CHAPTER 9

CHEMISTRY

Doctoral Theses

074. AFSAR ALI
Coordination Complexes With Appended Functional Groups: Hydrogen Bonded Networks and Heterobimetallic Complexes.
Supervisor : Dr. Rajeev Gupta
Th 18995

Abstract

The study aims at providing a strategy to synthesize self - assembled structures where a coordination complex has been touted as the building block and to accomplish such a strategy, several coordination complexes of pyridineamide based bidenate and tridentate ligands have been used as the building blocks. Further, such building blocks either offer H-bond donor / acceptors groups (phenol, catechol or amide) that form the self-assembled structures or appended pyridine groups that produce discrete $\{M_2^{2+}\text{-}M_1^{3+}\text{-}M_2^{2+}\}$ heterobimetallic complexes (where M_1^{3+} = Co or Fe and M_2^{2+} = Co, Cu Zn, Cd and Hg). Finally presence of Lewis acidic metals in heterobimetallic complexes has been utilized by demonstrating several organic transformation reactions.

Contents

1. Introduction to Metallo-ligands as the building blocks to generate self-assembled networks. 2. Synthesis, charaterization and self-assembly of Pyridine-amide based Bidentate and Tridentate ligands appended with phenol and catechol groups. 3. Synthesis, characterization and self-assembly of Co^{3+} complexes with pyridine-amide based tridentate ligands appended with phenol and catechol groups. 4. Synthesis characterization and self-assembly of Co^{3+} complexes with pyridine-amide based bidentate ligands appended with phenol and catechol groups. 5. Part A : Synthesis and characterization of $\{Co^{2+}\text{-}M^{3+}\text{-}Co^{2+}\}$ and Cu^{2+} - M^{3+} - $Cu^{2+}\}$ heterobimetallic complexes using Co^{3+} and Fe^{3+} complexes as the building blocks.

5. Part B. Application of {M_2^{2+} - M_1^{3+} - M_2^{2+}} (M_1 = Co^{3+} or Fe^{3+}; M_2 = Zn^{2+}, Cd^{2+}, Hg^{2+} Co^{2+}, Cu^{2+}) heterobimetallic complexes in organic transformation reactions.

075. AGGARWAL (Neha)
Synthesis of Novel O-Aryl Glycosides, Aminocoumarins and Chromonyldihydropyridines and Study of their Anticancer and Antitubercular Activities.
Supervisor : Prof. Ashok K. Prasad
Th 18985

Abstract

The study achieved the simultaneous synthesis and separation of both the anomers of O-arylribofuranosides, i.e. natural β- and unnatural α-anomers from D-ribose using biocatalyst in one of the crucial step to develop an efficient and green methodology to produce both the anomers and it is found during our study that Lipozyme TL IM in DIPE at 40-42 ^{0}C selectively and most efficiently deacylates that acyl moiety derived from the C-5 hydroxyl group of only the a-anomer over the other acetoxy moieties of O-aryl-α, β-D-ribofuranosides.

Contents

076. ANWAR JAHAN
Transformations in Organic Compounds.
Supervisor : Prof. M. Kidwai
Th 19008

Abstract

The study reveals that the propargylamines are major skeletons and synthetically versatile key intermediate for the preparation of many nitrogen-containing bilogically active compounds and are synthesized by one-pot three components A^3-coupling and aldehydes, alkynes and amines. Finally the development of new synthetic methods and the role of recyclable solid acid catalyst

in organic transformations, also report an efficient recyclable A^3-coupling reaction (via C-H activation) catalyzed by Bafion ®NR50. A mixture of aldehydes, secondary amines and phenylacetylene in CH_3CN are stirred at 70-80 ^{0}C under a nitrogen atmosphere in the presence of Nafion ®NR50. The formation of propargylamines is confirmed by spectral analysis.

Contents

1. Nafion NR50 catalyzed A^3-coupling for the synthesis of propargylamines via C-H activation. 2. A novel and highly efficient method for the synthesis of dithiocarbamates and its evaluation as anticancer and antibacterial agents catalyzed by CAN in PEG-H_2O system. 3A. Polyethylene glycol : A recyclable solvent system for the synthesis of benzimidazole derivatives using CAN as catalyst. 3B. Potassium carbonate (K_2CO_3) catalyzed synthesis of thiohydantoins in polyethylene glycol as an efficient and reusable solvent medium. 4A. Cerium(III) chloride as a highly efficient catalyst for one-pot three-component mannich reaction. 4B. A novel methods for the synthesis of tetrahydrobenzo[a]-xanthen-11-one derivatives using cerium(III) chloride. 5. Gold(II) chloride ($HAuCl_4$-$3H_2O$) in PEG : A new catalytic system for the synthesis of functionalized spirochromenes. 6. Dodecylphosphonic acid (DPA) : A highly efficient catalyst for the synthesis of 2H-indazolo[2,1-b] phthalazine-triones under solvent-free conditions.

077. ARYA (Anu)
Synthesis of Triazolylated Nucleosides, Coumarins and Coumarinyldihydropdyrimidinones and Selective Biocatalytic Acylation & Antifungal Activity Studies on Coumarins.
Supervisor : Prof. Ashok K. Prasad
Th 18998

Abstract

The study achieved the synthesis of a series of coumarin0, aryl- and alkyl- conjugated 1,2,3-triazolylnucleosides via, click reation and to synthesize the target compounds, the first key substrate, 3'-deoxy-3'-azido-5-methyluridine is prepared in seven steps from readily available D-xylose.

