process. The fourth part of this chapter discuss synthesis of $(1-x)Ba(MgTa)O - (x)Ba(MgTa)O$ ($0 < x < 1.0$) by one pot metathesis process. All the ceramics synthesized in the chapter II were systematically characterized and their properties were reported in detail. Chapter III discuss the Ba-Mg-Nb complex perovskite system. This chapter discuss synthesis and characterization of $(1-x)Ba(MgNb)O - (x)Ba(MgNb)O$ ($x = 0, 0.005, 0.01, 0.02$). The microwave dielectric properties are in the range: $\epsilon \sim 31$, $Q.f$ between 37000 to 74000 GHz, τ varies between 21 - 24 ppm/ $^{\circ}C$. Chapter IV discuss the synthesis of new members of $BaMM'O$ system, where $M=Co, Mg, Zn$ and $M'=Ta, Nb$ by one pot metathesis process. For most of the compositions XRD pattern shows reflections due to both $BaMM'O$ and $BaMM'O$ phase. Promising dielectric properties were observed for all the compositions in MHz frequencies. Attempt to synthesize $BaMgNbO$ at $1350^{\circ}C$ led to tri phasic mixture of $Ba(MgNb)O, BaMgNbO$ and $BaNbO$.

Contents

1. Introduction 2. Ba-Mg-Ta system 3. $Ba_8MM'_6O_{24}$ ($M=Zn^{2+}, Co^{2+}, Mg^{2+}$ and $M'+Ta^{5+}, Nb^{5+}$) by one pot metathesis process. Publications and conferences.

11. CHAKRABORTY (Pinki)
Synthesis Characterization and Applications of Selected Novel Inorganic, Organic and Hybrid Layered Compounds.
 Supervisor: Prof. Rajamani Nagarajan
Th 23284

Abstract
(Not Verified)

Describes the synthesis of inorganic and organic layered materials and fabrication of inorganic layered solids with PMMA was studied. In chapter 1, a brief outline on the synthetic methods employed for the generation of layered materials. Chapter 2 deals with the synthesis of acetate containing layered double hydroxides (LDHs) and their usage in various applications. Section 2.1 deals with synthesis and characterization of acetate containing zinc- yttrium LDH. Additionally, attempts to synthesize LDH with organic anions and dodecylsulfate (DS) by self-assembly process was attempted and used for removal of dyes. In section 2.2, results of the trials involving hydrolysis of manganese salts using bromine water and hydrogen peroxide (H₂O₂) have been presented. For acetate salt, drastic change was noticed in PXRD and was used for oxidation and reduction processes and its role as contrast agent in MRI. Section 2.3 describes the generation of compounds holding Ni and La by hydrolysis and mechano-chemical route and their characterization using techniques. Section 2.4, the synthesis and characterization of layered salts consisting zinc and transition metals (Mn, Fe, Co and Ni) by co-precipitation method using KOH. Section 2.5 describes the simultaneous hydrolysis of acetates of Ca and Y or Gd. Synthesis and characterization of LDHs by co-precipitation is challenging because of formation of calcium carbonate. In Chapter 3, a single step polymerization of aniline using H₂O₂ and transition metal salts has been described and its adsorption capacity towards methyl orange (MO) dye was studied. Chapter 4 deals with use of acetate intercalated Zn-La, Zn-Y, Ni-La and DS-intercalated Zn-Y LDH to obtain PMMA composites. The dispersibility of composites was studied by PXRD and TEM analysis. General conclusions arising from these investigations along with futuristic prospects are presented at the end.

Contents

1. Background of the research work
 2. Inorganic layered compounds
 3. Ordered organic polymers
 4. Inorganic- organic layered polymer compounds
 5. Conclusions and list of publications
12. CHAUDHARY (Swati)
Characterization of DNA Structures Formed at Single Nucleotide Polymorphic (SNP) Sites of Human GRIN1 and APOE Genes.
 Supervisor: Prof. M. Thirumal
 Th 23275

Abstract
(Not Verified)

The unusual secondary structures formed by repetitive DNA sequences provide an alluring platform to study their role in gene regulation. The occurrence of Single Nucleotide Polymorphism (SNP) in a regulatory region of a gene may influence the gene's function which could play a role in human diseases. The DNA makeup can be altered due to distinctive secondary structures formed at genomic SNP sites which may influence the gene expression. In this work, the promoter region of human *GRIN1* gene and the coding region of human *APOE* gene were investigated in search of significant SNP sites. In *GRIN1* gene, -855(G/C) site was found to be associated with Schizophrenia syndrome in some population, while +2985(T/C) of *APOE* gene was known to be involved in Alzheimer's disease (AD). Structural characterization of these SNP sites was carried out in order to understand the etiology of concerned diseases. With the help of several biochemical and biophysical studies, it was found that the G-rich promoter sequence of *GRIN1* gene containing G-allele (GRIN1) forms an octameric parallel G-quadruplex structure, while its C-counterpart (GRIN1M) remains unstructured single stranded. A base change from G→C unable the sequence to form G-quadruplex structure which might be playing a significant role in the normal functioning of the gene, while single stranded C-allele

might result in reduced gene expression. A GC-rich sequence of *APOE* gene containing T-allele (APOE22T) represents the APOE3 isoform of the gene. It forms hairpin at low strand concentration and antiparallel G-quadruplex at high strand concentration, while its C-allele (APOE22C) representing APOE4 isoform forms hairpin as well as duplex structures at all the strand concentrations. The structural difference between the two alleles results in the altered gene expression leading to AD. Also, the G-quadruplex-berberine interaction studies were performed to enhance our knowledge of efficient quadruplex-binding ligands.

Contents

1. Introduction 2. Materials and methods 3. Bioinformatics analysis of *GRIN1* and *APOE* genes 4. Structural characterization of DNA sequence having SNP site of Human *GRIN1* gene promoter region 5. Structural characterization of DNA sequence having SNP site of Human *APOE* gene coding region. 6. G-quadruplex-ligand interactions 7. Conclusions and bibliography.

13. CHAUHAN (Himani)
Synthesis, Characterization and Applications of a Few Nanostructured Metal Chalcogenide Semiconductors.
 Supervisor: Dr. Sasanka Deka
Th 23775

Contents

1. Introduction to metal chalcogenic semiconductors and their applications 2. Experimental details for synthesis, characterization and application of nanostructured materials 3. Interesting optical properties of 2D CdSe/CdS core@shell dot-in-hexagonal platelet nanoheterostructures and its gold hybrid (CdSe@CdS-Au) for photocatalysis under direct sun light 4. Graphene stacked SnS₂ nanodiscs and nanosheets with efficient carrier separation for photocatalyzed multiple reactions 5. Development of surfactant free SnS nanorods, SnS₂ nanosheets and RGO/SnS₂ nanocomposites synthesized by solvothermal/hydrothermal route as new supercapacitor material 6. Direct partial cation exchange of Cd⁺² by Zn⁺² in 2D hexagonal CdSe/CdS core@shell. Summary of the thesis. Future scope of work. List of publications.

14. CHOPRA (Rashi)
Study of Corrosion Inhibition Properties of some Pyrazine Compounds for Mild Steel Corrosion in Sulphuric Acid.
 Supervisor: Prof. S.M.S. Chauhan
Th 23296

*Abstract
(Verified)*

The thesis focuses on the study of corrosion inhibition properties of some pyrazine compounds for mild steel corrosion in sulphuric acid. Chapter 1-Introduction It deals with the introduction to the world of corrosion and electrochemical aspect of corrosion. Chapter 2-Literature Survey The literature review of the work done in the area of corrosion of mild steel in acidic medium and use of inhibitors as a competent method to control corrosion has been described. Chapter 3- Experimental Procedure It explains the experimental setup and procedure undertaken for different techniques. Chapter 4- Gravimetric Measurements This chapter involves the principles and results of the most primitive gravimetric technique employed. Chapter 5- Electrochemical Impedance Spectroscopy (EIS) This chapter summarizes the investigation of inhibition characteristics of pyrazine compounds using

electrochemical technique. Chapter 6- Galvanostatic Polarization and Linear Polarization Resistance Technique Galvanostatic polarization and Linear Polarization Resistance studies were carried out to show the extent of corrosion inhibition. Chapter 7- Potentiostatic Polarization Technique This chapter describes the establishment of the passive behavior of all the inhibitors. Chapter 8- Temperature Kinetics Study This deals with the effect of temperature on the corrosion rate and calculation of various thermodynamic parameters for the adsorption process of inhibitor moiety on mild steel using temperature kinetics. Chapter 9- Quantum Chemical Calculation This chapter discusses the Quantum chemical or theoretical calculations using Hyperchem 8.0.6 package to supplement the experimental findings of other techniques. Chapter 10-Surface Morphological Studies Scanning electron microscopy (SEM)-Energy Dispersive Atomic X-Ray (EDAX) spectroscopy and Atomic force microscopy (AFM)) were carried out on inhibited and uninhibited mild steel samples to analyze their surface morphology. Chapter 11- Conclusion All the results obtained from different techniques were in good correlation each other, indicating that the studied pyrazine derivatives act as efficient inhibitors against corrosion of mild steel in acidic medium.

Contents

1. Introduction 2. Literature review 3. Experimental procedure 4. Gravimetric measurements 5. Electrochemical impedance spectroscopy 6. Galvanostatic polarization technique 7. Potentiostatic polarization technique 8. Temperature kinetics studies 9. Quantum chemical calculations. Surface morphological studies 11. Conclusions and list of publications.

15. DHANDA (Ritu)
Synthesis of Graphene-Supported Metal Alloy and Mixed-Metal Oxide Nanocatalysts for Organic Transformation Reactions.
 Supervisor: Prof. M. Kidwai
Th 23283

Abstract (Not Verified)

Due to important practical applications, graphene based nanocomposites (NCs) has attracted wide attention in the field of modern catalysis. The present research work represents synthesis, characterization of graphene based bimetallic alloy and mixed-metal oxide nanoparticles and their applications as highly efficient catalyst in industrially important organic transformation reactions. The observed application oriented results manifested the acceptability of these NCs as potential candidate to resolve many issues related to chemical science. During this research work, we have successfully synthesized various two component (Ag/graphene, Pd/graphene and Cu O/graphene) and three component (AgNi/graphene, RuNi/graphene, CuPd/graphene and CuFe O /graphene) nanostructures by *in situ* growth of nanoparticles over graphene sheets either via one pot co-reduction or co-precipitation method. Various compositions of different alloy nanomaterials were synthesized by varying precursor's amount. As-prepared nanostructure were well characterized by TEM, HR-TEM, FT-IR, SEM, STEM-HAADF, EDS, XRD, ICP, UV-Vis and Raman techniques to determine their phase purity, morphology and various intrinsic properties. Thereafter, present nanostructures were studied in catalytic studies which can be discussed as: 1. AgNi/graphene NCs were examined in nitroarenes reduction with ammonia borane and sodium borohydride as reductant. 2. RuNi/graphene ternary NCs were used in hydrogen production from ammonia borane hydrolysis and reduction of nitro/nitrile compounds. 3. CuPd/graphene NCs were employed for synthesis of propargylamines via cross dehydrogenative coupling between tertiary amine and terminal alkyne via C-H activation. 4. CuFe O /graphene NCs were used in oxidative coupling of various benzylamine to corresponding imines in neat condition. As-prepared NCs showed excellent catalytic properties owing to small sized, surfactant free nanoparticles, synergistic effect between various components, high electronic conductivity and large surface area. All NCs also showed excellent recyclability. In

addition, synthesis and catalytic mechanism for all NCs was proposed and discussed in thesis by examining various studies.

Contents

1. Introduction 2. Reduced graphene oxide supported AgNi alloy nanocatalyst for nitroarenes reduction reaction 3. Reduced graphene oxide supported RuNi alloy nanoparticles as a highly active catalyst for hydrolytic dehydrogenation-hydrogenation reactions 4. CuPd/RGO nanocomposites as a highly efficient catalyst for cross dehydrogenative coupling of tertiary amines with terminal alkynes 5. Magnetic CuFe₂O₄/RGO nanocomposites for solvent free oxidative coupling of amines to imines. 6. Summary, future scope and list of publications.

16. GAIJON (Panmei)
Synthesis, Characterization and Application of Clay Polymer Composites.
 Supervisor: Prof. Monika Datta
Th 23286

Abstract
 (Not Verified)

The objective of this work is to synthesize clay polymer composites which have advanced properties of pristine polymers. Due to the cost effective and light weight of the new hybrid composite materials have attracted a large number of researchers. This composite material was to be used as an alternative of the existing, non-renewable and as fire retardant materials. Polymer clay composite materials have attracted huge number of researchers due to its several advanced and optimized properties (electrical, thermal and mechanical) than constituents. These properties have explored its multi fold industrial applications such as adsorbent for water purification, barrier film for packaging, sheet for automobile and fire retardant coating film. Generally, formation of clay polymer composite generates adsorption capacity, expansively of clay optimizes hardness for automobiles, and mechanical properties for heat release. The significance of application of wide range polymer also symbolize with the term "Plastic Age" for current time. Thus, in recent times, many of the traditional materials like wood, stone, concrete and metals are replaced by the polymers and polymer industry is one of the burgeoning industries. On the basis of industrial applications three polymers including Polyvinyl chloride (PVC), Poly (methyl methacrylate) (PMMA) and Polystyrene (PS) were selected for synthesis of the clay polymer composite material and which was used in various fields on large scale as well as have various applications. These polymers were used for preparation of its clay composite.

Contents

1. Introduction to clay polymer composite 2. Recent review of literature 3. Methodology 4. Synthesis of poly (vinyl chloride)- organo vermiculite composite film 5. Synthesis of poly (methyl methacrylate)- organo vermiculite composite film 6. Synthesis of polystyrene-organo vermiculite composite film 7. Application of organo vermiculite polymer composite as flame retardant material 8. Summary of the reported work.

