

CHAPTER 11

CHEMISTRY

Doctoral Theses

101. AGARWAL (Shweta)
Self-Assembly of Functional Porphyrins and Related Heterocycles.
Supervisor : Prof. S. M. S. Chauhan
Th 16842

Abstract

Phthalocyanines are 18p-electron-conjugated macrocycles with unique physicochemical properties. Phthalocyanines have been used as dyes. Spectroscopic findings support that neutral-OH containing resorcin[4]arenes bind fluoride anion more effectively through non-covalent interactions due to smaller size and high electronegativity.

Contents

1. Coordination Bonds in the Self-Assembly of Functional Zinc Metalloporphyrins in Solution. 2. Non-Covalent interactions in the self-assembly of symmetrical and unsymmetrical phthalocyanines and porphyrazines. 3. Hydrophobic and other non-covalent interactions in 5,10-bis(1-methylpyridinium-4-yl)-15,20-di(4-alkoxyphenyl)-21H,23H-porphyrin ditosylates and related amphiphilic porphyrins. 4. Hydrogen-bonding in self-assembly of functional porphyrins. 5. Interactions of anions with self-assembled resorcin [4] arenes, pyrogallol[4] arenes and octahydroxypyridine[4]arenes.

102. ARORA (Indu)
Study of Some Organic Compounds as Corrosion Inhibitors for Mild Steel in Acidic Medium.
Supervisor : Prof. Gurmeet Singh
Th 16637

Abstract

Analyses the inhibition of corrosion of Mild Steel in 0.5M sulphuric acid in presence of three different enzymes- Pepsin, Papain and Rennin at different concentration and temperatures. The study was carried out at four different concentrations for the inhibitor (0.25%, 0.5%, 0.75% and 1.0%) and four temperatures (298K, 308K, 318K and 328K) using the following techniques. 1. Galvanostatic Polarization Studies, 2. Temperature Kinetics Studies, 3. Potentiostatic Polarization Studies, 4. Electrochemical Impedance Spectroscopy, 5. Scanning Electron Microscopy (SEM), 6. Atomic Force Microscopy (AFM).

Contents

1. Introduction. 2. Literature survey. 3. Experimental techniques. 4. Galvanostatic polarization studies. 5. Temperature kinetics. 6. Electrochemical impedance spectroscopy. 7. Potentiostatic polarization studies. 8. Scanning electron microscopy. 9. Atomic force microscopy. 10. Conclusions. Bibliography.

103. BAKSHI (Ruchi)
Synthesis and Characterization of Copper (II), Manganese (II) and Iron (III) Complexes of Some Multidentate Bis Benzimidazolyl Diamide Ligands with Varying Spacer Groups and their Utilization as Catalysts for Oxidation of Some Organic Substrates.

Supervisor : Prof. Pavan Mathur
 Th 16631

Abstract

Describes the synthesis and characterization of Copper (II), Manganese (II) and Iron (III) complexes with multidentate bis benzimidazolyl diamide ligands with varying spacer groups and their utilization as catalysts for oxidation of some organic substrates. The ligands comprise of two biologically important groups i.e. amide and benzimidazole. Amide group being the basic unit in many biomolecules. Imine-N atom of benzimidazole is similar to the imidazole nitrogen of histidine which is known to be the coordinating atom in several copper, manganese and iron metalloenzymes. Benzimidazoles are therefore good mimics of Histidines; these multidentate ligands therefore provide a local coordinating environment similar to that exist in the metalloenzymes.