Contents

1. Synthesis of 3'-substituted 1,2,3-Triazoly Inucleosides. 2A. Synthesis and antifungal acitivity of novel azido and 1,2,3-Triazole

containing coumarins. 2B. Enzymatic stereoselective acylation studies on novel azido and 1,2,3-Triazole containing coumarins. 3. Synthesis of novel coumarinyldihydropy- rimidinones and their N-acylates. Summary.

078. ATTRI (Pankaj)
Influence of Ammonium Ionic Liquids on the Structure and Stability of Biomolecules.
Supervisor : Dr. P. Venkatesu
Th 19003

Abstract

The study finds out that anion variation has significantly larger effect on the Mb structure than cation variation. Further showed that a combination of spectroscopic studies of NMR measurements can be used to characterize the refolding ability of ILs. The results suggest that TEAP, DEAP and TMAP are effective refolding additives for Mb from quenched thermally denatured protein structure whereas Mb does not get refolded in the rest of ILs. Further the experimental results conclude that all combinations by kosmotropic anion and chaotropic cation cannot stabilize the biomolecuels. Finally ILs can provide better protein stability for the use in biocatalytic process.

Contents

1. Introduction and review of literature. 2. Materials and experimental techniques. 3. Structural basis for the enhanced stability of protein model compounds and their functional groups in ammonium ionic liquids (ILs). 4. Influence of ammonium ionic liquids on the structure and stability of α-chymotrypsin. 5. Influence of ammonium ionic liquids on the structure and stability of succinylated con A. 6. Influence of ammonium ionic liquids ont he strucutre and stability of myoglobin. 7. Conclusions.

079. AVDHESH KUMAR
Green Approach for the Synthesis of Ag, Cu, Ni, Co, Zn, Al Nanoparticles and their Catalytic Applications.
Supervisor : Dr. Sulekh Chandra
Th 18999

Abstract

The investigation illustrates simple, greener and significant methods for the synthesis of zinc nanoparticles through the

reduction of zinc nitrate in liquid media with reducing agent, surface areas to volume ratio of solid-supported metal nanoparticles (1-25 nm) nanoparticles can be used a scatalyst in organic synthesis and transformation.

Contents

080. AVNEET KAUR

Synthesis, Characterization of Some Transition Metal Complexes Containing N and S Donor Ligands.

Supervisors : Prof. Gurmeet Singh and Prof. N. K. Kaushik

Th 19002

Abstract

The study of some Transition Metal Complexes Containing N and S Donor Ligands describes the synthesis and structural studies of complexes of Ni(II), Cu(II), Co(III) and Zn(II) with dithiocarbamate ligands and Pd(II) and Pt(IV) with thiohydrazide ligands. Characterization and thermal studies of these complexes are carried out using various physico-chemical methods. Few of the synthesized complexes have been investigated for their cytotoxicity against various tumor cell lines. Biological studies against certain bacterial and fungal strains are also carried out.

Contents

1. Introduction. 2. Methods and materials. 3. Physico-chemical studies. 4. Thermal studies. 5. Biological studies. Summary and References.

081. BARAK (Anil)
Synthesis and Characterization of Amphiphilic Block copolymers Through Anionic Polymerization.
Supervisor : Dr. K. Tharanikkarasu
Th 18996

Abstract

The study finds out that all the PTBA-b-PEO-b-PTBA triblock copolymers and (PS)2-b-PEO-b-(PS)2 H-shaped block copolymers prepared through living anionic polymerization show superiority in terms of molecular weight and chain architecture, block copolymers showed self-assembly behavior in water and from colloidal solutions and the colloidal solution thus formed exhibit very low polydispersity index. The narrow particles size distribution could be explained on the basis of superior quality block copolymers and their efficient self assembly behavior.

Contents

1. Introduction. 2. Aim on objective of present investigation. 3. Synthesis and characterization of polyacrylate-b-poly(ethylene oxide)-b-polyacrylate triblock copolymers from diphenylethylene terminated poly (ethlene oxide). 4. Synthesis and characterization of polyztyrene-b-poly(ethylene oxide)-b-polystyrene H-shaped block copolymers from diphenylethylene terminated poly (ethylene oxide). 5. Synthesis and characterization of poly (styrene-acrylate)-b-poly(ethylene oxide)-b-poly(styrene-acrylate) H-shaped block copolymers from diphenylethylene terminated poly(ethylene oxide). 6. Preparation and characterization of micelles from polyacrylate triblock and polystyrene H-shaped block copolymers. 7. Summary and conclusions.

082. BEENA
Synthesis and Biological Activity Evaluation of Cyclohexane-1, 2-diamine, Metronidazole, Curcumin and Thymol Derivatives.
Supervisor : Diwan S. Rawat
Th 18980

Abstract

The study finds out that mono-functionalized symmertrical or unsymmetrical diamines are important intermediates for the synthesis of many biologically important pharmacophores. Selective and efficient protecting reasgents and mild reaction conditions are often required for sequential protection and deprotection of polyfunctional molecules. The preferential protection of one of the primary amine group of cyclohexane-1, 2-diamine is carried out using literature methods. Different protective groups such as $(Boc)_2O$,[59] CBZ,[60] tosyl, [61] Fmoc[62] are exoplored but out of all these, $(Boc)_2O$ in dioxane gave good results.