17. GOEL (Rahul)
Design, Synthesis and Characterization of Nanomaterials using Self-assembling β -Amino Acid Containing Model Peptide Systems for Biomedical Applications.
 Supervisor: Dr. Alka Gupta
Th 23278

Abstract
 (Not Verified)

Self-assembly play a vital role for the generation of nanosized peptide-based materials. These materials due to their biocompatibility have been considered to be very useful in drug delivery, tissue engineering, gene delivery, and other biomedical systems. Researchers have extensively worked in this area of research. In this area, a novel approach that has emerged in recent years with significant potential and improved physiological stability is the use of β -amino acids. Judicious substitution of α -amino acids with β -amino acids in the peptides of interest leads to mimic good to excellent stability, affinity and function. β -Amino acid residue is considered to be a valuable addition to ensemble of peptide backbone modifications. The aim of present research work was to design nanostructures based on β -amino acid sequences and make them potentially active for drug and/or gene delivery applications. This thesis entitled "Design, synthesis and characterization of nanomaterials using self-assembling β -amino acid containing model peptide systems for biomedical applications" includes: (i) designing short oligomers based on β -alanine using theoretical simulations which will have potential to self-assemble into vesicular structures, (ii) synthesis of designed peptide sequences by means of solid phase and/or solution phase peptide synthesis procedures and verifying their structural and self-assembling properties with theoretical results, (iii) investigation of the self/coassembling features of peptide sequences loaded with antiparkinson's drug L-Dopa, anticancerous drug curcumin and antiinflammatory/antipyretic drug aspirin, as the model drugs, (iv) the interactions between peptide nanoassemblies with the said drugs and model dye molecules eosin and fluorescein sodium salt, (v) study of encapsulation and *in vitro* release kinetics of peptide/drug conjugates, (vi) investigation of the cellular toxicity of peptide/plasmid DNA complexes and uptake.

Contents

1. Introduction 2. Materials and methods 3. Synthesis, characterization, and fabrication of nanostructures from self-assembling β -alanine homotetrapeptide, H- β Ala- β Ala- β Ala-NH₂, and their potential use in drug delivery applications 4. Synthesis, characterization, and fabrication of nanostructures from self-assembling amphiphilic mixed α/β -tetrapeptide, H- β Ala- β Ala-Lys-Ala-NH₂, and their potential use in drug delivery applications 5. Synthesis, characterization, and fabrication of cationic nanostructures from self-assembling amphiphilic mixed α/β -pentapeptide, H-Lys- β Ala- β Ala-Lys- β Ala-OEt, and their potential use in drug delivery and gene delivery applications 6. Summary, references and list of publications.

18. GOYAL (Madhusudan)
Electrochemical, Surface Characterization and Corrosion Inhibition of Mild Steel in Acidic Medium by Quaternary Phosphonium Compounds.

Supervisor: Prof. Gurmeet Singh

Th 23301

Abstract (Not Verified)

Corrosion is inevitable, but its effect can be substantially reduced". Corrosion control is processes aimed at reducing the rate of corrosion to a tolerable level. Among several methods of corrosion control/inhibit, such as cathodic protection, anodic protection, coating & alloying, etc., the use of inhibitors is one of the most practical/synthesize methods to secure metal against acid corrosion due to its excellent mechanical and cheap cost. The quality of a compound to serve as potent inhibitor is dependent on its ability to interact with π -orbital and/or nature of adsorption on a metal surface, electrostatic attraction between the charged metal and charged inhibitors molecules, capable of making bonds with the surface of metal through electron transfer, etc. The Quaternary phosphonium compounds fulfill the necessary requirements of being a good inhibitor of corrosion of metals. The thermally stable and therefore, these are suitable for reactions carried out even at higher

temperatures up to 400 K. Keeping this in mind, it was decided to explore some new compounds belonging to phosphonium class as corrosion inhibitors. The names of the phosphonium compounds are enlisted as follows:

1. Methoxycarbonylmethyl Triphenyl Phosphonium Bromide (MCMTPPB)
2. Decyl Triphenyl Phosphonium Bromide (DTPPB)
3. Isopentyl Triphenyl Phosphonium Bromide (IPTPPB)
4. Ethoxycarbonylmethyl Triphenyl Phosphonium Bromide (ECMTPPB)

The effect of these compounds on the corrosion of mild steel in 0.5 M H₂SO₄ was studied in the presence and absence of four organic inhibitors. The various techniques which were used to study corrosion inhibition are as follows:

1. Galvanostatic Polarization Studies
2. Electrochemical Impedance Spectroscopy
3. Temperature Kinetics Studies
4. Scanning Electron Microscopy
5. Atomic Force Microscopy
6. Quantum Chemical Calculations

• The results obtained from both experimental and theoretical studies indicated that the trend of the inhibition efficiency of inhibitors is:

$$\text{DTPPB} > \text{ECMTPPB} > \text{MCMTPPB} > \text{IPTPPB}$$

Contents

1. Introduction 2. Literature Review 3. Experimental Procedures 4. Galvanostatic Polarization Studies 5. Potentiostatic Polarization Studies 6. Electrochemical Impedance Spectroscopy 7. Temperature Kinetic Studies 8. Scanning Electron Microscopy 9. Energy Dispersive X-ray Spectroscopy 10. Atomic Force Microscopy 11. Quantum Chemical Calculations 12. Conclusions.

19. KATYAL (Divya)

Theoretical Models for the Dynamics of Star, Dendrimer and Comb-of-Comb Polymers in Random and Shear Flows.

Supervisor: Prof. Rama Kant

Th 23299

Abstract (Not Verified)

The objective of the present thesis is to develop a theoretical formalism to investigate the dynamics of flexible branched polymers with arbitrary topology in two types of external flows, viz., random and shear flows. Although the formalisms are generalized for various complex topologies of polymers, we have particularly focused on three important branched structures: stars, dendrimers and comb-of-comb-network polymers. The modeling of flexible branched polymers is done within the framework of generalized Gaussian structure approach while the random flow is accounted through Matheron-de-Marsily flow model. The dynamics is evaluated through relevant physical quantities, viz. average square displacement (ASD) and velocity autocorrelation function (VACF). The attempt has been made to understand the two main aspects. First is the effect of the polymer topology on the dynamics which is analyzed by varying the generations, spacer lengths, number and length of branches. Second is the influence of random flow on the dynamics by varying flow parameters, like flow exponent (α), root-mean-square velocity of flow (V_r) and flow strength (W_r). The dynamics of the flexible branched polymers displays an anomalous diffusive behavior in random flows where the larger polymers move faster than smaller ones. Moreover, we have investigated the impact of long-range hydrodynamic interactions (HIs) based on the preaveraged Oseen tensor. The introduction of the HIs in the random flows quantitatively speeds up the dynamics with the enhancement of the magnitude of the ASD. The stretching dynamics of star polymer with increasing flow strength predicts shape transition which involves initial radial symmetry to partial contraction followed by complete elongated radial contraction. This anomalous behavior with increasing flow strength shows analogy with the "swimming octopus". Finally the dynamics of flexible branched polymers in non-random steady shear

flows was analysed showing the expected behavior of larger polymers moving slower than smaller ones.

Contents

1. Introduction to the polymer dynamics 2. Dynamics of generalized Gaussian polymeric structures in random layered flows 3. Dynamics of branched polymers in random layered flows with intramolecular hydrodynamic coupling: star and dendrimer 4. Anomalous stretching dynamics of tagged monomer of branched polymer in random flows 5. Dynamics of comb-of-network polymers in random layered flows 6. Theory for the dynamics of arbitrary topology polymer under steady shear flows 7. Summary and future prospects.

20. KHANNA (Garima)
Development of Novel Synthetic Methodologies for the Synthesis of Oxazine , Triazole, Spirooxindole and Pyrimidine Hybrids using Green Approaches.
 Supervisor: Prof. J. M. Khurana
Th 23777

Contents

1. Synthesis of novel 1,3-oxazine hybrid heterocycles using multicomponent approach in green reaction media 2. Metal free synthesis of 1,4-disubstituted 1,2,3-triazoles and benzo/ naphtha-fused 1,2,3-triazoles 3. Catalyst free synthesis of spiro[indene-2,2'-naphthalene]-4'-carbonitriles and spiro[naphthalene-component reaction in ethylene glycol An efficient catalyst free synthesis of diversified bis(spirooxindoles) via one-pot three component reaction 5. An efficient one-pot synthesis of functionalized benzo[a]chromeno[2,3-c]phenazine derivatives via four component domino protocol using [NMP]H₂PO₄ 6. Summary and conclusions. List of publications.

21. KHOLIYA (Rohit)
Development of Facile Synthetic Strategies for Medicinally Important Molecules, Biological Evaluations and Mechanistic Investigations.
 Supervisor: Prof. Diwan S. Rawat
Th 23302

Abstract (Not Verified)

In chapter 1, the effect of structural modifications on the linker of the previously synthesized 4- aminoquinoline-pyrimidine hybrids has been studied in order to examine their antiplasmodial activity and pharmacokinetic behavior. The terminal free -NH of diamine linker was substituted with appropriate aryl/heteroaryl functionality (1,3-benzodioxole and thiophene). The resulted compounds showed moderate to excellent *in vitro* antiplasmodial activity against both the strains (W2 and D6) of *P. falciparum*. In addition, to understand the mechanism of action; heme binding and molecular docking studies of best active compounds were performed. ADME properties were predicted to assess the pharmacokinetic behaviour of the synthesized compounds. In chapter 2, molecular hybrids comprising indole-triazole and indole-pyrimidine pharmacophores have been synthesized since these pharmacophores are well known for their wide range of biological activities including anti-TB activity. Synthesized compounds were evaluated for their *in vitro* antimycobacterial activity against Mtb H37Rv strain which showed moderate activity. In chapter 3, benzothiazole and benzimidazole derivatives were designed as possible antitubercular

agents. This design was based on the literature that proposes functionalization of benzothiazole and benzimidazoles may improve their anti-TB activity. In chapter 4a, we explored the catalytic potential of tetrabutylammonium glycinate [TBA][Gly] ionic liquid for the one-pot, three-component synthesis of 3-substituted indoles and indolyl-4*H*chromenes. [TBA][Gly] ionic liquid was found to be an efficient, recyclable and biodegradable organocatalyst for selective synthesis of 3-substituted indoles and indolyl-4*H*-chromenes with excellent yields in short reaction time. In chapter 4b, a novel polyvinyl alcohol-sulphonic acid (PVA-SO₃H) catalyst has been synthesized and used for the *N*-formylation of different aromatic/aliphatic amines by utilizing simple formamides. Further, PVA-SO₃H catalyst is recyclable and is amenable to microwave synthesis which significantly shortened the reaction time to afford *N*-formylated amines.

Contents

1. N-H functionalized aminoquinoline-pyrimidine hybrids: effect on the Antiplasmodial Potency 2. Synthesis of indoleamide-triazole and indoleamide-pyrimidine hybrids as anti-tubercular agents 3. 2,6-disubstituted benzothiazole and 2,5-disubstituted benzimidazole derivatives as anti-TB agents 4a. [TBA][Gly] ionic liquid promoted multi-component synthesis of 3-substituted indoles and indolyl-4*H*-chromenes 4b. Polyvinyl alcohol-sulphonic acid (PVA-SO₃H): a novel and recyclable organocatalyst for *N*-formylation of amines under metal free and neat condition 5. Summary and Publications.

22. MALIK (Vidhu)
Synthesis and Characterization of Materials of Interest for Catalytic and Photocatalytic Applications by Solid State Chemistry Approach.
 Supervisor: Prof. S. Uma
Th 23294

Contents

1. Introduction 2. Investigation of bismuth containing materials 3. Investigation of oxides of lithium ion possessing rocksalt superstructure 4. Oxides and osynitrides containing rare earth (Ce³⁺, Sm³⁺, Gd³⁺, Dy³⁺, Y³⁺) cations 5. Appendices and list of publications.

23. MANCHANDA (Prinka)
Design and Synthesis of Kinase Inhibitors, Antimicrobial Agents.
 Supervisor: Prof. Sunil K. Sharma
Th 23317

Abstract (Verified)

The work presented in Chapter 1 entitled "Design, Synthesis and Evaluation of Kinase Inhibition Potential of Pyridylpyrimidinylaminophenyl Derivatives" describes the design and development of Pyridylpyrimidinylaminophenyl (PPAP) amides. Scaffolds based on benzopyran-2-one, benzopyran-4-one acids etc. have been conjugated with PPAP amine to form novel amide/cyclic amide derivatives and evaluated their kinase inhibition potency. The work presented in Chapter 2, entitled "Glucitol Based Cyto-compatible Non-ionic Amphiphilic Architectures for Encapsulation of Non-polar Dyes and Drugs" describes the design, synthesis and biophysical characterization of novel *D*-glucitol based non-ionic amphiphilic architectures constructed using biocompatible synthons as the hydrophilic component. Furthermore, aromatic units have been incorporated as hydrophobic part. Both, polar and non-polar components have

been grafted on glucitol backbone *via* '1,3-cycloaddition'. Self-assembling properties in an aqueous medium have been investigated *via* dynamic light scattering (DLS) and surface tension measurements. Applicability of the synthesized amphiphiles in bio-medical applications have been provided by evaluating their cytotoxicity profile in addition to the ability of the self-assembled aggregates to solubilize hydrophobic dyes and drugs. The work presented in chapter 3 entitled "Synthesis of Triazolylated Quaternary Ammonium Derivatives of Benzopyran-2-ones as Lead Antimicrobial Agents" describes the synthesis of twelve novel compounds conjuring varied pharmacophores i.e. benzopyran-2-one, triazole unit, alkyl chain and quaternary ammonium group. All of the synthesized triazolylated benzopyran-2-one derivatives, were screened for antibacterial activity against four pathogenic bacterial strains. The compound bearing C alkyl chain, methoxy substituents at C-5 and C-7 position and the quaternary ammonium group was found to be most active. The work presented in chapter four entitled "Pathogen Sensing by Boronic acid Functionalized 2D Nanomaterials" describes the synthesis of boronic acid functionalized covalently modified thermally reduced graphene oxide. The modified graphene was subsequently employed for sensing of pathogenic *E.coli* using fluorescence spectroscopy.

Contents

1. Design, synthesis and evaluation of kinase inhibition potential of pyridylpyrimidinylaminophenyl derivatives 2. Glucitol based cyto-compatible non-ionic amphiphilic architectures for encapsulation of non-polar dyes and drugs 3. Synthesis of triazolylated quaternary ammonium derivatives of benzopyran-2-ones as a lead antimicrobial agents 4. Pathogen sensing by boronic acid functionalized 2D nanomaterials 5. Summary and publications.