1. Introduction. 2. Synthesis and characterization of ligands and theory of techniques used in the present study. 3. Synthesis, structural, spectral, electrochemical studies of copper(II) complexes with bis benzimidazolyl diamide ligands and their oxidase activity. 4. Synthesis, spectral, electrochemical studies of manganese(II) complexes with bis benzimidazolyl diamide ligands : Superoxide quenching and oxidation of hindered phenol/aniline. 5. Synthesis, spectral, electrochemical studies of iron(III) complexes with bis benzimidazolyl diamide ligands : Oxidation of aminophenol and alkyne.
104. BEDI (Amarpreet Kaur)
Corrosion Inhibition of Mild Steel by Some Antibiotics in Acidic Medium.
 Supervisor : Prof. Gurmeet Singh
Th 16626

Abstract

Entails the use of the some antibiotics as corrosion inhibitors for mild steel in sulphuric acid. The antibiotics studied are Ciprofloxacin (CIP), Norfloxacin (NOR), Gatifloxacin (GATI) and Ofloxacin (OFLO). The results are summarized as follows : The antibiotics were found to be effective corrosion inhibitors for mild steel in sulphuric acid. There is no appreciable shift observed in E_{corr} values indicating that all these compounds are mixed inhibitors. An increase in temperature was seen to decrease the inhibition efficiency. The extent of inhibition increases with the increase in the concentration of the inhibitor. the anodic tafel slopes are greater than the cathodic tafel slopes which can be interpreted as an indicator that anodic character is more predominant in these CIP, NOR, GATI and OFLO mixed type inhibitors. These are passivating inhibitors. CIP and GATI follows Freundlich adsorption isotherm, NOR follows Temkin adsorption isotherm whereas OFLO follows Frumkin adsorption isotherm. All these can be ascertained by R^2 value. All inhibitors show chemisorption on mild steel surface (since $E_a > 80 \text{ kJ mol}^{-1}$). the RMS values are found to be lowered in the presence of inhibitor solution which indicates that all antibiotics are effective inhibitors.

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 calculations. 11. Conclusions. Bibliography.

105. BHANDARI (Mamta)
Alloxan-Dialuric Acid System : Insights into the Diabetogenic Activity of Alloxan.
 Supervisor : Prof. Rita Kakkar
Th 16841

Abstract

Deals with a computational study on the diabetogenic activity of the pyrimidine derivative, alloxan, which is used to induce diabetes in laboratory animals as a result of the specific necrosis of the pancreatic β cells. The resulting insulinopenia causes a state of experimental diabetes mellitus called 'alloxan diabetes'. The reduction product of alloxan, dialuric acid, has also been shown to be diabetogenic in animals, and to cause ultrastructural changes identical to those observed in response to alloxan. Correlates the biological activity of three derivatives of alloxan with their structure because of the limited data available. This indicated a correlation with the lipophilicity of the derivatives.

Contents

1. Introduction. 2. Computational techniques. 3. Molecular structure and tautomerism of alloxan. 4. The alloxan - Dialuric acid redox cycle reduction products. 5. Reaction of alloxan and its derivatives with glutathione. 6. Metal ion complexes of alloxan. 7. Concluding remarks. Appendix and Bibliography.

106. BHATT (Ranjan Kumar)
Synthesis of Novel Porphyrin Analogues through Peripheral Functionalization of meso-Tetraphenylporphyrins.
 Supervisor : Dr. Mahendra Nath
Th 16635

Abstract

Synthesises peripheral functionalization of mesotetra aryl porphyrins further, in the study, nickel(II) 2-imino-5,10,15,20-tetraphenylporphyrins were used precursors for the synthesis of novel β -substituted porphyrinic thiazolidinone conjugates.

Addition of mercaptoacetic acid to refluxing solution of nickel(II) 2-iminotetraphenylporphyrins in toluene affords porphyrinic thiazolidinone product in moderate to good yield. Describes the synthesis, characterization and photophysical properties of meso-substituted iminoporphyrins and their porphyrin thiazolidinone conjugates. Provides a variety of new photosensitizers. Besides this, porphyrins have also been equipped with variety of therapeutic agents for better biological activity. Some of these exhibited various biological activities as antiviral, antimalarial and antiameobic agents. This intrigued the porphyrin chemists to explore the functionalization of porphyrin periphery by incorporating biologically active moieties.