Contents

083. BHARDWAJ (Bharti)
Synthesis & Biological Profile of Some Novel Benzofurans, Benzotriazoles & Spiroindoles & Phytochemical Investigation of Floral Part of Callistemon Lanceolatus.
Supervisors : Prof. S. C. Jain and Dr. Sunita Bhagat
Th 19004

Abstract

The study chosen benzofuran as one of the scaffold in the couse of research and revealed that compounds containing sulfones possess various biological activities. Further use of sulfones has been diversified to herbicidal, antifungal and plant growth stimulants and sulfone as another bioactive moiety for target molecule. Heterocyclic secondary amines deserves special attention as these constitute an important part of various drugs, available in the market possessing anti-inflammatory, anti-HIV, fungistatic, bacteriostatic, antileukemic and anticonvulsant acitivitie. Besides these, aliphatic secondary amines are also present in a large number of biologically active compounds.

Contents

7-N-heterocyclyl)hepty)benzofurans. 2. Synthesis of some novel aminoalkylated 1H-benzotriazoles of biological importance. 3. synthesis and biological evaluation of 2-(5-(aryl/heteroaryl)-4H-[1,2,4]triazol-3-yl)benzfurans. 4A. Synthesis of novel 3'-(2-mercaptobenzimidazole-5-yl) spiro[indoline-3,2'-thiazolidine]-2,4'-diones.4B. Synthesis of nvel N'-(2-oxoindolin-3-ylidene)benzofuran-2-carbohydrazides via greener approach. 5. Phytochemical investigation of floral part of callistemon lanceolatus.

084. DAS (Maumita)

Studies on Nano-Structured Zirconia Based DNA Biosensors for M. Tuberculosis Detection.

Supervisors : Dr. R. Nagarajan and Dr. B. D. Malhotra

Th 19006

Abstract

The study deals with thin film fabrication of nano-structured ZrO_2, CHIT, CNT and their nanocomposite onto gold (Au) and indium-tin-oxide (ITO) coated glass substrates. Electrochemcial, self-assembly and lectrophoretic techniques have been employed to fabricate ZrO_2, CHIT, CNT and their composite with enhanced electrochemical characteristics. The nanostructured films have been utilized to immobilize single stranded DNA (ssDNA) specific to Mycobacterium tuberculosis (M. tuberculosis) via different immobilization methods [N-ethyl-N'-3(-dimethylaminoproply) corbodimide (EDC)-N-hydroxysuccinimide (NHS) chemistry, avidin-biotin coupling or affinity interaction between zirconia and the oxygen atom of the phosphate backbone of DNA. The prepared bioelectrodes have been investigated for their biosensing characteristics.

Contents

085. DHIRAJ KUMAR

Application of 1,4-dihydropyridine Scaffold for the Synthesis of Highly Functionalized di- and Tetrahydropyridines of Biological Importance.

Supervisor : Dr. Rakesh Kumar

Th 19007

Abstract

The study investigates that widespread occurrence and different bilogical activities associated with nitrogen heterocyclic compounds have made them important targets for synthetic chemists. Cladobotryal which is a metabolite of the fungus Caldobotrium varium, is first described in 1998 and reported to inhibit the growth of plant pathogens belonging to Oomyceta. Consequently, Cladobotryal may be useful as an agricultural fungicide and also reported to show moderate activity against some drug-resistant bacteria such as methicillin-resistant Staphylococcus aureus.

Contents

086. DHRA (Gulshan Kumar)

Polymer Electrolyte Membranes for Fuel Cell Applications.

Supervisor : Dr. K. Tharanikkarasu

Th 18982

Abstract

The study focus on to improve water stability of the sulfonated polymides and one such attempt is the corss-linking, but higher cross-linking brings out the brittleness in the resulted polyamides films in the dry states and so to reduce this problem

of cross-linking, very low percentage of cross-linking is required. Further the study has synthesized two novel triamines cross-linking agents one with stilbene and flexible ether linkage containing moiety and other with oxy-dibenzene basd structure.

Contents

1. Introduction. 2. Aim and objective of the presentation investigation. 3. Synthesis and characterization of cross-linked sulfonated polyimide membranes through novel stilbene containing triamine cross-linker. 4. Synthesis and characterization of cross-linked sulfonated polyimide membranes through novel oxy-dibenzene containing triamine cross-linker. 5. Synthesis and characterization of sulfonated polyimide membranes using novel stilbene containing non-sulfonated diamine. 6. Summary and conclusions.

087. ELUMALAI, P.
Palladium(II) and Platinum(II) Complexes of sym N,N',N" - Triarylguanidines : Eforts Directed Towards the Understanding of Mechanistic Aspects of C-H Activation Process.
Supervisor : Dr. N. Thirupathi
Th 19089

Abstract

Describes the results obtained from synthesis and conformational studies of sym N,N',N"-tris-(2,5-xylyl)guanidine ($LH_2^{2,5\text{-xylyl}}$) and the reactivity studies of this and other known sym N,N',N"-triarylguanidines (LH_2^{Aryl}) with palladium(II) and platinum(II) salts/presursors. New compounds synthesized in the present investigation have been characterized by various spectroscopic data. In addition, selected compounds have also been characterized by single crystal X-ray diffraction data.