24. MAQSOOD AHMED

Functionalized Molecular Sieve Materials as Potential Catalysts and Catalytic Support.

Supervisor: Dr. A. Sakthivel

Th 23297

Abstract (Verified)

The thesis entitled "Functionalized Molecular Sieve Materials as Potential Catalysts and Catalytic Support" is to be submitted to University of Delhi. It describes the *in-situ* as well as *ex-situ* synthesis of various functionalized microporous and mesoporous molecular sieves, characterization and their catalytic applications. Three different types of microporous silicoaluminophosphates (viz. SAPO-37, SAPO-5 and SAPO-34) with different framework type were functionalized with various organosilane by *in-situ* synthesis. The organo functionalized materials were thoroughly characterized by various and analytical spectroscopic techniques. The resulting materials show promising activity towards various organic transformations. Subsequently mesoporous SBA-15 was functionalized with organosilane ligand via post synthesis grafting method and utilized as support for anchoring cobalt carbonyl cluster. The resulting material exhibited good catalytic activity towards hydroformylation of 1-octene. The thesis content is divided into six chapters. First chapter focuses the general introduction and literature background related to the importance on development of functionalized microporous and mesoporous molecular sieves and their applications. The Second chapter describes the experimental techniques used in the material synthesis and characterization. Further procedures on evolution of catalytic activities of the functionalized materials were also included. The third chapter describes the *in-situ* synthesis of amine functionalized microporous SAPO-37 by using microporous seed precursor. Thoroughly characterized material was used for β -amino alcohol formation via epoxide ring opening with aniline. The fourth chapter deals on preparation of amine functionalized AFI type SAPO-5 material and its catalytic application towards phenoxylation of propylene oxide under solvent free conditions. The fifth chapter concerned with preparation of amine functionalized chabazite (CHA) type SAPO-34 microporous materials and its catalytic application for synthesis of cyclic carbonate via cycloaddition of CO on epoxides. The sixth chapter illustrates the

covalent grafting of cobalt carbonyl cluster on functionalized mesoporous SBA-15 molecular sieve and its applications towards hydroformylation of 1-octene.

Contents

1. Introduction 2. Experimental methods 3. In situ preparation, characterization and catalytic application of various amine functionalized microporous SAPO-37 4. Amine functionalized AFI type microporous SAPO-5 materials: preparation, unique solvent extraction of template and its catalytic application 5. Amine functionalized chabazite type SAPO-34 as a potential catalyst for preparation of cyclic carbonate via cycloaddition of CO₂ on epoxide 6. Covalent grafting of cobalt carbonyl cluster on functionalized mesoporous SBA-15 molecular sieve and its applications towards hydroformylation of 1-octene 7. Future scope of the work and List of publications.

25. MUKESH KUMAR

Synthesis of Metal Alloy and Metal Oxide Nanoparticles for Novel Catalytic Applications.

Supervisor: Dr. Sasanka Deka

Th 23288

Abstract (Not Verified)

Due to important practical applications, nanocatalysts have attracted wide attention in the field of modern catalysis research. Among different nanomaterials, metal alloys and metal oxides have been studied extensively due to their shape and size controlled excellent catalytic performance. Among inorganic nanomaterials, Ag based nanostructures are very important due to their low cost, catalytic activity, antibacterial activity and optical properties. During this research work, we have successfully synthesized various one-component (Ag, Ni), two-component (AgNi, Ag@Ni and Ag@Ag.Ni) and three-component (Cu.O-CuO/Graphene, Ag-Cu.O/Graphene and AgNi/C) nanostructures by hydrothermal/solvothermal and one pot high temperature colloidal co-reduction methods. Various morphologies and compositions of nanomaterials were controlled via optimizing various reaction conditions like reaction time, temperature, precursors and other reagents etc. As-prepared nanomaterials were well characterized by TEM, HRTEM, FT-IR, SEM, STEM-HAADF, EDS, XRD, BET, UV-Vis, Raman and cyclic voltammetry to determine their phase purity and various intrinsic properties. Thereafter, present nanomaterials were studied in catalytic studies which can be discussed as: 1. AgNi alloy NPs were examined in nitroarenes reduction, dye degradation and oxidative coupling of amine to azo compounds. 2. AgNi/C ternary nanocomposites were used as a cathode material for electrochemical hydrogen evolution reaction in 1.0 M H₂SO₄. 3. Ag@Ag.Ni, core-graded alloy shell (CGAS) NPs were employed for synthesis of biologically active 3-substituted indoles via three component coupling at ambient condition in aqueous medium. 4. Reduced graphene supported yolk type Ag-Cu.O hybrid NPs were used as electrode material in supercapacitor study. As-prepared nanomaterials showed excellent catalytic properties owing to their size, shape and synergistic effect. In addition, synthesis and catalytic mechanism is also discussed in thesis for all nanostructures by pre and post catalytic studies.

Contents

1. Introduction 2. Nanoparticles synthesis, characterization and catalytic techniques 3. Five-fold twinned Ag_xNi_{1-x} (x=0.2-0.8) alloy NPs as highly active catalyst for multiple reduction and degradation reactions 4. Role of surfactant directed Ag_{1-x}Ni_x alloy nanocatalyst in oxidative coupling of amines 5. Electrochemically activated AgNi/C NCs as outstanding cathode material for hydrogen evolution reaction 6. Fabrication of magnetic Ag@Ag_xNi_y core/graded-alloy-shell nanostructures for the synthesis of biologically important 3-substituted indoles 7. RGO supported yolk type asymmetric Ag-Cu₂O hybrid nanoparticle electrodes for

high performance electrochemical hybrid supercapacitors 8. Summary and future scope and list of publications.

26. NARANG (Uma)
Synthesis, Reaction and Applications of Selected Newer Functional Porphyrinoids.
 Supervisor: Prof. Ramesh Chandra and Prof. S. M. S. Chauhan
Th 23289

Abstract
 (Not Verified)

The thesis entitled: "Synthesis, Reaction and Applications of Selected Newer Functional Porphyrinoids" has been divided into five chapters. In chapter 1, the singlet oxygen quantum yields of synthesized porphyrin tweezers has been studied using DPBF by indirect method and the effect of substituents on the tweezer for singlet oxygen generation has been analyzed. The tweezer with electron withdrawing group has been found to be most suitable for generation of singlet oxygen. In Chapter 2, synthesis of triazole linked porphyrin-pyrene dyads has been carried out and have been used in sensing of mercury ions. Thus, novel dyads by connecting metalloporphyrin unit with pyrene through a triazole moiety via click reaction have been developed. All the dyads have been synthesised by following simple click reaction. Dyads selectively bind to Hg ions. Spectroscopic studies indicate transmetalation takes place in dyads. These changes can also be detected through naked eyes. In Chapter 3, the synthesis of various substituted cobalt phthalocyanines has been carried out and have been used as catalyst for synthesis of 2-Substituted Benzimidazoles, Benzothiazoles and Benzoxazoles from Substituted Benzyl Alcohols. In Chapter 4, the synthesis of triazine substituted porphyrin has been carried out and its application in surfactant assisted self-assembly into supramolecular nanoarchitectures has been studied by various spectroscopic techniques. The studies reveal that synergistic effect of four point hydrogen bonding and hydrophobic interactions play an important role in self assembly of synthesized porphyrin and has been utilized in the synthesis of nano structures. In Chapter 5, a new model of porphyrin photosensitizer for DSSC having two carboxylic acid groups, serving as anchoring groups that bind to TiO₂ has been synthesised. Presence of two anchoring groups, extended conjugation through meso linked triazolyl group and appropriate values of band gaps make the synthesized porphyrin a good candidate for a dye sensitized solar cell.

Contents

1. Synthesis of conformationally flexible porphyrin tweezers and their application in generation of singlet oxygen 2. Synthesis of porphyrin-triazole-pyrene dyads and their uses in detection on mercury and their supramolecular interactions 3. Synthesis of selected cobalt phthalocyanines and their application in the synthesis of 2-substituted benzimidazoles starting from benzyl alcohols 4. Synthesis of triazine linked porphyrins and their application in surfactant assisted self-assembly into supramolecular nanoarchitectures 5. Porphyrins as sensitizers in dye sensitized solar cell via click reactions.

27. NATRAJAN (Mookan)
Bioinspired Model Complexes Mimicking the [FeFe] Hydrogenase Enzyme Active Site.
 Supervisor: Dr. Sandeep Kaur
Th 23774

Abstract

Contents

1. An introduction and scope of the work done 2. Diiron (I) propanedithiolate and benzenedithiolate complexes with tris(aromatic) phosphine ligand relevant to the [FeFe] hydrogenase active site 3. Synthesis and electrocatalysis of diiron monothiolate complexes: Small molecule mimics of the [FeFe] hydrogenase enzyme 4. Tetranuclear iron complex (μ_4 -Sulfido-bis(μ -2-furylmethanethiolato) bis[tricarbonyliron](Fe-Fe)); Substitution into electrocatalytic proton reduction 5. Mononuclear iron carbonyl complex [Fe(μ -bdt)(CO)₂(PTA)₂] with bulky phosphine ligand: Minimal model for the [FeFe] hydrogenase enzyme active site. Summary and conclusion. List of publications.

28. NEEMA CHAND

Magnetic Chitosan Nanocomposites for Removal of Heavy Toxic Metals.

Supervisor: Dr. P. S. Jassal

Th 23318

*Abstract
(Not Verified)*

The study provides potential application of magnetic chitosan nanocomposites (MCN) for the removal of heavy toxic metal ions from industrial wastewater. In the present work, MCN were synthesized in two simple steps. The first step involved the production of Fe₃O₄ nanoparticles that were used as magnetic core to instill magnetic properties to the MCN. Fe₃O₄ nanoparticles were produced by chemical co-precipitation and thermal decomposition and subsequently coated with chitosan to form MCN. Co-precipitation technique involved the precipitation of Fe²⁺ and Fe³⁺ ions in the presence of a base. Solvothermal technique used FeCl₃·6H₂O as a precursor, ethyleneglycol as a reducing agent and chitosan as a surface-modification agent. The morphology and chemical component of prepared nanocomposites were studied using spectroscopic techniques. MCN were applied to remove heavy metal ions from aqueous medium by virtue of chitosan that is coordinated on the surface of the Fe₃O₄ nanoparticles. The interaction between chitosan and heavy metal ions is reversible, which means that adsorbed ions can be extracted from chitosan in weak acidic deionized water. On the basis of above mentioned reasons, synthesized MCN were used as a recyclable tool for the removal of heavy metal ions. Adsorption performances of MCN for toxic metal ions namely Zn, Cd, Pb, Cu, Ni, Co, Fe and Cr ions were studied using 797 VA computer (Metrohm, Switzerland) which provides both qualitative and quantitative analysis of the metal ions present in the given sample via current-voltage graph. Investigations were also carried out to assess the concentration of Pb, Fe, Zn, Cd, Co, Cu, Cr and Ni metal ions in the water samples collected from Yamuna and Hindon Rivers flowing through the city of Delhi. Adsorption experiment was carried out in river water samples using MCN as an adsorbent to justify its potential for the removal of heavy metal ions.

Contents

1. Introduction 2. Review of previous work 3. Scope and object of present work 4. Materials and method 5. Adsorption of Ni²⁺ and Co²⁺ metal ions by magnetic chitosan nanocomposites: isotherms study 6. Adsorption of Zn²⁺, Cd²⁺, Pb²⁺ and Cu²⁺ metal ions by magnetic chitosan nanocomposites: Thermodynamic study 7. Adsorption of Cr⁶⁺ and Fe³⁺ metal ions by crossed-linked magnetic chitosan nanocomposites: Reaction kinetics 8. Determination of toxic metal ions in Yamuna metal ions in Yamuna and Hindon rivers 9. Summary, references and list of publications.

29. NEERAJ KUMARI
Application of Naturally Occurring Clay Minerals for the Synthesis of Nano Pigments as Colorant.
 Supervisor: Prof. Ramesh Chandra
Th 23295

Abstract
 (Not Verified)

The main objective of the present study is to remove the various types of cationic (Crystal violet, Victoria blue, Malachite green, Thioflavin T, Chrysoidine Y and Safranin O) and anionic dyes (Indigo carmine) from aqueous media using clay minerals {Montmorillonite (Mt), Bentonite (Bent) and Vermiculite (Vt)} and their synthetically modified form {organo Montmorillonite (OMt), organo Bentonite (OBent) and organo Vermiculite (OVt)} using batch extraction studies and used them as valuable added products, clay based nano pigments without creating second generation waste. From batch extraction studies, it was found that cationic dyes shows more interaction toward negatively charged pristine clay minerals and anionic dye shows more interaction toward positively charged organo clays (the surface of clay minerals become positively charged after treating with 2% CPC as confirmed from zeta potential values) due to their electrostatic interaction. The cationic dyes are found in the interlayer of Mt and Bent and on surface whereas they are found on surface of Vt, OMt, OBent and OVt. Indigo carmine dye was found on surface of pristine clay minerals and organo clays as confirmed from XRD pattern and surface charge analysis. The thermal stability of dye increased after interaction with clay minerals. The particle size of dye treated clay minerals and organo clays was found <300nm (mainly in case of pristine Mt, Bent and organo Mt, Bent). On the basis of their particle size, dye treated colored residues are known as clay based nano pigments. The clay based nano pigments can be easily dispersed in polymer matrix (PMMA and PVC) to form polymeric films and it was observed that polymer films containing organo clays and organo clays based dye nano pigments were more transparent and bright colored due to hydrophobic nature of organo clays which shows better compatibility with hydrophobic polymer than pristine clay minerals.