Contents

1. An overview on the synthesis and peripheral functionalization of meso-tetraarylporphyrins. 2. Synthesis and spectroscopic characterization of β -imino-5,10,15,20-tetraphenylporphyrins and β -substituted porphyrinic thiazolidinone conjugates. 3. Synthesis, characterization and photophysical study of novel meso-substituted porphyrinic thiazolidinones. 4. Synthesis of meso-tetraphenylporphyrins with π -conjugated β -substituents via Knoevenagel condensation reactions. 5. Synthesis and spectroscopic investigation of hydrazonomethyl-tetraphenylporphyrins, meso-substituted triazonoporphyrins and porphyrinic azacycloalkane analogues. 6. Summary. Bibliography.

107. BRAHMA (Raju)
Synthesis and Biological Activity Evaluation of Novel 4-Aryldihydropyridines, 4-Alkylated Mono- / Dihydroxy and Acyloxycoumarins and Coumaryldihydropyrimidinones.
 Supervisor : Prof. Ashok K. Prasad
 Th 16641

Abstract

Describes synthesis and antifungal and antibacterial activity evaluation of 4-aryl-1, 4-dihydropyridines important pharmacological feature of these molecules came in sight in 1970. Evaluates antimicrobial activity of new coumarin molecules which are synthetically derived from resorinol (1,3-dihydroxybenzene) and pyrogallol (1,2,3-trihydroxybenzene), Pechmann condensation reactions were carried out followed by acylation reactions to obtain monohydroxy-, and dihydroxycoumarins and their clyates and have designed and synthesixed a total of 27 compounds. Attempts to find out

possible synergistic biological property by combining two different biologically active molecular fragments. the study attempted designing and synthesis of a total of six alkyl 4-(7-aminocoumarin-4-yl)-6-methyl-3, 4-dihydropyrimidin-2-one-5-carboxylates by adlpting multi-step organic synthetic methodologies to obtain the coumaryldihypprimidinone molecules and evaluated their antiplatelet activities. the results of the experiments suggest that the compounds have low to moderate antiplatelet activities.

Contents

1. Synthesis and antifungal and antibacterial activity evaluation of novel 4-Aryl, 4-dihydropyridines. 2. Synthesis and antimicrobial activity evaluation of 7-Hydroxy- and 7, 8-dihydroxy- 4-alkylcoumarins and their acylates. 3. Synthesis and antiplatelet activity evaluation of Alkyl 4- (7-carbethoxyaminocoumarin-4-yl)-6-methyl-3, 4-dihydropyrimidin-2(1H)-one-5-carboxylates. 4. Summary. Bibliography.

108. CAO PEI
Synthesis of Natural Products Based Bioactive Compounds.
 Supervisor : Prof. V. S. Parmar
Th 16615

Abstract

The increased levels of expression of cell adhesion molecules on the endothelial cells alter the adhesive property of the vasculature, leading to indiscriminate infiltration of the leukocytes across the blood vessels, which results in inflammation. A critically regulated expression of these adhesion molecules is, therefore highly essential for maintaining normal and healthy homeostasis in the body. Ethyl 3¹,4¹,5¹-trimethoxycinnamate has been isolated for the first time from a natural source, Piper longum, and it significantly blocked the adhesion of neutrophils to endothelium in a time- and concentration-dependent manner. Importantly, its inhibitory effect was found to be reversible. These findings have implications in developing compounds with a better therapeutic index against various inflammatory diseases. The methoxy cinnamates synthesized in the present study showed lowering of ICAM-1 expression and we found the best results with p-t-butylphenyl 2¹,3¹,4¹-trimethoxycinnamate as it significantly blocked the adhesion of endothelial monolayer. this novel compound caused the inhibition of TNF- α induced expression of ICAM-1 on

endothelial cells to the extent of 86% at IC_{50} value of 25 $\mu\text{g/ml}$ with MTD value of 63 $\mu\text{g/ml}$. The dimethylchromanyl acrylates synthesized in the present study showed lowering of ICAM-1 expression and we found the best results with p-t-butylphenyl 3-[2,2-dimethyl-3,4-dihydro-(2H)- benzopyran-6yl]-2E-prop-2-enoate as it significantly blocked the adhesion of endothelial monolayer. this novel compound caused the inhibition of TNF- α induced expression of ICAM-1 on endothelial cells to the extent of 84% at IC_{50} value of 76 $\mu\text{g/ml}$ with MTD value of 125 $\mu\text{g/ml}$.