Contents

1. Introduction. 2. Results and discussion. 3. Experimental section.

088. GARG (Ankur)
Synthesis and Spectroscopic Properties of Novel β Functionalized 5,10,15,20-Tetraarylporphyrins and Diporphyrin Analogues.
Supervisor : Dr. Mahendra Nath
Th 19000

Abstract

The study emphasised that porphyrins are π-conjugated macrocycles, which have been found to be of great interest in diverse areas such as artificial photosynthesis, catalysis, molecular sensing, electrooptics, and medicine. They are capable to bind with variety of metal ions and play a number of critical biological functions including oxygen transport, light harvesting, energy and electron transfer etc. Thus porphyrins are often referred as “pigments of life”. They have also been proved as promising candidates to be used in the development of new molecular materials with imporved electro- and photochemical properties. These chromphores display interesting photophysical, photochemical and eletrochemical properties due to their unusual electronic structure and play vital roles in photosynthesis, cellular respiration, and act as a component of metalloenzymes. The basic tetrapyrrolic skeleton of porphyrin in present in many natural pigments such as heme, chlorophyll, bacteriochlorophyll, vitamin B_{12} and cytochromes.

Contents

089. GUPTA (Shweta)
Synthesis of Anisotropic Nanostructures at the Interface, their Characterization and Applications.
Supervisors : Prof. Rita Kakkar and Dr. Renu Pasricha
Th 18977

Abstract

The study presents on overview of current research in the area of anisotropic nanomaterials in noble metal nanoparticles, in particular, with an introduction to the advancement of growth of anisotropic nanoparticles, followed by several detailed important synthetic protocols for making anisotropic nanomaterials.

Contents

1. Introduction. 2. Characterization technique. 3. Synthesis of gold nanostructures by citric acid reduction unexplored areas. 4. Effect of halide ions in transmetallation reaction between silver nanoparticies and chloroaurate ions : Means to build anisotropic nanostructures. 5. Interlinked assembles of nano gold using diamines. 6. A langmuir blodgett study : Graphene-gold complxes with excellent photocatalytic properties.7. Conclusions.

090. HEMANT KUMAR
Studies in Phthalocyanine Based Organic Solar Cells.
Supervisors : Dr. P. Venkatesu and Dr. Suresh Chand
Th 18990

Abstract

The objective of the thesis is to achieve a deep understanding of the working mechanism, performance limiting parameters of phthalocyanine based OSCs and to improve the device performance. Phthalocyanine compounds are important class of organic materials which have found potential applications in organic electronic devices. These materials exhibit good absorption in UV-visible regions where absorption spectra possesses high energy Q bands which follows red shift when hydrogen in metal free phthalocyanine complex is replaced by Zn metal and blue shift for Cu metal. It supports the fact that the covalent character increases from Zn to Cu based phthalocyanines.

Contents

1. Introduction. 2. Experimental techniques and procedure. 3. Studies on materials used in the preparation of OSCs. 4. Studies on effect of interface layer on PCE of OSCs. 5. Studies on temperature effect on PCE of OSCs. 6. Studies on the origin of V_{oc} in OSCs.

091. JOSHI (Megha)
Base-Mediated Regio-And Stereoselective Intermolecular Hydroamination of Alkynes.
Supervisor : Dr. Akhilesh Kumar Verma
Th 19090

Abstract

Describes the addition of amines onto C-C multiple bonds is

rising as a powerful techniques for the synthesis of imines, enamines or other nitrogen containing molecules used in diverse biological activities. Deals with the addition of various N-heterocycles onto symmetrical internal alkynes. Describes the preferential addition of N-heterocycles onto halo-arylalkyne over N-arylation under catalytic conditions.

Contents

1. Hydroamination : A general introduction. 2. Base-mediated hydroamination of internal alkynes. 3. Base-mediated hydroamination of terminal alkynes. 4. Preferential addition of N-Heterocycles onto Haloarylalkynes over N-Arylation. Appendixes and summary.

092. JYOTI

Investigation of Oxides Containing Sb5+ with Ilmenite and Pyrochlore Related Structures : Soft Chemical Synthesis, Structure and Applications.

Supervisor : Dr. S. Uma

Th 18997

Abstract

The study focuses on the alternate approaches for the synthesis of oxide materials and investigation of their structural and photocatalytic properties. In the preparative solid state chemistry, often the knowledge of structural chemistry and reactivity patterns of the solids have been found to be useful in synthesizing a avriety of new solids possessing novel structures and hence unique properties. Recognizing the limitations of the conventional 'heat-and-beat' methods, alternate synthetic strategies for the preparation of wide variety of metal oxies are being developed.