Contents

1. Introduction 2. Synthesis of clay based pigments 3. Application of nano pigments. Result, discussion and conclusions.

30. PRADEEP KUMAR
Strategies for N/O-Heterocycles Synthesis via [3+2] Cycloaddition, Axidation, Staudinger Reaction and Alkyne Activation.
 Supervisor: Prof. Akhilesh Kumar Verma
Th 23776

Abstract
 (Not Verified)

We have demonstrated chemoselective azidation of *o*-alkynyl aldehydes *via* 6-*endo dig* electrophilic cyclization over [3+2] cycloaddition reaction using the silver catalyst. The reaction proceeded with high 6-*endo-dig* regioselectivity and confirmed by X-ray crystallographic studies. This chemistry is general and expected to find application in a variety of organic synthesis. The method appeared to be very general and compatible with differently substituted starting materials having different electronic properties increasing its applicability to various functional groups. Further, we have demonstrated the solvent controlled chemoselective addition of NaN towards *o*alkynylaldehydes. The synthesis of azido-iodo pyranoquinolines and pyridines were achieved by *via* electrophilic iodocyclization in acetonitrile solvent for the synthesis of azido-iodo-pyranoquinolines and pyridines. The protocol also extended for the synthesis of bromo-derivatives of azido-pyranoquinolines by using NBS instead of molecular iodine. While the [3+2] cyclo-addition reaction for the synthesis of triazole product was facilitated in DMSO solvent. After that we have shown the application of Staudinger reaction in the synthesis of Benzonaphthyridines and naphthyridines by using triphenylphosphine. The reaction proceeds at room temperature in methanol solvent under metal free conditions. Further the deuterium

labeling experiments supports the proposed reaction pathway and the incorporation of deuterium at C-4 position in the Benzonaphthyridines validated the tautomerization and proton transfer steps. In last, we have developed Rh-catalysed noval approach for the synthesis of quinolines from hydrazine protected 2-aminoacetiphenone and alkynes. We have first time reported the base free activation of hydrazones and employed it for the synthesis of functionalised quinolines. The oxidant and ligand free catalysis also provided the economical route for these types of reactions. The protocol has high functional group tolerance as well as applicable for the synthesis of bis-quinolines from 1,4 and 1,3- dialkynes. Further scope and experimental studies for better understanding of mechanistic pathway are in due course.

Contents

1. Chemoselective azidation of *o*-alkynyl aldehydes over [3+2] cycloaddition: An access to the noval azidopyranoquinolines 2. Axidation *vs* [3+2] cyloaddition: Controlled chemoselectivity of sodium azide towards *o*-alkynyl aldehydes 3. Application of the staudinger reaction: Synthesis of benzo naphthyridines and naphthyridines employing azido/iodo-pyranoquinolines and pyridines 4. Rhodium (III) triggered reverse reactivity of anilines towards alkynes in C-C and C-N bond formation: A new approach for the synthesis of. Summary of the work. Copies of the publications.

31. PRASHANT KUMAR

Metal-Free Strategies for the Synthesis of Benzimidazo [1,2-*a*]quinazolines, 2,3-Dihydroquinazolin-4(1*H*)-ones and Coumarin-3-Carboxamides.

Supervisor: Dr. B. K. Singh

Th 23282

Abstract (Not Verified)

The work presented in Chapter I entitled "Metal-Free, Microwave-Assisted, Base-Mediated C-N Bond Formation/Cleavage for the Synthesis of Benzimidazo[1,2-*a*]quinazoline Derivatives" describes an efficient, metal-free, microwave-assisted, base-mediated approach for the synthesis of benzimidazo[1,2- *a*]quinazolines from readily available building blocks. In this chapter, a microwave-assisted, metal-free, base-mediated protocol for the synthesis of benzimidazo[1,2-*a*]quinazolines from *N*-(2-benzimidazolyl)-2-aminobenzamides and 2-halogenated benzaldehydes has been described. This newly developed methodology not only overcomes the drawbacks of the previous approaches, but also employs readily available starting materials, exhibits a broad substrate scope, offers operational simplicity and provides an easy access to a wide range of benzimidazo[1,2-*a*]quinazoline derivatives without using any metal. The work presented in Chapter II entitled "Metal-Free, Microwave-Assisted Synthesis of 2-Aryl/Alkyl-3-(1*H*-benzo[*d*]imidazol-2-yl)-2,3-dihydroquinazolin-4(1*H*)-one Derivatives" describes an efficient approach for the synthesis of 2-Aryl/Alkyl- 3-(1*H*-benzo[*d*]imidazol-2-yl)-2,3-dihydroquinazolin-4(1*H*)-ones under microwave-assisted and metal-free conditions. In this chapter, a microwave-assisted protocol for the synthesis of 2,3-dihydroquinazolin-4(1*H*)-ones from *N*-(2-benzimidazolyl)-2-aminobenzamides and benzaldehydes under metal-free conditions has been described. This newly developed methodology was found to show good functional group tolerance and a wide range of differently substituted derivatives could be synthesized in good to excellent yields. The work presented in Chapter III entitled "Metal-Free, Regioselective, Dehydrogenative Cross Coupling Reaction for the Synthesis of Coumarin-3-carboxamides via C-H Functionalization" describes a highly efficient, single-step, metal-free synthetic approach for the synthesis of coumarin-3-carboxamides and 3- aroyl coumarin. In this present chapter, a methodology for the regioselective C-3 functionalization of coumarins and azacoumarin with formamides and aldehydes using TBPB (*tert*-butylperoxybenzoate) has been described. This newly developed methodology provides a convenient, cost effective and shorter route to access products with excellent regioselectivity.

Contents

1. Metal-free, microwave-assisted, base-mediated C-N bond formation/cleavage for the synthesis of benzimidazo[1,2-a]quinazoline derivatives 2. Metal-free, microwave-assisted synthesis of Aryl/Alkyl-3-(1H-benzo[d]imidazole-2-yl)-2,3-dihydroquinazolin-4(1H)-one derivatives 3. Metal-free, regioselective, dehydrogenative cross coupling reaction for the synthesis of coumarin-3-carboxamides via C-H Functionalization 4. Summary.

32. PRAVEEN KUMAR

Synthesis, Characterization and Evaluation of Biocompatible Nanomaterials for the Delivery of Anticancer Agents.

Supervisor: Dr. Aruna Chhikara

Th 23780

Contents

1. Introduction 2. Synthesis and characterisation of poly(ethylene glycol)-*co*-acrylic acid based nanogels for delivery of doxorubicin 3. *In vitro* release mechanism, biological evaluation of doxorubicin loaded poly(ethylene glycol)-*co*-acrylic acid nanogels to cancer cells 4. Co-administration of etoposide and vorinostat via disulfide cross-linked biodegradable polymeric nanogels: synthesis, biodegradation, characterization and antitumor activity 5. pH and redox responsive biodegradable nanogels for the delivery of doxorubicin. Summary. Appendix.

33. PREETI

C*-Envelopes and Tensor Products of Operator Systems.

Supervisor: Prof. Ajay Kumar

Th 23770

Contents

1. Introduction 2. Operator system nuclearity via C*-envelope 3. Embeddings of exact operator systems 4. Nuclearity of operator system inductive limits 5. Polynomial-induced matrix ordering for operator spaces and operator systems. Bibliography. Notations. Index.

34. RADHIKA N.P.

Synthesis, Characterization and Catalytic Applications of Hierarchical and Nano Zeolites for Friedel-Crafts Alkylations.

Supervisor: Prof. Rita Kakkar

Th 23320

Abstract
(Not Verified)

The aim of the research work presented in this thesis is to study the synthesis and characterisation of nanocrystalline non-hierarchical and hierarchical zeolites ZSM-5 and beta and to analyse their catalytic performance in industrially significant alkylation reactions. Alkylation is a valuable tool in the synthesis of aromatic hydrocarbons. It is carried out in the presence of Friedel-Crafts catalysts along with mineral acids. However, these traditional homogeneous catalysts are toxic, moisture-sensitive and non-recyclable. In order to address these drawbacks, there has been a surge of interest in the scientific community to develop alternate solid acid catalysts. Previous reports involving bulk commercial zeolite

catalysts revealed that when employed for such organic transformations, they are required in large amounts, work under extreme reaction conditions, yield mixtures with low selectivity towards desired products and get deactivated fast. These problems arise because of the high diffusion resistance and easy pore blocking in bulk zeolites. Comparatively, in nano zeolites and hierarchical zeolites, there is a larger fraction of external active sites and greater accessibility of inner active sites. Hence, these forms of zeolites may catalyse reactions involving bulky substrates that may hitherto be unattainable with commercial zeolites. These merits associated with modified zeolites impelled our investigation on nano and hierarchical zeolites as novel materials for catalysing alkylation of aromatics under ambient conditions. Zeolites, if to be industrially used as catalysts for fine chemical synthesis, have to be synthesised under controlled laboratory conditions. In this regard, we have studied the effectiveness of vacuum concentration-coupled hydrothermal method to obtain nano-dimensional crystals and crystals with secondary porosity, in minimum amount of time. Hence, this study is an attempt to assess and develop suitable protocols for the facile synthesis of nano and hierarchical zeolites, characterise the zeolites synthesised and further explore their application in catalysing selected alkylation reactions.

Contents

1. Synthesis and applications of nanocrystalline and hierarchical zeolites: advances so far 2. Materials and experimental techniques 3. Nanocrystalline zeolite ZSM-5 as an efficient catalyst in benzylation of anisole 4. Nanocrystalline hierarchical ZSM-5: an efficient catalyst for the alkylation of phenol with cyclohexene 5. Synthesis, characterisation and catalytic efficiency of nanocrystalline zeolite beta in *tert*-butylation of aniline 6. Synthesis, characterisation and catalytic efficiency of nanocrystalline hierarchical zeolite beta in *tert*-butylation of phenol 7. Conclusions, perspectives, bibliography and appendices.

35. RAM BHAGAT
Synthesis and Characterization of Biomass/waste Derived Carbon Supports for Pseudo-capacitive Nanoparticles and their Applications in Electrochemical Capacitors.

Supervisor: Dr. Raj Kishore Sharma
Th 23312

Abstract (Verified)

Depending upon availability, cost factor, renewability and eco-friendly different kinds of biomass/waste have been utilized to prepare valuable carbon nanomaterials. In chapter 1, summarizes synthesis of carbon nanomaterials from biomass/waste materials and their basic charge storage mechanism in supercapacitors. Chapter 2 summarizes all characterization techniques that were used. In chapter 3, oxygen-enriched, light weight carbon monolith is synthesized from agarose. Monolith synthesized at 900 °C, exhibits large surface area (625 m² g⁻¹), high charge storage (302 F g⁻¹ at 5 mV s⁻¹) and good cycle life over 5000 charge/discharge cycles. Chapter 4 discusses non-biodegradable and health-hazardous soot particles (obtained from combustion of wood, coal and diesel) for preparation of activated carbon nanomaterials which shows large surface area (~870 m² g⁻¹) with significant presence of oxygen content (18 wt%). Synergistic effect results in high charge storage (409 F g⁻¹). In chapter 5, mesoporous carbon aerogel (CA) is prepared from mustard oil soot particles and exhibits high charge storage performance with large surface area (1032 m² g⁻¹) and low bulk density (0.144 g cm⁻³). Polyaniline spikes were further immobilized over CA to enhance overall power density (7.9 kW Kg⁻¹) and high energy density (55.6 Wh Kg⁻¹). In Chapter 6, 3-D meso/microporous carbon aerogel with large

surface area (2000 m² g⁻¹) and high electrical conductivity are derived from sugarcane juice. Carbon aerogel exhibits its electrochemical stability in both acidic and basic media. Chapter 7 summarizes carbon templated nickel-shells (NS) is synthesized using waste packing foam. Nanofibres of α -Ni-Co(OH)₂ is prepared over NS current collector. An asymmetric cell is fabricated with a very high energy (107 Wh kg⁻¹) and power (7 kW kg⁻¹) storage capacity with good electrochemical characteristics. Chapter 8 summarizes all the results of the entire research work.

Contents

1. Introduction 2. Characterization Techniques 3. Self-activating oxygen rich holey carbon monolith derived from agarose biopolymer for electrochemical capacitor 4. Functionalized activated carbon derived from hazardous-soots for charge storage 5. Vegetable oil derived carbon aerogel for the growth of hierarchical polyaniline spikes and their application in solid-state symmetric/ asymmetric supercapacitor 6. Biomass derived conducting and oxygenrich mesoporous carbon and their nickel cobaltite nanocomposite for energy storage 7. Carbon template Ni-shell catalyzed growth of Ni-Co(OH)₂ and their symmetric/asymmetric supercapacitive performance 8. Conclusions and list of publications.

36. RANA (Neha)

Biocatalytic Separation of Epimeric Furanosugars, Synthesis of Bicyclic- & Spiro- Nucleosides and Isoindoloquinolines.

Supervisor: Prof. Ashok K. Prasad

Th 23314

Abstract
(Not Verified)

In chapter I, a successful separation of a 1:1 mixture of epimeric furanosugars by enzymatic acetylation and subsequent synthesis of bicyclic nucleosides, *i.e.* 3'-O,4'-C-methyleneuridine and 2'-O,4'-C-methylene-xyloouridine have been accomplished. In chapter II, an efficient and environment friendly chemoenzymatic methodology for the synthesis of targeted nucleosides, 3'-azido-3'-deoxy-2'-O,4'-C-methylene- α -L-ribofuranosyl thymine and 3'-azido-3'-deoxy-2'-O,4'-C-methylene- α -L-ribofuranosyl uracil was found to be superior than classical method and led to the improvement in the overall yields. The improvement in yields in chemo-enzymatic methodology may be due to its less reaction time and easy deacetylation in the last step. In chapter III, a simple methodology for the synthesis of conformationally restricted spirocyclic nucleosides containing a hydroxyl substituents at C-1" position has been achieved, *i.e.* 3'-O-benzyl-5'-O,1"-C-ethylene-1"-hydroxy- β -D-ribofuranosyl thymine, uracil, cytosine, adenine and 5'-O,1"-C-ethylene-1"-hydroxy- β -D-ribofuranosyl thymine *starting* from 4-C-hydroxymethyl-1,2:5,6-di-O-isopropylidene- α -D-gulofuranose which in turn was synthesised from commercially available diacetone-D-glucose following literature procedure. In conclusion, a concise and efficient route is followed for the synthesis of C-4'-spiro-furanoribonucleosides of thymine, uracil, cytosine and adenine, which may be useful for therapeutic application. In chapter IV, synthesis of isoindolo[2,1-a]quinolin-11one derivatives was carried out using *N*-aryl-3-hydroxyisoindolin-1-ones, which in turn was synthesized from substituted anilines and phthalic anhydride by following literature procedures. *N*-aryl-3-hydroxyisoindolin-1-ones and vinyl acetate under Lewis acid-catalysed anhydrous conditions led to the synthesis of corresponding isoindolo[2,1-a]quinolin-11-one derivatives. This is the first report of the use of vinyl acetate as a dienophile for the inverse-electron demand Diels–Alder reaction with *N*-acyliminium cations as dienes.