Contents

1A. Synthesis and anti-inflammatory activity of novel methoxycinnamates. 1B. Synthesis and anti-inflammatory activity of novel dimethylchromanyl acrylates. 2. Highly stereoselective "Greener" trans addition of π -type nucleophiles to (3S, 7S)-3-Trifluoroacetamido-7-methoxycaprolactam. Summary. Bibliography.

109. CHANDRA (Charu)
Study of Corrosion Inhibition of Brass by Some Leaf Extracts in Acidic Medium.
 Supervisor : Prof. Gurmeet Singh
Th 16835

Abstract

Discusses about the experimental set up for various corrosion inhibition studies like Galvanostatic Polarization Studies, Potentiostatic Polarization Studies, Electrochemical Impedance Spectroscopy (EIS) Temperature Kinetics Studies, Scanning Electron Microscopy (SEM) and Atomic Force Microscopy (AFM). Explains the theoretical and mathematical details of the galvanostatic polarization technique. It discusses the results obtained from Tafel curves about the corrosion inhibition of brass in acidic medium using various leaf extracts as corrosion inhibitors. It also proposes the mechanistic details of the corrosion inhibition process and gives an idea of the latest research being conducted using this technique. Explains adsorption and its importance in corrosion chemistry. Deals with anodic dissolution of brass in nitric acid in the presence of 0.5%, 1%, 2% and 3% solution of leaf extracts as corrosion inhibitors at 298K. Explains the use of scanning electron microscope (SEM) in corrosion studies. Explains the use of atomic force Microscopy (AFM) in studying the corrosion inhibition of brass.

1. Introduction.
 2. Literature survey.
 3. Experimental procedures.
 4. Galvanostatic polarization studies.
 5. Temperature kinetics.
 6. Potentiostatic polarisation studies.
 7. Electrochemical impedance spectroscopy (EIS).
 8. Scanning electron microscopy.
 9. Atomic force microscopy.
 10. Conclusions. Bibliography.
110. DAS (Palash Jyoti)
Synthesis and Characterization of Polyethyleneoxide Based Triblock Copolymers Through Anionic Polymerization.
Supervisor : Dr. K. Tharanikkarasu
Th 16840

Abstract

PS-b-PEO-b-PS triblock copolymers have been synthesized by using telechelic bromine-terminated poly(ethylene oxide) through living anionic polymerization. Well-defined PS-b-PEO-b-PS triblock copolymers was successfully synthesized by sing telechelic bromine-terminated poly(ethylene oxide) through living anionic polymerization, this methods if not suitable for the end-fictionalization of polymeric chain as well as anionic polymerization of another monomer after the formation of PS-b-PEO-b-PS triblock copolymers, as the PS-b-PEO-b-PS triblock copolymer chain end is not living. Diphenylethylene terminated polyethylene oxide was synthesized which is a novel macroinitiator.

Contents

1. Introduction.
2. Aim and objective.
3. Synthesis of polystyrene-b-poly(ethylene oxide)-b-polystyrene triblock copolymers using bromine terminated poly(ethylene oxide).
4. Synthesis of polystyrene-b-poly(ethylene oxide)-b-polystyrene triblock copolymers using diphenylethylene terminated poly(ethylene oxide).
5. Synthesis of poly(methyl methacrylate)-b-poly(ethylene oxide)-b-poly(ethylene oxide)-b-poly(methyl methacrylate) triblock copolymers using diphenylethylene terminated poly(ethylene oxide).
6. Preparation and characterization of reverse micelles from polystyrene-b-poly(ethylene-oxide)-b-polystyrene triblock copolymers.
7. Summary and Conclusions. Bibliography.