Contents

1. Introduction. 2. Characterization techniques. 3. Synthesis and characterization of ilmenite and pyrochlore polymorphs of $AgSbO_3$ and evaluation of their photocatalytic activities. 4. One step hydrothermal synthesis of M(II)Sb2O6 (M=Cd and Zn) type antimonats and their photocatalytic properties. 5. Synthesis and characterization of Cu^{+} incorporated ($Na_{0.39}Cu_{0.68}Sb_2O_{62}.0H_2O$) pyrochlore oxide and its photophysical properties. 6. Room temperature ion exchange synthesis of Sn^{2+} containing pyrochlore type oxides and their photocatalytic activities.

093. KAPOOR (Vinita)
Theoretical Studies on Molecular Designing of Novel Electrically Conducting Polymers and Biopolymers Using Genetic Algorithm.
Supervisor : Prof. A. K. Bakhshi
Th 18988

Abstract

The study investigated the effect of change in secondary structure, change of basis set, effect of hydration / solvation shell as well as the effects of H^+ and Li^+ binding to the peptide group (in the presence of anions represented by point charges θ) on the electronic structure and conduction properties of aperiodic poly (gly, ala, ser) chains, and also investigated the effect of replacing alanine residue in the polypeptide chain with leucine residue.

Contents

094. KARAM CHAND
Synthesis of Novel Pyridin-2-(1H)-One, Benzopyran-2(1H)-One, and Quinolin-2(1H)-One Derivatives & Sar Study of their Anticancer and Antiplatelet Activities.
Supervisor : Prof. Sunil K. Sharma
Th 19001

Abstract

The investigation has synthesized a series of 6-acetoxy-2-alkyl-4-methylquinolin-2-one derivatives starting from p-anisidine and studied their Calreticulin Transacetylase (CRTAase), antiplatelet activities. The potency of these quinolones having acetozy group as substituent are then evaluated for the CRTAase catalysed modulation of proteins, such as inhibition of cystolic glutathione-S-transferase (GST) and inhibition of platelet aggregation. Among the compounds screened, 4-methyl-2-oxo-1, 2-dihydroquinolin-6-yl acetate is found to be the superior

substrate to platelet CRTAase and emerged as the most promising antiplatelet agent. However, the introduction of N-alkyl ester and alkyl group (C_2 / C_4 / C_6 / C_8 / C_{10}) at C-3 position of 4-methyl-2-oxo-1,2-dihydroquinolin-6-yl acetate resulted in almost complete loss of activity, while O-alkyl ester i.e. ethyl 2-(6-acetoxy-4-methylquinolin-2-yloxy)acetate results in marginal decrease in the antiplatelet activity.

Contents

1. Design and synthesis of novel pyridin-2(1H)-one derivatives and evaluation of their anticancer activity. 2. Characterization of 4-methyl-2-oxo-1,2-dihydroquinolin-6-yl acetate as an effective antiplatelet agent. 3. Synthesis of novel benzopyran-2(1H)-one based chalcone derivatives and their anticancer activity evaluation.

095. KHATTAR (Raghvi)
Synthesis, Spectral and Structural Characterization of Some Iron (III), Nickel (II) and Copper (II) Transition Metal Ion Complexes with N-Substituted Bis-Benzimidazolyl Based Ligands.
Supervisor : Prof. Pavan Mathur
Th 18976

Abstract

The investigation reveals the synthesis and characterization of transition metal ion complexes with bidentate N-Picolylated-1,3(bis-benzimidazolyl)propane [PGAB](L1) and tridentate N-Picolylated-bis(2-benzimidazolylmethyl)ether [PDGB](L2), Bis(1-(4-nitrobenzyl)-benzimidazol-2-ylmethyl)ether [NBDGB)(L3) ligands. These ligands have been chosen to study spectral, electrochemical and structural aspects of Iron(III), Nickel(II) and Copper (II) metal ion complexes.

Contents

1. Introduction. 2. Theory of spectroscopic methods utilized in the identification of ligands, their metal complexes synthesis of ligands. 3. Synthesi, spectral and structural characterization of Iron (III) complexes with N-Picolylated-bis(2-Benzimidazolylmethyl) ether [PDGB] (L2) and Bis(1(4-nitrobenzyl)-benzimidazol-2-ylmethyl)ether [NBDGB](L3). 4. Synthesis, spectral and strucutural characterization of nickel (II) complexes with N-Picolylated-bis (2-benzimidazolylmethyl)ether [PDGB(L2) and Bis(1-(4-nitrobenzyl)-benzimidazol-2-ylmethyl)ether [NBDGB] (L3). 5. Synthesis, spectral and structural characterization of

copper (II) complexes with bidentate N-Picolylated-1,3 (bis-benzimidazoly) propane [PGAB](L1), tridentate N-Picolylated-bis (2-benzimidazolylmethyl)ether [PDGB)(L2) and Bis(1-(4-nitrobenzyl)-ether [PDGB](L2), and Bis)1-(4-nitrobenzyl)-benzimidazol-2-ylmethyl)ether [NBDGB](L3) ligands.