Contents

1. Enzymatic separation of epimeric 4-C-hydroxy methylated furanosugars: Synthesis of bicyclic nucleosides 2. Synthesis of novel 3' -azido-3'- α -L-ribo configured nucleosides: A comparative study between chemical and chemo-enzymatic methodologies 3. Synthesis of conformationally restricted C-4'-spirofurano-ribofuranosyl nucleosides 4. Synthesis of isoindoloquinolines *via* inverse demand diels-alder reaction 5. Summary and list of publications.

37. RATNESH KUMAR

Electrochemical Investigation of Power Spectrum Based Theories on Rough Pt Electrode: E, EC', EE and EDL Response.

Supervisor: Prof. Rama Kant

Th 23298

*Abstract
(Verified)*

Surface of a solid electrode ubiquitously possesses morphological disorder which greatly influences their kinetics and transport properties. Also, the anomalies in electrochemical phenomena are governed by the characteristic phenomenological lengths and their interactions with the morphological length scales. Some of these characteristic lengths are significantly influenced by the viscosity of the electrolyte. Purpose of current thesis is to quantitatively study the influence of electrode roughness and electrolyte viscosity using impedance, chronoamperometry and cyclic voltammetry (CV) techniques. We experimentally corroborate the recently developed power spectrum based theories of one step electron transfer (E) process for chronoamperometry, CV and impedance, two step electron transfer (EE) for CV, coupled catalytic reaction (EC') for chronoamperometry, and electric double layer (EDL) impedance response on rough Pt electrodes. Impedance response of EDL is studied in NaNO₃ in aqueous and viscous medium (90% glycerol). Data are analyzed through the EDL theory, which accounts for the compact and diffuse layer relaxations under the influence of the heterogeneity, roughness and sluggish charge transfer. Similarly, impedance measurements are carried out in mixture of potassium ferro-ferricyanide (in 3M NaNO₃) and viscous medium (in 3M NaNO₃+glycerol) at various applied potentials to corroborate the theory involving charge transfer step. Chronoamperometric and CV measurements are carried out in: (i) solution of K₃Fe(CN)₆ and K₄Fe(CN)₆ in 3M NaNO₃ at various compositions of glycerol and (ii) ferrocene in [bmim][BF₄] RTIL on nanoparticles deposited Pt and validated with the theory of reversible charge transfer. Chronoamperometric response is also studied in potassium ferrocyanide in the presence of excess ascorbic acid and compared with the theory for EC'. CV measurement is performed in ethyl viologen in TBAP dissolved in acetonitrile to compare with theory for two electron transfer system. Finally, the roughness influenced measurements in viscous medium cause anomalous temporal delay and dilation as predicted by our contemporary theories.

Contents

1. Introduction 2. Experimental validation of debye-falkenhagen dynamics of electric double layer in viscous medium on heterogeneous Pt electrode 3. Anomalous warburg impedance on rough Pt electrode: influence of viscosity, solution resistance and potential bias 4. Influence of viscosity on chronoamperometry of reversible redox system on rough and nanoparticles deposited Pt electrode: aqueous/glycerol and RTIL medium 5. Chronoamperometric study of EC' reaction on rough Pt electrode 6. Cyclic staircase voltammetry for one and two electron transfer reaction schemes on rough Pt electrode 7. Summary and prospects.

38. RAWAT (Pooja)

Unconventional Synthesis of Crystalline Solids: Selected Example along with their Application for the Removal of Environmental Carcinogenic Pollutants.

Supervisor: Prof. Rajmani Nagarajan
Th 23290

Abstract
 (Not Verified)

This thesis entitled "Unconventional synthesis of crystalline solids: Selected few examples along with their application for the removal of environmental carcinogenic pollutants" to be submitted by Ms. Pooja Rawat, Department of Chemistry, University of Delhi for the award of the degree of Doctor of Philosophy. The thesis is divided into six chapters with subsections: Chapter 1 deals with the various synthetic methodologies to realize crystalline inorganic solids along with their structural description. Structure and applications of inorganic solids have also been highlighted. Chapter 2 deals with the investigation of the mechanochemical synthesis of metal oxides from metal peroxides [Zn, Cd] precursor using different source of metal powders. Soft chemical synthesis of M(OH)F (Zn, Cu, Cd) and their application as photo catalyst for dye degradation process are discussed in Chapter 3. Further the application of M(OH)F as a single source precursor for the synthesis fluoride doped metal oxides was also demonstrated. Discussions of double perovskite mixed metal fluorides are described in chapter 4 in two sub sections. In section 4.1, wet chemical synthesis of K GaF and its application as a host material for doping of rare earth ions (Eu, Tb, Er, Yb) for further upconversion studies has been discussed. Composite of up-converting compositions with optically transparent polymer, PMMA has been fabricated to demonstrate its practical utility. In section 4.2, mechanochemical synthesis of A PdF (A= Rb, K) and its further applicability as catalyst for the removal of carcinogenic Cr and as a photocatalyst for the removal of organic pollutants has been examined. Chapter 5 describes our attempts to synthesize some ternary sulfides using soft chemical methods. Further oxidation of sulfide to mixed metal sulphates. Application of sulfate as a catalyst for the reduction reaction has been elaborated. The conclusions arising from all these investigation are summarized and discussed in Chapter 6.

Contents

1. Introduction to the importance of unconventional synthesis of crystalline inorganic solids has been emphasized along with the application of such compounds
 2. Mechanochemical synthesis of metal oxides using metal peroxide precursors and their applications for the degradation of aqueous dye solutions under UV-visible radiation
 3. Synthesis of M(OH)F (M= Cu, Cd and Zn) by suspension reaction and their application as a photocatalyst as well as a precursor for the synthesis of F-doped metal oxide
 4(a). Wet-chemical synthesis, structural characterization and optical properties of rare-earth doped halo perovskite K_3GaF_6
 4(b). Mechanochemical oxidation of Pd(II) to Pd(IV) mediated by ammonium fluoride towards the synthesis of A_2PdF_6 (A=K, Rb) along with their catalytic role in environmental remediation
 5. Synthesis of ternary sulphides by the decomposition of metal thiourea precursors and their oxidation using H_2O_2 as an oxidizing agent forming mixed metal sulphates
 6. Conclusion and future prospects.

39. REDDY (Panyala Linga)
Design and Application of Nanomaterials for Organic Transformations & Synthesis of Medicinal Hybrids.
 Supervisor: Prof. Diwan S. Rawat
Th 23315

Abstract
 (Not Verified)

Chapter 1a describes the C-N cross coupling of aryl chlorides with various alkyl/aryl amines catalyzed by copper nanoparticles impregnated on alumina/silica support ($Cu(0)@Al_2O_3/SiO_2$). The catalyst offers significant advantages such as brevity, milder reaction conditions, excellent

yields and high functional group tolerance for C-N cross coupling. Moreover, this atom-economical methodology does not require an additional ligand or co-catalyst/activator. The robustness of the catalyst was examined by reusing it for five consecutive runs. Chapter 1b describes "sodium citrate" assisted hydrothermal method for CuI nanoparticles for the synthesis of 2-substituted benzimidazoles by the cyclization of o-phenylenediamines and various aldehydes. Short reaction times, easy and quick isolation of the products, excellent yields and air/O as oxidant are the main advantages of this procedure. Chapter 2 describes cobalt oxide nanoparticles impregnated on an alumina-silica (Co O @Al O /SiO) support for the hydrazine mediated chemoselective transfer hydrogenation of nitroarenes and synthesis of 2-substituted benzimidazoles *via* oxidative coupling of benzyl alcohols/amines with ophenylenediamine. Chapter 3 describes environmentally benign and eco-friendly cobalt based catalytic system (Co(0)- Co O @Al O /SiO) for the catalytic hydrogenation of nitroarenes and C-C unsaturated bonds in a green solvent (EtOH) and under mild reaction conditions (20 to 60 psi H). The catalyst prepared has high functional group tolerance towards various other reducible functional groups like esters, amides, nitriles, carbonyls and halogens. The catalyst also can be recovered by simple filtration and recycled for further runs without loss in its catalytic activity. Chapter 4 describes the synthesis and anti-plasmodial activity of 4-aminoquinoline-pyrimidine and 4-aminoquinoline-purine hybrids against CQ-sensitive (D6) and CQ-resistant (W2 and Dd2) strains of *P. falciparum*. Heme binding studies were performed on the most active hybrids and found these compounds form a stable 1:1 complex with heme, suggesting that heme may be one of the possible targets of these hybrids.

Contents

1(a). Cu(0)@Al₂O₃/SiO₂ NPs: an efficient reusable catalyst for the C-N cross coupling reactions of aryl chlorides with amines and anilines 1(b). CuI nanoparticles mediated expeditious synthesis of 2-substituted benzimidazoles using molecular oxygen as the oxidant 2. Co₃O₄@Al₂O₃/SiO₂ catalyzed chemoselective transfer hydrogenation of nitro-arenes and oxidative coupling of benzyalcohols/amines with o-phenylenediamines 3. Hydrogenation of nitro-arenes and unsaturated C-C bonds over supported transition metal nano catalysts 4. Synthesis of 4-aminoquinoline-pyrimidine and 4-aminoquinoline-purine based molecular hybrids as antimalarial agents 5. Summary, list of publications and patent.

40. SAHOO (Priya Ranjan)
Synthesis and Applications of Photoactive Multifunctional Materials.
 Supervisor: Dr. Satish Kumar
Th 23287

Abstract (Verified)

The research work embodied in the thesis entitled "Synthesis and applications of photoactive multifunctional materials" has been divided into six chapters namely: chapter 1. Light triggered switches as heavy metal ion sensors; tool for sensing heavy and transition metal ions. Chapter 2. Photoactive naphthopyrans for ion sensing; chapter 3. Protective spirooxazine as Fe and CN chemosensor; chapter 4. Spiropyran and other organic motifs as photoactive digital pH sensor; chapter 5. Photophysical studies of light responsive polymers; chapter 6. Novel heterocycles as selective optical metal ion sensor. The chapter 1 of the thesis provides an overview of the photoresponsive behavior and metal complexation tendency of photochromic receptors developed till today (up to 2016). The chapter 2 of thesis describes the design, synthesis, characterization and evaluation of several naphthopyran receptors. The chapter 3 of the thesis deals with the synthesis, characterization and evaluation of spirooxazine based receptors. The chapter 4 of the thesis deals with the synthesis of spiropyran and other organic motif based sensing materials. The pH responsive strips were successfully fabricated for potential

applications in pH monitoring. The chapter 5 of the thesis describes the preparation and characterization of spiropyran, naphthopyran based polymeric materials for reversible response. The chapter 6 includes synthesis and characterization of various fluorescent and colorimetric receptors. One of the receptor displayed selective fluorescence "turn-off" response towards Cu ions in aqueous methanol. The crystallized structure displayed polymorphism at the molecular level. The synthesized receptors complexed with Zn, Cu and Ni were also investigated using single crystal X-ray crystallography.

Contents

1. Light triggered switches as heavy metal ion sensors 2. Photoactive naphthopyrans for ion sensing 3. Photoactive spirooxazine as Fe³⁺ and CN⁻ chemosensor 4. Spiropyran and other organic motifs as photoactive digital pH sensor 5. Photophysical studies of light responsive polymers 6. Novel heterocycles as selective optical metal ion sensor.

41. SATYANAND KUMAR
Newer Approaches for the Heterocyclic Synthesis and Selective Fundamental Group Transformation in Organic Molecules using Metal Salts, Ionic Liquids and Nanoparticles.

Supervisor: Prof. Satish K. Awasthi

Th 23303

Abstract (Not Verified)

Newer approaches for the heterocyclic synthesis and selective functional group transformation in organic molecules using metal salts, ionic liquids and nanoparticles Chapter I describes auric chloride and gold nanospheres catalyzed efficient method for access pure aromatic, heteroaromatic and aliphatic tetrazoles by treatment of sodium azide with diverse functionalized nitriles in good yield without following a purification process. Advantages of reported protocol include simple work-up procedure, easy preparation and handling of the catalyst, high yields, elimination of dangerous and harmful hydrazoic acid formation. This report opens new dimensions in synthetic organic chemistry. Chapter II focuses on eco-friendly CAN catalyzed high yielding (3+2) cycloaddition to access substituted tetrazoles using various substituted aliphatic and aromatic nitriles. The protocol works smoothly with various substituents without potentially affecting the yield. This methodology reports simple work-up procedure, elimination of toxic hydrazoic acid formation to access pure tetrazoles without column chromatography. Chapter III throws light upon proline catalyzed high yielding (3+2) cycloaddition of sodium azide with various aryl nitriles (mononuclear, polynuclear and heteronuclear aryl nitriles, phthalonitrile, terephthalonitrile) and aliphatic nitriles in PEG-400 to access tetrazoles. Aromatic nitriles are more reactive than aliphatic nitriles. Electron releasing substituents on aromatic nitriles are more efficient than electron withdrawing substituent in this protocol. Chapter IV deals with ionic liquid catalyzed viable synthesis of carboxylic acids from nitriles with excellent yield in short time under mild condition. This protocol works smoothly with aliphatic, aromatic and heterocyclic nitriles having nitro, amino, alkyl and halogens, except amide. Chapter V describes gold nano particles and HAuCl catalyzed high yielding S Ar fluorine substitution to access aryl azides using aryl fluorides with sodium azide. Electron withdrawing groups in substrate assist the substitution while electron releasing groups retard. Moreover electron withdrawing groups at ortho and para to fluorine substantially enhance reaction rate. Halobenzenes are not suitable for this substitution.