111. GABA (Ritu)
DFT Study of Nanocrystalline TiO₂ : Relationships between Size, Structure and Reactivity.
 Supervisor : Prof. Rita Kakkar
Th 16613

Abstract

Studies the nanocrystalline titanium dioxide, with an idea to better understanding the relationship between its structure and reactivity. Determines the structures and stabilities of nanocrystalline TiO₂, a material finding various applications. Analyses of the stoichiometric structure with size, and the 17 unit crystal is the first cluster that shows partial retention of the anatase morphology. the band gap reduces significantly with size. Clusters of this size were taken up for subsequent examination of cation and anion defects, both charged and neutral. this threw up interesting revelations in the form of new bonds, some titanium atoms becoming trivalent, the excess electron residing in a titanium 3d orbital, leading to the experimental observation of paramagnetism. As a test case, adsorption of acetaldehyde on the nanosurface was investigated, and it was found that spontaneous dissociation occurs. This result is significant, since acetaldehyde is one of the most harmful volatile organic compounds.

Contents

1. Introduction. 2. Computational techniques. 3. Structures and stabilities of anatase TiO₂ nanocrystals. 4. Structures and stabilities of small TiO₂ clusters. 5. Fundamental point defects in nanocrystalline TiO₂. 6. Adsorption of acetaldehyde on the TiO₂ nanosurface. 7. Conclusions & perspectives. Bibliography.

112. GAURAV
Synthesis of Novel Bioactive Indolylchalcones and Partial Esters of Diols and Encapsulation Studies with Amphiphilic Polymers.
 Supervisors : Prof. V. S. Parmar and Prof. A. C. Watterson
Th 16639

Abstract

Synthesizes a series of aryl 2-methylpropanoates by the alkylation of 3-hydroxy-2-hydroxymethyl-2-methylpropanoic acid with benzyl bromide and 4-fluorobenzyl bromide, respectively

using KOH as base and DMF as the solvent at 100 °C. After the successful synthesis of aryl 2-methylpropanoates, we employed two different approaches to get the desired monoacylated derivatives by using the lipases. Attempts chemo-enzymatic condensation copolymerization of polyethylene glycol (Mn-900) with dimethyl 5-aminoisophthalate. After the successful synthesis of amino polymer, it was converted to the acylated amino amphiphilic polymers by attaching the acyl moieties by simple acylation reactions. Used the N-acylated amphiphilic copolymers for the encapsulation of the bio-active molecules, β -carotene and curcumin to develop their nano-formulations. In summary, two novel amphiphilic copolymers and one known amphiphilic copolymer were synthesized and characterized from their ^1H & ^{13}C NMR and IR spectra. The ability of these polymers to form self assembled structures in solution provides enormous potential in drug delivery studies. the polymers were evaluated for their drug encapsulation capacity using hydrophobic drugs, curcumin and β -carotene.

Contents

1. Synthesis and antiplatelet activities of novel indolylchalcones.
 2. Selective biocatalytic transesterification reactions and Aryl 3-hydroxy-2-(hydroxymethyl)-2-methylpropanoates.
 3. encapsulation studies with chemo-enzymatically synthesized amphiphilic polymers.
 4. Summary. Bibliography.

113. GUPTA (Anjali)
Synthesis of Nucleic Acid Building Blocks and Analogs of Naturally Occurring Bio-Active Compounds.
 Supervisor : Dr. Sunil K. Sharma
Th 16628

Abstract

Undertakes the synthesis of novel thiol - modified PNA building blocks in which the sulfhydryl group is incorporated in the side chain instead of PNA backbone moiety. In total 25 quinoline derivatives were synthesized having different functionalities e.g. methoxy, hydroxyl, acetoxy, trifluoromethyl, etc. All the compounds synthesized are fully characterized by their physical and spectral data. Of the 25 compounds synthesized, 11 are novel and reported for the first time. All the compounds were screened for various biological activities viz. antiplatelet aggregation activity, and antituberculi activity. Benzofuran derivative compounds synthesized, 10 are novel and reported for the first time.