096. LUMB (Anshika)
Deoxygenations with Nickel Boride, Oxidations with $NaBrO_3$-[bmim]HSO_4, Green Synthesis of Xanthenes, Pyranopyrimidines and in Vitro antioxidant Studies.
Supervisor : Prof. J. M. Khurana
Th 18987

Abstract

Studies some novel synthetic methods, which include (i) facile deoxygenation of telluroxides, tellurones and selenones with nickel boride at ambient temperature, (ii) $NaBrO_3$ / [bmim]HSO_4: a versatile system for the selective oridation of 1,2-diols, α-hydroxyketones and alcohols, (iii) microwave mediated synthesis of 12-aryl-8,9,10,12-tetrahydrobenzo[α]xanthen-11-ones in solvent less conditions, (iv) acid catalyzed syntheses of naphthoquione scaffolds in aqueous media and their antioxidant activity, (v) synthesis and in vitro evaluation of antioxidant acitivity of diverse naphthopyranopyrimidines and tetrahydrobenzo[α]xanthen-11-ones.

Contents

097. MALIK (Ritu)
Design and Synthesis of Azaheterocycles of Medicinal Interest & Phytochemical Investigation of Saurauia Napaulensis.
Supervisor : Prof. S. C. Jain
Th 19005

Abstract

Medicinal plants are new getting more attention than over because theyhave potential of myriad benefits to society or indeed to all mankind, especially in the field of medicine and pharmacology. The medicinal value of these plants lies in bioactive phytochemical constituetns that produce definite physiological action on the human body. Some of the important bioactive phytochemical constituents are alkaloids, essentail oils, flavonoids, tannis, terpenoids, sapoinins, phenolic compounds and many more. These natural compounds formed the foundations of modern prescription drugs as we know today. The study undertook the biological evaluation and phytochemical studies of the extract of bark of Saurauia napaulensis using bioassay guided technique and have also screened the extract of S. napaulensis for various biological activities such as antimicrobial and anti-oxidants.

Contents

098. MANOCHA (Alzu)
Understanding Biochemical Mechanism Involved in Development of Dictyostelium Discoideum.
Supervisors : Dr. S. K. Awasthi and Dr. Rajesh S. Gokhale
Th 18983

Abstract

The investigation explore the studies on MPBD and DIF1 using the novel approach of genetic disruption couples with chemical complementation provides a new insight into Dicty biology and the development of the high throughput assay system for α-KG- dependent enzymes provides a tantalizing opportunity to decipher the functions of this large family of enzymes in Dicty.

Contents

1. Review of literature. 2. Comparative phenotypic and genotypic analysis of DiPKSI and DiPKS37 mutants with DiPKS1/37 double mutant. 3. Investigation of functional role of MPBD by synthesis of MPBD-biotin analogue. 4. Biochemical characterization of Fe(II)/α-KG-dependent enzymes. Summary and conclusions.

099. MD. MERAJUL ISLAM
Theoretical Models for Spectroelectrochemical Absorbance and Chronocoulometric Transients Under Potentiostatic Condition on Rough Electrodes.
Supervisor : Prof. Rama Kant
Th 18994

Abstract

The study investigates rough optically transparent electrodes (OTEs)-electrolyte interface by using spectroelectrochemistry (SEC) and chronocoulometry techniques. SEC is a couples technique of spectroscopy and electrochemistry the advantage of the two different techniques are combined which provides the versatile utility to understand the electron-transfer, spectroscopic study and surface processes and results obtained have wide range of applicability such as in the development of the electrochromic devices, light emitting diodes, solar cells, photovoltaics, carbon nanostructures, graphene and biomolecules.

Contents

1. Spectroelectrochemical and chronocoulometrical responses at rough electrodes : An introduction. 2. Theory of absorbance-transients of a redox reaction at an optically trnasparent rough electrode. 3. Theory of chronoabsorptometry of a pseudo first-order cat-alytic process at an optically transparent rough electrode. 4. Generalization of the anson equation for fractal and nonfractal rough electrodes. 5. Theory of chronocoulometry of a pseudo first-order catalytic process at a rough electrode. 6. Conclusions.

100. MOHSINEEN WAZIR
Theoretical Investigation of Biopolymers and Conducting Polymers Using Ant Algorithm.
Supervisor : Prof. A. K. Bakhshi
Th 18978

Abstract

The study explore that AA is an efficient tool which can enable researchers to design conducting polymers with pre-specified electronic properties and is a probabilistic technique which has the advantage of giving an optimum solution by searching just 30% of the solution space. The result obtained show that the electronic properties and optimum solutions of type-I copolymers are governed by the lowest band gap constituent homopolymer. The band gap of a type-I copolymer is almost the same whereas that of a type-II copolymer is less than that of the lowest band gap homopolymer.

Contents

101. NUSRAT JEHAN
Design and Synthesis of Pharmacophores Based on Nitrogen Heterocycles & Phytochemical Investigation of Leaves of Callistemon Lanceolatus.
Supervisor : Prof. S. C. Jain
Th 18991

Abstract

The study has developed new triazolybensimidazoles, a series of novel 1-[3-aryl-4H-[1,2,4]-5-ylmethyl]-2-substitited-1H-benzimidazoles and have synthesized from benzimidazoles and using different substituted-benzaldehydes/furfuraldehyde/thiophene-2-carboxaldehyde and the intermediates along with the final compounds formed have been fully characterized by their detailed spectral studies.

Contents

thesis of novel 1-(6-N-(substituted)aminohexyl)-1H-benzimidazoles of biological importance. 2B. Synthesis of 1-(6-N-(substituted)aminohexyl)spiro(1',3'-dioxolane-2',3-indoline)-2-ones. 3. Synthesis of 3-(2-benzofuran-2-yl-2-oxoethylidene) indolin-2-ones & their chemical modification. 4. Phytochemical investigation of leaves of callistemon lanceolatus.