Contents

1. Synthetic application of gold nano particles and auric chloride for the synthesis of 5-substituted 1-H tetrazoles 2. (NH₄)Ce(NO₃)₆ as an inexpensive, eco-friendly, efficient catalyst for the synthesis of 5-substituted 1-H tetrazoles from Nitriles 3. Proline catalysed one-pot synthesis of 5-substituted-1-H-tetrazoles in metal-free

condition using PEG-400 4. An efficient one pot method for synthesis of carboxylic acids from nitriles using recyclable ionic liquid [bmim] HSO₄ 5. Selective aromatic fluorine substitution by azide using gold (III) chloride and gold nanoparticles under moderate reaction conditions 6. Summary and publications.

42. SETHI (Komal)
Metal Containing Hybrid Nanoparticles: Synthesis, Characterization and some Biomedical Applications.
 Supervisor: Dr. Indrajit Roy
Th 23307

Abstract
 (Not Verified)

This thesis is divided into eight chapters, where first three chapters include introduction, literature review, and experimental and characterization techniques. The last eighth chapter of the thesis discusses about the conclusion of entire research work and the remaining four chapters are briefly discussed here: Fourth chapter titled as "Microemulsion mediated synthesis of titanium dioxide nanoparticles, characterization and application in drug delivery". In this chapter, we have designed and fabricated titanium dioxide nanoparticles (both in oil-in-water and water-in-oil microemulsion) for application in cell imaging and drug delivery. Fifth chapter entitled as "Organically modified titania nanoparticles for sustained drug release applications". Organically modified titania nanoparticles (ORTM) were synthesized in AOT/BuOH/water micellar system at a room temperature. ORTM nanoparticles encapsulate lipophilic molecules and release it in a sustained and pH dependent manner. The organic-modification to titanium dioxide nanoparticles provides improved colloidal stability, better drug loading, and sustained release behavior. Sixth chapter titled as "Iron carboxylate, metal organic framework for magnetically guided drug delivery". In this work, we have synthesized iron carboxylate metal organic framework using iron as a metal center and 2-amino benzene dicarboxylate as a ligand. These nanoframeworks have been synthesized in a micellar medium using two different coordinating solvent. The NMOFs were effectively used to load lipophilic entities (dye/drug) and showed a sustained and slow drug release. The S-NMOF and F-NMOF nanoparticles are found to be robustly uptaken by cells and the uptake was further enhanced over the application of external magnetic field. Seventh chapter entitled as "Metal sulphides as photoactive agents". In this research work, we have synthesized various metal sulphides such as cadmium sulphide (CdS), copper sulphide (CS), copper indium sulphide (CIS), and copper indium zinc sulphide (CIZS) in an oil-in-water microemulsion system for photoactivated applications such as photocatalysis, photodynamic therapy, and photothermal therapy, etc.

Contents

1. Introduction 2. Literature review 3. Experimental and characterization techniques 4. Microemulsion mediated synthesis of titanium dioxide nanoparticles, characterization and application in drug delivery 5. Organically modified titania nanoparticles for sustained drug release applications 6. Iron carboxylate metal organic framework for magnetically guided drug delivery 7. Metal sulphides as photoactive agents 8. Conclusion and publications.

43. SHAILJA KUMAR
Imaging and Drug Delivery Application Doped Gadolinium Nanoparticles.
 Supervisor: Dr. Rakesh Kumar Sharma
Th 23279

Abstract
(Not Verified)

The thesis is divided into three chapters: CHAPTER 1 FITC-Dextran entrapped and silica coated gadolinium oxide nanoparticles for synchronous optical and MRI applications. Nanoparticles of size 18nm were prepared in water-in-oil micromulsion Gd O core show paramagnetism which is affirmed by the NMR proton peak and by VSM analysis. Entrapment efficiency of nanoparticles was calculated to be 62.5%. The fluorescence of the entrapped dye is confirmed by the UV-visible and fluorescence spectroscopy. Nanoparticles behave as non-releasing system. SRB assay of nanoparticles on HEK-293 and A-549 cells indicated non-cytotoxic nature. These particles have the potential to be efficiently used for optical and MR imaging. CHAPTER 2 PEG coated and doxorubicin loaded multimodal Gadolinium oxide nanoparticles for simultaneous drug delivery and MRI. UV-Visible and fluorescence spectrum confirmed optical activity of nanoparticles. The paramagnetic nature of nanoparticles was affirmed by NMR proton peak broadening. Nanoparticles were efficiently uptaken by A-549 cells. Nanoparticles exhibit fluorescence. pH dependent and sustained drug release pattern was observed for nanoparticles. Cell viability assay performed on cancerous cell lines revealed cytotoxic nature of particles. These nanoparticles promises potential applications in cancer therapy and imaging. CHAPTER 3 Rose Bengal conjugated and dextran coated gadolinium oxide nanoparticles for diagnostic imaging. Nanoparticles of 17nm size show H-NMR line broadening. Optical activity of nanoparticles was confirmed by UV-Visible and fluorescence spectrum. Time dependent release of RB in pH=7.4 and pH=5.0 revealed that nanoparticles are non-releasing system. Nanoparticles are efficiently uptaken by cells. SRB assay performed on cancerous (A-549 and U-87) and normal (HEK- 293) cell lines, show no cytotoxic effect of nanoparticles. Therefore, such nanoparticles can be efficiently used for bio-imaging and optical tracking.

Contents

1. Introduction 2. Literature review 3. Experimental and characterization Techniques 4. FITC-dextran entrapped and silica coated gadolinium oxide nanoparticles for synchronous optical and magnetic resonance imaging applications 5. PEG coated and doxorubicin loaded multimodal gadolinium oxide nanoparticles for simultaneous drug delivery and magnetic resonance imaging 6. Rose Bengal conjugated and dextran coated gadolinium oxide nanoparticles for diagnostic imaging 7. Conclusions, appendix and publications.

44. SHANKAR (Deval Sathiyashivan)
Tripodal Molecules with Aromatic Cyclic Trimer Motif.
 Supervisor: Dr. Dhanraj T. Masram
Th 23292

Abstract
(Not Verified)

The present work deals the design, synthesis, nuclear magnetic resonance (NMR) studies, Single-crystal X-ray diffraction (SC-XRD) analysis, and density functional theory (DFT) calculations of family of tripodal molecules with/without cyclic aromatic trimer motif. These tripodal molecules were synthesized from substituted benzimidazole and tri-bromo-aromatic compounds. The obtained results indicate that the steric groups furan/thiophene/pyridine/substituted phenyl at the 2-position of the benzimidazolyl and alkyl (methyl/ethyl) at the centre of benzene scaffold play a role in arranging cyclic aromatic trimer motif in the tripodal molecules. The first chapter begins with a general introduction where the literature data related to the cyclic aromatic trimer motif in synthetic molecules. This also sets the stage for the scope of the work carried out in the current thesis. The second chapter involves synthesis, NMR characterization, SC-XRD analysis of a family of tripodal molecules with/without steric ethyl groups at the central benzene scaffold and with mono-aromatic group

(furan/thiophene/pyridyl group) at 2-position of the benzimidazolyl unit. The results reveal that the introduction of three ethyl groups into a central benzene scaffold of furan/thiophene/pyridyl substituted benzimidazolyl based tripodal molecules enhances the edge-to-face C–H... π interactions, thereby favouring the aromatic cyclic trimer motif, in solution and solid state. The third chapter involves synthesis and characterization of a family of mono-/di-/tri methoxyphenyl substituted benzimidazolyl based molecules with/without alkyl substituted spacers. Among the nine molecules in this chapter, one molecule adopts perfect symmetrical cyclic aromatic trimer motif, stabilized through edge-to-face C–H... π interactions, similar to the theoretically predicted symmetrical cyclic benzene trimer cluster. The fourth chapter involves synthesis, NMR characterization analysis of a family of tripodal molecules with/without steric ethyl groups at the central benzene scaffold and with bi-aromatic/alkylsubstituted mono-aromatic group (bithiophene/biphenyl/alkylthiophene) at the 2-position of the benzimidazolyl unit. The fifth chapter involves the conclusions and the future prospective of the synthesized tripodal molecules.

Contents

1. Introduction 2. Steric group enforced aromatic cyclic trimer conformer in tripodal molecules 3. Crystallographic evidence of perfect symmetrical cyclic benzene trimer motif with close contacts (4.8Å) in tripodal molecule 4. Cyclic aromatic trimer motif in lengthy aromatic unit substituted benzimidazolyl-based tripodal molecules 5. Conclusion, future aspects and list of publications.

45. SANJAY KUMAR
Matrix Games with Fuzzy Payoffs.
 Supervisor: Dr. Ratnesh R. Saxena
Th 23771

Contents

1. Introduction 2. Game matrix with triangular fuzzy numbers 3. Game matrix with trapezoidal fuzzy numbers 4. Game matrix with triangular Intuitionistic fuzzy numbers 5. Game matrix with trapezoidal Intuitionistic fuzzy numbers. Bibliography.

46. SHARMA (Dhanjay)
Preparation of Inorganic Composite Materials by Intercalation of Layered Double Hydroxides and their Applications.
 Supervisor: Dr. A. Sakthivel and Prof. N. Thirupathi
Th 23293

Abstract *Not Verified)*

The thesis entitled “Preparation of Inorganic Composite Materials by intercalation of Layered Double Hydroxides and Their Applications” is to be submitted to University of Delhi. It describes the synthesis, structural characterization and catalytic applications of various organic surfactants, silicate moiety intercalated and noble metal supported layered double hydroxide or hydrotalcite (HT) type materials. The developed materials showed efficient catalytic activity on hydroformylation of olefins, oxidation of alcohols, hydroisomerization of 1-octene and bi-functional electro-catalyst for oxygen evolution reaction (OER) and oxygen reduction reaction (ORR) involved in water splitting reaction. The thesis content is divided into six chapters. The first chapter describes general introduction reviewing the literature related to monometallic and bimetallic layered double hydroxides materials, and discusses their importance in the areas of catalysis and other applications. The second chapter describes synthetic protocol a series of silicate and organic surfactants intercalated various monometallic (cobalt), bi-metallic and noble metal containing hydrotalcite and hydrotalcite type materials. The third chapter depicts systematic approach on preparation of silicate intercalated monometallic cobalt hydrotalcite (Co-

HT) materials, characterization and its catalytic application on alcohol oxidation. The fourth chapter is focused on synthesis of different organic surfactants intercalated monometallic cobalt hydrotalcite materials which demonstrated as bi-functional electro-catalysts for OER and ORR involved in water splitting reaction. The fifth chapter describes synthesis of layered cobalt rhodium hydrotalcite (CoRh-HT) type materials which were utilized for the hydroformylation of olefins. The role of rhodium ions on enhancing the selectivity towards linear aldehydes during hydroformylation reactions was discussed. The sixth chapter demonstrates the synthesis of uniformly dispersed rhodium nanoparticles supported on silica intercalated magnesium aluminum hydrotalcite (RhMAHT) materials, its systematic characterizations and showed promising catalytic activity in the hydroisomerization of 1-octene.

Contents

1. Introduction 2. Experimental methods 3. Silicate anion intercalated monometallic cobalt hydrotalcite (CoHT-Si) a potential catalyst for alcohol oxidation 4. Surfactant intercalated cobalt layered double hydroxide: Preparation, characterization and its bi-functional electrochemical application 5. Rhodium incorporated monometallic cobalt hydrotalcite-type materials: Preparation and its applications for the hydroformylation of alkenes 6. Hydroisomerization of 1-octene on rhodium nanoparticles supported on silicate intercalated magnesium-aluminium hydrotalcite 7. Future scope of the work and list of publications.

47. SHARMA (Kumkum)

Interaction Study of Small Molecules with Serum Albumin Proteins and Applications of Organocatalyst in Asymmetric Synthesis.

Supervisor: Prof. Satish K. Awasthi

Th 23274

Abstract (Not Verified)

The results of research work incorporated in thesis entitled “*Interaction Study of Small Molecules with Serum Albumin Proteins and Applications of Organocatalyst in Asymmetric Synthesis*” are presented in four chapters: Chapter I entitled “Study of interaction of coumarin with serum albumins using spectroscopic techniques and molecular docking” describes biophysical, spectroscopic and molecular docking study for interaction of triazole-substituted 7-hydroxy coumarin derivatives with BSA/HSA. Fluorescence quenching with increasing CUMs concentration occurred. Binding constant of CUMs with BSA/HSA from fluorescence emission was $\sim 10^6$ Lmol⁻¹. Conformational changes were observed in secondary structure of serum albumin with CUMs in CD spectra, confirmed by molecular docking. Chapter II entitled “Study of interaction of naturally occurring flavonoids with human serum albumin using spectroscopic techniques and molecular docking” elucidates interaction of naturally occurring flavonoids with HSA, studied using UV-vis, fluorescence, CD and molecular docking. Fluorescence study showed quenching of HSA by flavonoids via static mechanism revealing strong binding. CD studies unveiled decreasing of α -helicity in conformational structure of HSA, confirmed by molecular docking. Chapter III entitled “Design and synthesis of triazole-substituted s-triazine derivatives and their biological applications” describes design and synthesis of series of triazole-substituted s-triazine derivatives by three consecutive nucleophilic substitution of s-triazine moiety followed by triazole formation through CuI catalyzed click reaction. These derivatives were checked for *in vitro* antimalarial activity against *P. falciparum* (3D7 strain) and antibacterial activity against *S. aureus*, *E. coli*, *P. aeruginosa* and *B. cereus* bacterial strains. Chapter IV entitled “Enantioselective Solvent-Free aldol reaction of isatin and alkylation of oxindole: Catalyzed by s-Triazine based L-proline asymmetric organocatalyst” explicates synthesis and asymmetric catalytic activities of s-triazine substituted L-proline based organocatalysts for enantioselective solvent-free aldol reaction of isatin with aliphatic ketones and mono-alkylation

of *N*-Boc 2-oxindole with aliphatic and aromatic alkylating agents. The catalytic results were proficient with excellent yield and high enantioselectivity.

Contents

1. Interaction study of coumarins with serum albumins using spectroscopic techniques and molecular docking 2. Interaction study of naturally occurring flavonoids with human serum albumin using spectroscopic techniques and molecular docking 3. Design and synthesis of triazole-substituted s-triazine derivatives and their biological applications 4. Enantioselective solvent-free aldol reaction of isatin and alkylation of oxindole: Catalyzed by s-triazine based L-proline asymmetric organocatalyst 5. Summary and list of publications.