All these compounds are well characterized from their physical data (1H, 13C, IR, UV and Mass spectrometry). All the compounds were screened for varied biological activities e.g. transacetylase activity, antiplatelet aggregation activity, antibacterial and antifungal activity and good preliminary results were obtained.

Contents

1. Synthesis of thiol modified building blocks of peptide nucleic acid. 2. Design and synthesis of quinolin-2-one derivatives and evaluating their biological. 3. Synthesis of benzofuran derivatives. Bibliography.

114. GUPTA (Deepti)
Structural Properties of Maleic and Fumaric Acids and Catalytic Role of Metal Oxides in their Degradation : A DFT Study.
 Supervisor : Prof. Rita Kakkar
Th 16612

Abstract

Deals with a computational study on the structural properties and isomerization reaction mechanisms of maleic acid (MA) and fumaric acid (FA). These acids are the most frequently encountered intermediates during the degradation of organic wastes and, therefore, the study of the structural and spectroscopic properties of these acids, their anions and their degradation has fascinated scientists for the past many years. Also, the existence of a low-barrier hydrogen bond (LBHB) in hydrogen maleate has made the study of the maleic acid monoanion a topic of intensive scientific research. The importance of the maleate ion in biochemistry as an inhibitor of transaminase reactions and of fumaric acid esters in curing psoriasis led us to study the structural properties of the two acids, as well as their monoanions and dianions. The increasing amount of non-biodegradable pollutants requires the development of new powerful, clean and safe decontaminant technology. In view of this, the adsorption of maleic and fumaric acids has been studied on metal oxides such as TiO₂ (anatase). Adsorption of these acids has been studied using a discrete TiO₂ moiety also. The industrial production of fumaric acid is achieved by the catalytic isomerization of maleic acid. The most common catalyst is thiourea, a toxic compound. Attempts to explore alternate, more benign, catalysts.

1. Introduction. 2. Computational techniques. 3. Structures and isoforms of fumaric acid and its anions. 4. Structures and isoforms of maleic acid and its anions : Characterization of the low barrier hydrogen bond in hydrogen maleate. 5. The maleic acid to fumaric acid isomerization. 6. Catalytic role of titanium dioxide in the isomerization and degradation reaction mechanisms of maleic acid. 7. Concluding remarks. Bibliography.
115. KHARKWAL (Mamta)
Synthesis, Characterization and Photophysical Properties of Mixed Metal Oxides Containing Titanium.
Supervisor : Dr. S. Uma
Th 16629

Abstract

Describes the experimental studies carried out on the Synthesis, Characterization and Photophysical Properties of Mixed Metal Oxides containing titanium. Gives details about the various materials, preparation method and basic principles of various analytical techniques such as Powder X-Ray Diffraction, UV-Visible Spectroscopy, Raman Spectroscopy, fourier Transform-Infra Red spectroscopy (FTIR), thermogravimetric Analysis and Differential thermal Analysis (TGA & DTA), Differential Scanning Calorimetry (DSC), Scanning Electron Microscopy (SEM) and EDX analysis, transmission Electron Microscopy (TEM), Surface Area Measurements and Photoluminescence Spectroscopy that have been employed for the current investigation of titanium containing mixed metal oxides. Describes the synthesis of precursors for the various metal titanates $M\text{TiO}_3$ ($M = \text{Cd}, \text{Zn}, \text{Mn}, \text{Co}, \text{Ni}$) via coprecipitation method using oxine as the ligand. The precursors were initially characterized by different techniques. Also describes the photophysical properties which include photocatalysis and photoluminescence of the various metal titanates and their precursors. for the first time, the application of CdTiO_3 (ilmenite and perovskite forms) as a photocatalyst for the decomposition of aqueous Methylene Blue (MB) dye solutions under UV and Visible light irradiation have been demonstrated.

Contents

1. Introduction. 2. Materials, method and characterization

techniques. 3. Results and discussion. 4. Photophysical properties. Bibliography, appendices.