102. PADMAJA (G. Vani)
Preparation of Nanosized I Tier Biocompatible Dendrimer with Silicon as a Core-Their Structural and Intrafacial Optimization.
Supervisor : Prof. Man Singh
Th 18992

Abstract

The researcher has synthesized polymeric dendrimeric supramolecules by using the polymric and amono acid component with semiconductor with silicon as the discrete molecular building block in the versatile supramolecular assemblies. Giant supramolecules with many multifunctional moieties and the biologically active sites are composed of subunits designed to perform specific tasks in biological, biochemical, biophysical, pharmacological areas etc. Self assembly of polymeric dendrimer systems are powerful tools for producing functional materials which combine several desired properties and could respond to external conditions.

Contents

1. Introduction. 2. Literature review. 3. Theory. 4. Chemical, experiment and calculations. 5. Result and discussion. 6. Summary anc conclusion.

103. RAJAKANNU (Palanisamy)
Synthesis, Structural Characterization and Photophysical Studies of Heteroleptic Re(I) Based Metallacycles.
Supervisor : Dr. M. Sathiyendiran
Th 18986

Abstract

The study concludes two hydroxy bridged rectangles 23 and 24 and four furan units exocyclically functionalized rectangle 25 are assembled using fac-$Re(CO)_3$ synthetic approach and characterized. This synthetic methods not only facilitates the incorporation of potentially biologically and materially desirable

moieties onto a discrete supramolecule at the exterior but also provides control over the number and location of functional units in the molecule. The rectangle 25 is regonizing planar aromatic molecules (naphthalene, anthracene and triphenylene) through $\pi\cdots\pi$ interactions between bpe moiety of rectangle and guest molecules.

Contents

1. Introduction. 2. Synthesis and charaterization of neutral altitudinal metallacyclic rotors. 3. Synthesis, characterization and photophysical studies of molecular cycles of rhenium complexes decorated with furan / thiophene. 4. Synthesis, characterization and photophysical studies of molecular cycles of rhenium complexes. 5. Synthesis, characterization and photophysical studies of molecular rectangles with / without furan decorating units.

104. RAWAT (Amit Kumar)
Synthesis, Covalent and Non-Covalent Interactions of Selected Porphyrinoids and Related Compounds.
Supervisor : Prof. S. M. S. Chauhan
Th 19087

Abstract

Describes synthesis of selected porphyrinogens, hexa porphyrinogen and their interactions with anions in different reaction conditions. Deals with synthesis of selected oxo-porphyrinogens, related macrocycles and their non-covalent interactions. Synthesis of hetero-porphyrinogens in acidic ionic liquids and their non-covalent interactions. Synthesis of functional core modified porphyrins in acidic ionic liquids and their non-covalent interactions and synthesis of 5-substituted dipyrromethanes and their uses in the synthesis of expanded porphyrins and core-modified expanded porphyrins

Contents

1. Synthesis of porphyrinogens, hexa porphyrinogen and their interaction with anions. 2. Synthesis of Oxo-porphyrinogenes, related macrocycles and their non-covalen interactions. 3. Synthesis of hetero-porphyrinogens in acidic ionic liquids and their non-covalent interaction. 4. Synthesis of functional core modified porphyrins in acidic ionic liquids and their non-covalen interactions. 5. Synthesis of 5-substituted dipyrromethanes and their uses in the synthesis of expanded porphyrins and ocre-modified expanded porphyrins.

105. SAVITA

Synthesis, Spectral Characterization and Biological Evaluation of Transition Metal Complexes of Some N,O and N,S Donor Schiff's Base Ligands.

Supervisor : Dr. Sulekh Chandra

Th18993

Abstract

The investigation deals with the result of physicochemical characterization on transition metal complexes of semicarbazide and thiosemicarbazide based ligands and transition metal that have been taken for study are Mn(II), Co(II), Ni(II), Cu(II). The complexes synthesized are characterized by elemental analysis, magnetic moments, IR, electronic and EPR spectral studies and newly synthesized ligands and their some of the complexes have also been screened against different bacterial and fungal species.

Contents

106. SHARMA (Sweta)

Design and Synthesis of Pyrazines, Imidazolones, Chromones and their Anticancer and Transacetylase Activities.

Supervisors : Dr. M. Thirumal and Prof. V. S. Parmar

Th 19088

Abstract

Describes the design and synthesis of furopyrazine scaffold as potential conformationally restricted dipeptidomimetics. Synthesis of C-3 aroylated 3,5-dichloro-2-(1H)-pyrazinones using NHC as catalyst. The silver (I) catalyzed synthesis of tetrasubstituted 2-imidazolones and the synthesis of novel chromones and their evaluation for anticancer and transacetylase activities.

Contents

aroylated 3,5-Dichloro-2-(1H)-pyrazinones using NHC as catalyst. 2. Silver (I) catalyzed synthesis of tetrasubsituted 2-imidazolones. 3. Synthesis of novel chromones and their evaluation for anticancer and transacetylase activities.