48. SHARMA (Pooja)
Composition Operators on Lorentz-Karamata-Bochner, Zygmund, L^2 and Double Sequence Spaces.
 Supervisor: Dr. Anuradha Gupta
Th 23772

Contents

1. Introduction 2. Non-normal composition 3. Generalized composition operators on Lorentz-Karamata-Bochner spaces and zygmund spaces. 4. Composition operators on double sequence spaces defined by a modules 5. Isometric composition operators. Scope for further research. Bibliography.

49. SHARMA (Sandeep)
Synthesis and Characterization of Some Metal Oxide Nanoparticles for Catalytic and Biomedical Applications.
 Supervisors: Dr. Rakesh Kumar Sharma and Prof. Surinder Kumar Sharma
Th 23306

Abstract
 (Not Verified)

Gallic acid, a polyphenolic compound has a potential to behave as a good stabiliser for preparing the stable hydrophilic metal and metal oxide nanoparticles. Gallic acid has ability to show altering reducing strength with changing the alkalinity of the system. This behaviour of gallic acid can be harnessed in making the different size of metal nanoparticles. Catalysis using different sizes of the GA-Ag NPs established the foundation that surface area is a critical factor to enhance the adsorption process which in turn increases the rate of given reaction. Silver nanoparticles efficiently catalysed the hydrolysis of chlorpyrifos, an organophosphate pesticide into less toxic compounds. It motivates us towards application of these nanoparticles in cleansing away the other hazardous chemicals prevalent in the environment. Green approach was adopted to synthesize gold and silver nanoparticles to highlight the usefulness of environmentally benign naturally occurring compounds as reducing agents as well as stabilising agents. Removal of harmful organic dyes from environment like rhodamine B, eosin yellow, toluidine blue etc. using gold nanoparticles paved us a way for doing sustainable chemistry. Water in oil microemulsion method was adopted to prepare ultra small sized gallic acid coated gadolinium oxide nanoparticles. GA-GO NPs were well dispersed and showed no cytotoxicity on PC-3 cell lines. GA-GO particles showed very strong relaxation of protons which makes it a potential candidate for MRI contrast agents.

Contents

1. Introduction. 2. Literature review 3. Instrumentation and experimental techniques. 4. Synthesis of gallic acid coated silver nanoparticles of different sizes as catalyst in

the reduction of aromatic nitro compounds. 5. Silver nanoparticles for the degradation of organophosphate pesticide (chlorpyrifos). 6. Green approach mediated synthesis of gold silver nanoparticles for removal of organic pollutants and antibacterial applications respectively. 7. Synthesis and characterization of ultra-small gallic acid coated gadolinium oxide nanoparticles as contrast agent for magnetic resonance imaging applications. 8. Conclusions and publications.

50. SHILPI PAL

Transition-Metal and Lewis Acid Promoted Synthetic Approaches to Multifunctionalization of *Ortho*-Arylalkynylaldehydes.

Supervisor: Prof. Akhilesh K. Verma

Th 23291

Abstract
(Not Verified)

The thesis entitled “*Transition-Metal and Lewis Acid Promoted Synthetic Approaches to Multifunctionalization of ortho-Arylalkynylaldehydes*” describes a versatile and an efficient synthetic methodology to produce a broad range of biologically important variety of oxazolo fused pyridoindoles, benzofurooxazolo pyridines, γ -carbolines, benzofuro[3,2-*c*]pyridines, oxidation of alkynes, oxidative esterification and difunctionalization of alkynes. The designed strategy represents Au(III)-catalyzed domino protocol in water which allowed a facile access to a vast variety of pyridoindole/benzofuropyridine fused oxazole using readily available starting materials in good yields with high regioselectivity under mild reaction conditions. The reaction proceeded with high 6-*endo-dig* regioselectivity. This methodology appeared to be very general and compatible with differently substituted starting materials having different electronic properties thus, increasing its applicability to various functional groups. It is likely that the efficiency of this environment friendly method combined with its operational simplicity will make it attractive for the construction of variety of heterocyclic compounds. Further, Ag(I) catalyzed investigation was extended for the synthesis of γ -carbolines and benzofuropyridines. *Ortho*-aldehyde assisted metal-free regioselective oxidation of alkynes have been investigated. We control the formation of iodo-cyclized product and simultaneously diketone and esterification of aldehyde with the equivalence of iodine and nature of base. The reaction proceeded with high regioselectivity and confirmed by X-ray crystallographic studies. The role of aldehydic group and electron rich substrate for the oxidation process was confirmed by control experiments. A deuterium labelling experiment supports the source of proton. Iodine- and solvent controlled selective synthesis of *ortho*-alkynyl esters and difunctionalization of alkynes from *ortho*-alkynyl aldehydes in mild reaction conditions have been developed. Developed novel oxidative esterification process, provides a powerful tool for the preparation of wide range functionalized benzofurans and thiophenone scaffolds. Further, difunctionalization of alkynes was achieved in *N*-methylindole substrate in regioselective and chemoselective manner.

Contents

1. Regio- and stereoselective domino synthesis of oxazolofused pyridoindoles and benzofurooxazolo pyridines from *ortho*-alkynylaldehydes 2. Domino synthesis of γ -carbolines and benzofuro[3,2-*c*] pyridines 3. *ortho*-Aldehyde assisted base controlled and metal-free regioselective oxidation of alkynes 4. Chemoselective behaviour of alcohol: Oxidative-esterification and difunctionalization of *ortho*-alkynylaldehydes 5. Summary of the work and publications.

51. SINGH (Abhishek Kumar)
Synthesis of Glycerol and Oligoglycerol Based Amphiphilic Architectures for Biomedical Applications.
 Supervisor: Prof. Sunil K. Sharma
Th 23304

*Abstract
 (Verified)*

Abstract of the thesis entitled "Synthesis of Glycerol and Oligoglycerol Based Amphiphilic Architectures for Biomedical Applications" describe the synthesis characterization and biomedical applications of amphiphilic architectures. The thesis is divided into four chapters. In the first chapter, an indigenous method has been developed to synthesize oligomers of glycerol using a domestic microwave and K₂CO₃ as a catalyst. The objective of our work was to compare the various processes and optimize the conditions for direct oligomerization of glycerol. Also, a simple purification method is reported to refine the final product by excluding small oligomers. In the second chapter, a cleaner and greener method has been developed and used to synthesize 14 different functionalized oligomer derivatives of glycerol in moderate 29%-39% yields over three steps. After successive regioselective enzymatic acylation of the primary hydroxyl groups, etherification or esterification of the secondary hydroxyl groups and chemoselective enzymatic saponification, the target compounds can efficiently be used as versatile building blocks in organic and supramolecular chemistry. In the third chapter, a new class of twinned amphiphiles was developed by utilizing "click chemistry" and acylation reactions on a chemoenzymatically synthesized aromatic spacer. Cryo-TEM measurements show the formation of globular, hreadlike or rod-like micelles as well as planar double-layer assemblies, depending on the amphiphile's molecular structure. The transport capacity study of amphiphiles carried using Nimodipine and Nile red. In the fourth chapter, a modular approach has been developed for the synthesis of a new family of nonionic amphiphiles consisting of biocompatible molecules, e.g. PEG of varied sizes (mPEG 550/350) as a hydrophilic moiety and oleic acid as a hydrophobic moiety. The resulting self-assembled architectures were studied for their transport behavior using 'Nile red' and 'nimodipine' as model dye/drug. Cytotoxicity, cellular uptake, and enzyme-triggered release studies were also performed.

Contents

1. A simple and efficient process for large scale oligomerization of glycerol by microwave irradiation
 2. Chemo-enzymatic synthesis of oligoglycerol derivatives as building blocks in supramolecular chemistry
 3. Aggregation behaviour of non-ionic twinned amphiphiles and their application as biomedical nanocarriers
 4. Synthesis of non-ionic chain amphiphilic architectures and their applications as biomedical nanocarriers
 5. Summary and paper published.

52. SINGH (Sunny)
Some Aspects of 3-D Multi-Excitonic Quantum Dots in Zero and Non-Zero Magnetic field via Exact Formalism.
 Supervisor: Dr. Ram Kuntal Hazra
Th 23281

*Abstract
 (Not Verified)*

Chapter-1, Introduction- The basic physics and fundamental concepts involved in the study of quantum dots (QD) and excitonic systems, essential in developing the formalism and a

thorough literature survey concerning the mesoscopic physics pertaining to excitonic systems in QD is articulated. Chapter-2, Exact formalism of an excitonic (e-h) system in 3-D Quantum dot- A novel formalism towards an exact variational solution to the coulomb correlations for charged carriers confined in parabolic potential (ω) under transverse magnetic field (ω) leading to an exact, finite summed, absolutely convergent solution in terms of Lauricella functions has been presented. Chapter-3, Elucidation of Electronic structure of 3-D excitonic systems- The study of energy level spectra of a 3-D excitonic system in He, SiO₂, BN and GaAs QD for interactive and non-interactive systems at different values of α ($\alpha = m^*/m$) have been presented. Chapter-4, Level Spacing Statistics, Specific Heat Capacity (C_v) and Magnetization (M)- The results of Level Spacing Statistics, C_v , M for He, SiO₂, BN and GaAs at different ω and α for a 3-D excitonic system are discussed. Chapter-5, Formalism of 3-D multi-excitonic systems- An exhaustive formalism discussing the exact variational approach for coulomb correlations between e-h/e-e/h-h in 3-D multi-excitonic QD systems via multipole expansion which can accommodate any number of charge carriers and the eigensolutions to trions and biexciton is developed. Chapter-6, Elucidation of Electronic structure of 3-D multi-excitonic systems- The results obtained from the comparative study of energy level spectra of multi-excitonic systems in He, MoS₂, CdSe and GaAs QD at different ω and α is presented. Chapter-7, Level Spacing Statistics, Specific Heat Capacity (C_v) and Magnetization (M) for 3-D Multi-excitonic systems- For a multi-excitonic system in He, MoS₂, CdSe and GaAs 3-D QD with ω , the results of the study of 3 thermodynamic properties at different ω and α are given.

Contents

1. Introduction 2. Exact formalism of an excitonic (e-h) system in 3D quantum dot 3. Elucidation of electronic structure of 3-D excitonic systems 4. Level spacing statistics, specific heat capacity (C_v) and magnetization (M) 5. Formalism of 3-D multi-excitonic systems 6. Elucidation of electronic structure of 3-D multi-excitonic systems 7. Level spacing statistics, specific heat capacity (C_v) and magnetization (M) for 3-D multiexcitonic systems 8. Bibliography and list of publications.

53. SRIVASTAVA (Smriti)

Click Chemistry Route to Triazole-linked Bicyclonucleosides and Coumarin-triazolylnucleosides: Fluorescence and Anti-tubercular Activity Studies of Some of Them.

Supervisor: Prof. Ashok K. Prasad

Th 23313

Abstract (Not Verified)

The thesis is divided into four chapters, *i.e.* Chapter I, Chapter II, Chapter III and Chapter IV. A brief account of each chapter is given below: The work presented in Chapter I entitled "Synthesis of Sugar Modified Triazole-linked Xylo/nucleoside Dimers: Monomers for the Synthesis of Neutral Nucleic Acid Analogs" describes the "click chemistry" approach for the synthesis of phosphate backbone modified triazole-linked, 2'-O,4'-C-bridged bicyclo xylo-nucleoside dimers, *i.e.* *N*-(3'-deoxy-2'-O,4'-C-methylene-5-methyluridine-3'-yl)-C-(5"-deoxy-2"-O,4"-C-methylene-*N*-benzoyl-xyloadenosine-5"-yl)-1,2,3-triazole (T-t-A) and *N*-(3'-deoxy-2'-O,4'-C-methylene-5-methyluridine-3'-yl)-C-(5"-deoxy-2"-O,4"-C-methylene-*N*-benzoyl-xylocytidine-5"-yl)-1,2,3-triazole (T-t-C). The work presented in Chapter II entitled "Chemo-enzymatic Synthesis of Bicyclo Xylo/triazolylnucleosides" describes the efficient separation of α - & β - anomers using lipase-catalyzed deacetylation reaction and further chemical transformations on the selectively deacetylated product leading to bicyclo xylo-triazolylnucleosides having thymine and uracil nucleobase, *i.e.* *N*-(2'-O,4'-C-methylene- β -D-

xylofuranosyl)-C -((uracil-1"-yl)methyl)-1,2,3-triazole and *N* -(2'-O,4'-C-methylene-β- D-*xylofuranosyl*)-C -((5"-methyluracil-1"-yl)methyl)-1,2,3-triazole in good yields. The work presented in Chapter III: entitled "Synthesis and Fluorescence Studies of Coumarin-triazolylbicyclonucleosides" describes the synthesis of eight novel coumarin-triazolylbicyclonucleosides, i.e. *N* -(3'-deoxy-2'-O,4'-C-methylene-β-D-*ribofuranosyl*-pyrimidine-3'-yl)-C - (coumarin-7-oxymethyl)-1,2,3-triazoles. The *N*-type preorganization of these synthesized compounds were demonstrated by determination of X-ray crystal structure of one of these derivatives. We have also carried out the photophysical studies of these modified nucleosides, which indicate the fluorescence enhancement in the triazolyl nucleoside conjugates as compared to the starting substrates for the click reaction i.e. 3'-azido nucleosides and 7-propargyloxycoumarins. The work presented in Chapter IV: entitled "Synthesis and Anti-tubercular Activity of Novel Coumarin-triazolylribosides" describes the synthesis of a series of β-D-*ribofuranosyl* coumarinyl-1,2,3-triazoles by Cu(I)-catalyzed cycloaddition reaction between azidosugar and 7-O-/7-alkynylated coumarins in good yields. We synthesized a small libraries of *N* -(β-D-*ribofuranosyl*)-C -(coumarin-7-oxymethyl)-1,2,3-triazole and *N* -(β-D-*ribofuranosyl*)-C -(coumarin-7-yl)-1,2,3-triazole. We have studied there *in vitro* anti-tubercular activities against *M. tuberculosis* sensitive reference strain H37Rv and multidrug resistant clinical isolate 591. Spectral data analysis unambiguously established structure of all synthesized compounds.