116. LOKESWARI (P)
Adsorptive Removal of Carcinogenic Textile Dyes from Water by Montmorillonite and Montmorillonite Nanocomposites.
 Supervisors : Prof. Monika Datta and Dr. R. K. Khandal
Th 16839

Abstract

The efficiency of montmorillonite and montmorillonite composites for the adsorptive removal of arsenic from aqueous solutions has been investigated. Makes way for the development of industrial important compounds, in the near future, which would in turn prove to be useful in removal hazardous chemical from water.

Contents

1. Introduction. 2. Reported literature. 3. Experimental. 4. Result and discussion. 5. Conclusions. 6. Future prospects. 7. Summary. Bibliography.

117. MAGOO (Devanshi)
Some Novel Synthetic Methodologies and Inhibition Studies of Urease.
 Supervisor : Prof. J. M. Khurana
Th 16633

Abstract

Presents some novel synthetic methods, namely (i) Facile deprotection and reduction of 1,3-oxathiolanes and dithiolanes using nickel borides, (ii) Application of [bmim] BF₄ ionic liquid and neat reaction conditions as green protocols for the synthesis of tetrahydrobenzo[a]xanthene-11-ones, (iii) Synthesis of novel benzo[g]chromene derivatives in water as solvent and under neat conditions and (iv) Efficient and green protocols for the synthesis of 2H-indazolo[2,1-b]phthalazine triones in water-ethanol and ionic liquid as reaction media. Focuses on inhibition studies of urease and is divided into (v) Standardization of indophenol assay for urease and (v) Inhibition studies of urease by substrate based analogues.

1. Facile deprotection and reduction of 1,3-Oxathiolanes and 1,3-Dithiolanes using Nickel Boride.
 2. PTSA catalysed one-pot synthesis of 12-Aryl-8,9,10,12-tetrahydrobenzo[a]xanthen-11-one in Ionic Liquid and under neat conditions.
 3. Efficient and green approach for the synthesis of 4H-Benzo[g]chromenes using catalytic CTAB in water and under neat conditions.
 4. Efficient one-pot syntheses of 2H-Indazolo[2,1-b]phthalazine-triones by catalytic H_2SO_4 in water-ethanol and in Ionic Liquid.
 5. Standardization of urease assay by indophenol method.
 6. Inhibition studies of urease by substrate based analogues.
 7. Summary and conclusions. Bibliography.
118. MISHRA (Neeraj Kumar)
Green Methodologies for Organic Synthesis Using Various Catalysts.
Supervisor : Prof. M. Kidwai
Th 16619

Abstract

The environmental legislations raised by the pollution prevention act of 1990 set the stage of green chemistry. Environmental concerns in research and industry are increasing with increasing pressure to reduce the amount of pollutants produced. Hence the challenge for a sustainable environment calls to develop the clean safe, effective, economical, catalyst recyclability and high yielding. The practice of green chemistry not only led to the environmental benefits but also economic and social advantages. Clark et.al reported metal nanoparticles as green technology. these provide us a strong encouragement for the development of Ullmann coupling using Cu nanoparticles as catalyst. Catalytic activity of Cu nanoparticles is further evaluated by the preparation of Mannich product i.e. β -amino carbonyl compounds derivatives. $NbCl_5$ as a catalyst of choice for many organic syntheses, thus biodynamic substituted quinoxalines were prepared using $NbCl_5$ in acetonitrile. In the continuation of green synthesis of polysubstituted tetrahydropyrimidines derivatives. Also prepared versatile biologically important Aza-Markovnikov's products using K_2CO_3 . Our methodology is a step ahead in the area of green catalytic system for the preparation of industrially important compounds.