107. SUNIL KUMAR
Application of Derivative Spectroscopy of α,b-Unsaturated Carbonyl Compounds (A Case Study of Testosterone & Its Interaction with Various Species).
Supervisor : Prof. Harish Chandra
Th 18981

Abstract

The study investigates that analytical power of derrivative technique is so versatile that it can unearth such informations which require very sophisticated instruments e.g., Circular Dichroism spectrometer. Through this technique one can unearth even such information which even CD spectrometer can't provide e.g., when recorded CD spectra of our target molecule in polar and hydroxylic solvents in the $\pi \rightarrow \pi^*$ region, featureless spectra without any vibrational transitions are observed while through technique observed beautiful spectra with all the expected features.

Contents

1. Introduction. 2. Review of literature. 3. Materials and methods. 4. Results and discussion. 5. Conclusion.

108. THAKRAL (Vaishali)
Solid State Chemistry of Novel Bismuth Containing Oxides : Synthesis, Structure and Investigation of Potential Photocatalytic Applications.
Supervisor : Dr. S. Uma
Th 19091

Abstract

Focuses on the synthesis of novel bismuth containing compounds, their crystal structure analysis by powder and single crystal X-ray diffraction, and the investigation of their potential applications. Describes the outcome of the investigation on the synthesis of Bi^{3+} containing mixed metal oxides and their structural and photocatalytic applications.

Contents

1. Introduction. 2. Characterization techniques. 3. Investigation of $Bi_4V_2O_{11-\delta}$ and bimievox (ME = Al, Ga) oxides for visible light photocatalysis. 4. Synthesis and structural investigation of a unique columnar phse in the Bi_2O_3-TeO_2-V_2O_5 system. 5. Raman spectroscopic study of the oxides with columnar structures in the Bi-Mo-O, Bi-Mo-V-O, Bi-Te-Mo-V-O and Bi-Te-V-O systems. 6. Investigation of the structural and photocatalytic properties of bismuth based mixed metal oxides with scheelite structure. 7. Investigation of the structural transitions in the solid solution between $BiCu_2VO_6$ and $BiZn_2VO_®$.

109. VASHISHT (Hemlata)
Corrosion Inhibition of Mild Steel by Some Phosphonium Compounds in Acidic Media.
Supervisor : Prof. Gurmeet Singh
Th 18989

Abstract

The work explore the use of phosphonium compounds as corrosion inhibitors for mild steel in sulphuric acid. The compounds studied are (2-Hydroxyethyl)triphenylphosphonium Bromide (HETPB), (2-Hydroxybenxyl)tri-phenylphosphonium Bromide (HBTPB), Tetrabutylphosphonium hydroxide 40 wt.% in H_2O (TBPH), Cyclopropyltriphenylphosphonium bromide (CPTPB), (4-bromobutyl) triphenylphosphonium broide (BBTPB) and (Polyethyleneglycol) triphenyl- phosphine (PEGTPP). The work is carried out at four different temperatures, viz., 298 K, 318 K and 328 K and at different concentrations and synergistic effect of KI on TBPH is also studied.

Contents

1. Introduction. 2. Literature survey. 3. Experimental procedure. 4. Galvanostatic polarization studies. 5. Temperature kinetics. 6. Potentiostatic polarization studies. 7. Electrochemical impedance spectroscopy. 8. Scanning electron microscopy. 9. Atomic force microscopy. 10. Quantum chemical analysis. 11. Conclusion.

110. VIJ (Kanika)
Synthesis, Characterization and Applications of Nickel Nanoparticles in Knoevenagel Condensation and Michael Addition Reactions.
Supervisor : Prof. J. M. Khurana
Th 18979

Abstract

The study explore some novel synthetic methods, which include properties, general synthetic approaches as well as the characterization of metal nanoparticles with emphasis on synthesis and catalytic applications of Ni nanoparticles, Ni nanoparticles mediated knoevenagel condensation of aromatic aldehydes with barbituric acids and their 2-thio analogues, synthesis of tetraketones and biscoumarins by domino Knoevenagel Michael addition reaction sequence in presence of PVP-stabilized Ni nanoparticles, synthesis of PEG-stabilized Ni nanoparticles for use as an efficient catalyst for the synthesis of 5-arylidene Meldrum's acids followed by tandem enol lactonization with active methylene compounds and PEG-stabilized Ni nanoparticles catalyzed synthesis of polyfunctionalized 2-amono-4H-pyrans with diverse substitution patterns by the reaction of aromatic aldehydes, malononitrile and α-(C-H) acids.

Contents

111. YADAV (Neesha)
Design, Synthesis and Characterization of Some Biologically Active Compounds.
Supervisor : Dr. Satish Kumar Awasthi
Th 18984

Abstract

The study deals with chalcones, coumarins and tetraoxanes have shown wide range of pharmacological acitivity and explore the synthesis of several novel substituted chalcone deivatives. Chalcones, considered as precursors of flavonoids and isoflavonoids, are abundant in edible plants. 1,3-diarylpropenone possess a wide range of biological activities, viz, antibacterial, antifungal, antitumour, anti-inflammatory and antimalarial and designed strategy of chalcones with different heterocyclic amines and methoxy group substitutions on A and B rings further twenty seven compounds are synthesized and their antimalarial and anticancer activities have been discussed in the chapter.

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