Contents

1. Synthesis of sugar modified triazole-linked *Xylo*-nucleoside dimers: monomers for the synthesis of neutral nucleic acid analogs 2. Chemo-enzymatic synthesis of bicyclo *Xylo*-triazolynucleosides 3. Synthesis and fluorescence studies of coumarin-triazolylbicyclonucleosides 4. Synthesis and anti-tubercular activity of novel coumarin-triazolylribosides 5. Summary, conclusions and list of publications.

54. SURBHI PRAKASH

Design and Synthesis of C-Functionalized Macrocyclic System to Conjugate Biomolecules for Multifunctional Imaging.

Supervisors: Prof. Shrikan Kukreti and Dr. A. K. Mishra
Th 23280

Abstract (Not Verified)

Chapter 1 discusses the role of radio-diagnosis and radio-therapy in managing and treating diseases. Chelating agents are the most crucial requirement in formulation of radiopharmaceuticals. Central aspect of the synthesis of radiopharmaceuticals is the design of new macrocyclic chelating system which can bind to metal ions with high stability and at the same time can be conjugated to biovectors without altering the properties of the vector. Chapter 2 shows the design, synthesis and evaluation of a 13 membered dioxo, diamide based macrocyclic system (DODAT). Potentiometric titrations were conducted with different metal ions in =2 and +3 oxidation state. The synthesized macrocycle was complexed with Tb(III) and then reacted with DPA to perform as a sensitive assay for endospore detection. DODAT was then modified from the carbon of the macrocyclic framework. The new C-substituted macrocycle, ATRIDAT was converted into bis-macrocycle by conjugating with 5-aminoisophthalic acid. Docking studies of bis-macrocycle have been performed on the CXCR4 receptors involved in the HIV entry and progression. Chapter 3 shows the synthesis of ATRIDAT-Biotin for PET imaging using biotin as the biovector for tumor recognition. In vitro and in vivo studies were done after radiolabeling with Ga. MTT assay, HABA Assay, Biotinidase stability assay, biodistribution studies and μPET imaging of Ga-ATRIDAT-Biotin have been conducted on A549 tumor mice models. Chapter 4 describes the synthesis and biological evaluation of an amino acid based derivative, ATRIDAT-NAC as PET diagnostic agent. N-acetyl cysteine was conjugated to ATRIDAT through S-alkylation to avoid free sulphur group getting involved in side

reactions and increases background activity. The synthesized compound was then radiolabeled with Ga. The transport of the compound in cells was found to be primarily through LAT receptors followed by ASC system. Cell binding assay, biodistribution and μ PET imaging has been done.

Contents

1. Introduction and review of literature
2. Design and synthesis of mono and bis-macrocyclic frameworks for different biomedical applications
3. Synthesis and preclinical evaluation of a biotinidase resistant ^{68}Ga -radioligand based on biotin/AV interaction for pretargeted tumor diagnosis
4. Synthesis and biological evaluation of S-alkylated N-acetylcysteine derivative for tumor imaging using pet.
5. Summary, conclusions and references.

55. TIWARI (Shelja)

On-Line Preconcentration and Speciation of Chromium using Solid Phase Extractants and Determination in Water Samples by Faas.

Supervisor: Dr. Reena Saxena

Th 23309

Abstract (Not Verified)

The thesis entitled "On-line Preconcentration and Speciation of Chromium using Solid Phase Extractants and Determination in Water Samples by FAAS" describes the use of various chemically and physically modified solid phase extractants in a hyphenated spectroanalytical system for chromium speciation in water samples. Increasing pollution caused by heavy metals has become a challenging problem throughout the world. Their toxicity is directly associated with their solubility in aquatic systems, resulting in their accumulation in living systems throughout the food chain. In the last decade, chromium has gained considerable attention because of the difference in the toxicity of its two most common oxidation states – Cr(III) and Cr(VI). Cr(III) is biologically essential for living organisms, while Cr(VI) is cancer causing. The carcinogenic activity of Cr(VI) is because it can penetrate through the cell membrane and oxidize biological material. The industrial discharge from various tanning, pigments and electroplating industries introduces Cr(VI) in surrounding water bodies. Thus, it is extremely important to determine the chromium content in water. The combination of flow injection on-line solid phase extraction (SPE) with FAAS has proven to be an effective system for trace element determination in various systems as it provides better sensitivity, effective removal of interfering ions, low cost and offers high sampling rate. Mini-columns packed with different solid phase extractants were used for the preconcentration of chromium species. The chemically modified SPEs were prepared via a series of chemical reactions for introduction of various functional groups on the surface of polymeric materials such as Dowex Optipore L493 (with dithizone), Amberlite XAD-16 (with α -benzoin oxime and salicylic acid) and multi walled carbon nanotubes (MWCNTs) (with L-arginine and tris (2-aminoethyl) amine). Unmodified polytetrafluoroethylene (PTFE) polymeric beads were used for speciation of Cr(III) and Cr(VI) using Iminodiacetic acid as complexing agent.

Contents

1. Introduction
2. Experimental
3. Preparation and characterization of solid phase extractants
4. Flow injection preconcentration system for speciation of chromium using solid phase extractants based on polymeric supports
5. Flow injection preconcentration system for speciation of chromium using solid phase extractants based on multi walled carbon nanotubes
6. Flow injection preconcentration system for

speciation of chromium using solid phase extractant based on polytetrafluoroethylene (PTFE) beads 7. Summary and list of publications.

56. TIWARI (Raju)
Synthesis, Characterization and Study of Electronic Properties of β -Functionalized 5,10,15,20-Tetraarylporphyrins.
 Supervisor: Prof. Mahendra Nath
Th 23311

Abstract
 (Not Verified)

The objective of this dissertation is to synthesize β -functionalized *meso*-tetraarylporphyrins and study their electronic properties. Since, functionalization of β -positions of porphyrins provides new molecules with improved electronic properties. Therefore, various β, β' -substituted and β, β' -fused *meso*-tetraarylporphyrins were prepared, which may be useful in various applications ranging from medicine to molecular device for electron transfer processes. The work presented in this thesis is divided into four chapters. The first chapter of this thesis presents a brief account on the synthesis and electronic properties of β -functionalized 5,10,15,20-tetraarylporphyrins. Chapter 2 discusses the synthesis and study of self-aggregation behavior of β, β' -pyrazine-fused *meso*-tetraphenyldiporphyrins. Chapter 3 describes an alternate synthesis of 2-diazo-3-oxo-5,10,15,20-tetraphenylchlorins and their electronic properties in addition to the mercuric ion recognition. Chapter 4 deals with the synthesis and photophysical properties of 2-nitro-3-(pyrrol-1-yl)-5,10,15,20-tetraarylporphyrins and pyrrolo[1,2-*a*]pyrazinoporphyrim analogues. The preliminary photophysical results are found to be encouraging and may prove useful for the designing of highly conjugated porphyrinic systems as light harvesting materials and photosensitizers in photodynamic therapy applications.

Contents

1. Synthesis and electronic properties of β -functionalized 5,10,15,20-tetraarylporphyrins: An overview 2. Divergent synthesis and study of self-aggregation behavior of β, β' -pyrazine-fused *meso*-tetraphenyldiporphyrins 3. 2-Diazo-3-oxo-5,10,15,20-tetraphenylchlorins: An alternate synthesis, electronic properties and mercuric ion recognition 4. Synthesis and properties of 2-nitro-3-(pyrrol-1-yl)-5,10,15,20-tetraarylporphyrins and pyrrolo[1,2-*a*] pyrazinoporphyrim analogues 5. Summary and publications.

57. YADAV (Sarita)
Synthesis and Characterization of Ag/Cu/Re-Core Based Supramolecular Coordination Complexes.
 Supervisor: Dr. Sandeep Kaur
Th 23319

Abstract
 (Verified)

The present work deals with the synthesis and characterization of Silver based metallacycles, Rhenium based metallacycles and Copper based complexes and their characterization by various spectroscopic techniques like H-NMR, COSY-NMR, FTIR, HR-MS, Elemental Analysis and SCXRD. The thesis also includes the electrochemical analysis of the Rhenium complex by cyclic voltammetric method. The thesis is divided into four chapters. The first chapter begins with the general introduction containing the literature data related to the methods of synthesis of complexes (metallacycles) of various shapes and geometry and their properties; explaining their importance in various fields of applications. This also sets the stage for the scope of the work carried out in the current thesis. The second chapter involves the synthesis and characterization

of Silver(I) based dinuclear, neutral and homoleptic metallacycles. These cyclic complexes were synthesized by one-step self-assembly procedure and characterized by various analytical techniques such as H-NMR, FTIR, Elemental analysis and mass spectroscopy. The crystal structures of the complexes have been discussed in detail. The third chapter deals with the synthesis, characterization and electrochemical investigations of the Rhenium based cyclic complexes. These complexes have been characterized by FTIR, H-NMR and Mass Spectrometry. The electrochemical investigations have been carried out in detail which concludes that the reductions were ligand based while the oxidations were metal based. The fourth chapter involves the synthesis and characterization of Copper(II) complex which was formed while synthesizing Copper metallacycles. The complex was characterized by various analytical techniques such as EPR and elemental analysis. The molecular and crystal structure of the complex was analysed by single crystal X-ray diffraction analysis.

Contents

1. Introduction and scope of the present work 2. Di-nuclear, homoleptic silver (I) metallacycles decorated free thiophenyl or thiomethyl units 3. Electrochemical aspects of restricted rhenium complexes with semi-rigid ligands 4. Synthesis and characterization of copper (II)- based trigonal complex. Summary, conclusion and publications.

58. YADAV (Sunil)

Coordination Complexes of Amide-Based Ligands: Synthesis, Characterization, Catalysis and Mechanistic Investigation

Supervisor: Prof. Rajeev Gupta

Th 23300

Abstract (Not Verified)

Chapter 1: Introduction: A brief survey on coordination chemistry with selected amide-based ligands This chapter summarizes selected examples of coordination chemistry with various amide-based ligands. Chapter 2: Manganese complexes of pyrrole- and indole-carboxamide ligands: Synthesis, structure, electrochemistry, and applications in oxidative and Lewis-acid assisted catalysis-shows the synthesis, structural, spectroscopic, electrochemical and catalytic properties of square-pyramidal and squareplanar Mn(III) complexes supported with pyrrole- and indole-carboxamide ligands. Electrochemical studies reveal highly negative Mn and moderately positive Mn redox potentials. In situ generated Mn species of the pyrrole-carboxamide ligands were characterized by absorption and electron paramagnetic resonance spectroscopy. Chapter 3: Cobalt complexes of pyrrole-carboxamide ligands as catalysts in nitro reduction reactions: Influence of electronic substituents on catalysis and mechanistic insights-presents the synthesis, characterization and catalytic properties of two square-planar Co(III) complexes. Binding studies provided evidence that the square-planar Co(III) complexes bind two equivalents of a substrate whereas mechanistic studies established the involvement of a Co -Co based redox cycle in the catalysis. Chapter 4: Synthesis and characterization of a Ni-NNP complex and its role in C-S and C-C crosscoupling reaction-describes the synthesis and characterization and catalytic property of a squareplanar Ni-NNP complex. Ni-NNP complex catalyzes cross-coupling of aryl halides with thiophenol and the reaction proceeds through a Ni-SPh compound which was isolated and structurally characterized. Mechanistic studies support the involvement of reversible Ni -Ni redox process in the catalysis whereas DFT studies advocate that the reaction proceeds via a concerted mechanism rather than step-wise route. Chapter 5: Palladium complexes in N PCI and N P environment: Synthesis, structure and catalysisdiscusses the synthesis, characterization and catalytic properties of two sets of square-planar Pd(II) complexes either in N PCI (1-3) or N P (4) coordination environment. Two sets of complexes display remarkable difference in catalysis as a result of difference in the coordination environment.

Contents

1. Introduction: A brief survey on and coordination chemistry with selected amide-based ligands 2. Manganese complexes of pyrrole- and indolecarboxamide ligands: Synthesis, structure, electrochemistry, and applications in oxidative and lewis-acid-assisted catalysis 3. Cobalt complexes of pyrrolecarboxamide ligands as catalysts in nitro reduction reactions: influence of electronic substituents on catalysis and mechanistic insights 4. Synthesis, characterization of Ni-NNP complex and its role in C-S and C-C cross-coupling reactions 5. Palladium complexes in N_2PCl and N_2P_2 environment: Synthesis, structure and catalysis 5. List of publications.

59. YADAV (Pooja)

Identification of Polypyrimidine Tract Binding Protein and Associated Splicing Factor as HIV-1 Integrase Interacting Host Protein and Biochemical Screening of Novel Synthesized Integrase Host Protein and Biochemical Screening of Novel Synthesized Integrase Inhibitors.

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Abstract
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The Human Immunodeficiency Virus (HIV) infection and Acquired Immunodeficiency Syndrome (AIDS) possess major health hazard worldwide since it was identified in 1981. HIV is categorized into two main types, HIV type 1 and HIV type 2. The virus attacks the human T-cell and thus hampers the overall immune system of the host. Combined Antiretroviral Therapy (cART), is a treatment regimen that consists of a combination of different classes of drug. However, the development of resistant strains has driven to focus on other targets of HIV. In the present study we have identified a new interacting partner of HIV-1 integrase, Polypyrimidine tract binding protein and associated splicing factor (PSF) through *in vitro* binding assays. PSF is a multidomain protein which is known to bind to the nucleic acid via its RRM domain. Along with its well-known function of splicing, it is also involved in transcriptional regulation, DNA repair, and Non-homologous end joining. We investigated its role in HIV-1 replication. The increase in transduction efficiency was observed in PSF knockdown cells. After we observed the change in knockdown cells, we overexpressed the cells with PSF plasmid and observed the decrease in virus transduction. The quantitative PCR data also revealed the difference in integration events and viral cDNA also. Based on our study and experimental data, we propose that the suppression of viral replication by PSF may be due to binding of this protein to integrase protein or to the integrase-HIV-1 cDNA complex and ultimately destabilizing the complex which leads to decline in the number of integration events. Other parts of our thesis

Contents

1. Review of literature 2. Identification of HIV-1 integrase interacting host cellular protein by *in vitro* assay 3. To study the role PSF in HIV replication 4. Biochemical screening of HIV-1 integrase strand transfer inhibitors from the library of synthesized anti-HIV compounds. Appendix.