1. Introduction. 2(I). Cu-Nanoparticles catalyzed O-arylation of phenols with Aryl halides via ullmann coupling. 2(II). Cu-Nanoparticles in PEG : An efficient and recyclable catalytic system for N-arylation of amines with Aryl halides. 3. Novel one-pot cu-nanoparticles catalyzed mannich reaction. 4. Niolium(V) pentachloride catalyzed synthesis of quinozoline derivatives at room temperature. 5A. A facile one-pot synthesis of polysubstituted-tetrahydropyrimidines using PEG. 5B. Synthesis of polyfunctional-tetrahydropyrimidines in recyclable Ionic liquids. 6. A green protocol for the markovnikov addition of N-heterocycles to vinyl esters using K_2CO_3 as catalyst. Summary.
119. MUKESH KUMAR
Novel Polymer-Montmorillonite Nanocomposites Through Controlled Radical Polymerization.
Supervisor : Dr. K. Tharanikkarasu
Th 16624

Abstract

A tetraphenylethane based novel thermal iniferter, 1,1,2,2-tetraphenylethane-1,2,-diyl bis(2-bromo-2-methylpropanoate) (TPEBMP), was prepared and used to polymerize methl, methacrylate and styrene in the absence of layered silicates to test CRP mechanism. After confirming CRP nature of the novel thermal iniferter using gel permeation chromatography, in the next step, CRP of the MMA and styrene was carried out in the presence of functionalized layered silicate using TPEBMP. The surface modification of sodium montmorillonite (Na^+ -MMT) was carried out by simple ion-exchange process using 2-methyloloxethyl benzyl ammonium bromide (MEBAB) and the resulting MEBAB-MMT was characterized by X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), thermogravimetric analysis (TGA), and FT-IR, GPC results confirm the presence of CRP mechanism in MMA and styrene polymerization in the presence of modified montmorillonite. Exfoliated and intercalated morphology of the nanocomposites was confirmed using powder XRD and TEM analysis. Na^+ -MMT was modified using the novel (4-vinylbenzyl)triethylammonium chloride(CTAC). The structure of VTAC was characterized by NMR and FT-IR spectroscopy. Surface modification of Na^+ -MMT with VTAC was confirmed by XRD, XPS, TGA, FT-IR spectroscopic techniques. The exfoliated and intercalated morphology of the layered silicates nanocomposites was confirmed using XRD and

TEM analysis. Thermal properties of polystyrene-layered silicates nanocomposites were studied using DSC and TGA analysis and results are compared with the virgin polymers. Polyurethane-layered silicates nanocomposites were prepared successfully using novel triethanolamine functionalized montmorillonite (TEA-MMT). the novel TEA-MMT was characterized by TGA, FT-IR and XRD analysis. Morphology of polyurethane-layered silicates nanocomposites were studied using XRD and TEM analysis. Thermal properties of the exfoliated and intercalated polyurethane-layered silicates nanocomposites were studied using DSC and TGA analysis and the results are compared with the virgin polymers.

Contents

1. Introduction. 2. Aim and objective of the present investigation. 3. Controlled radical polymerization of methyl methacrylate and styrene using novel thermal iniferter. 4. Intergallery controlled radical polymerization of methyl methacrylate and styrene using dimethylaminoethyl methacrylate functionalized montmorillonite. 5. Poly(methyl methacrylate) and polystyrene nanocomposites using 4-Vinylbenzyl functionalised montmorillonite with thermal iniferter. 6. Synthesis and characterization of polyurethane nanocomposites using novel triethanolamine functionalized montmorillonite. 7. Summary, conclusions . Bibliography.

120. PANDA (Siva Shankar)
Design and Synthesis of Some Novel Heterocyclic Pharmacophores and Biological Evaluation and Phytochemical Studies of Aporusa Octandra.
 Supervisor : Prof. S. C. Jain
Th 16616

Abstract

Deals with the synthesis of some novel bis spiro-indoles. Also deals with a clean, benign and aqua mediated synthesis of some pharmacologically active spiro heterocycles, and with a green protocol for the synthesis of 2-arylbenzimidazole. Describes synthesis of quinazoline and pyridine derived bioactive lead compounds and the design and synthesis of coumarin based antimicrobial agents. Further deals with the design and synthesis of novel fluorinated quinolines of medicinal importance and biological evaluation and phytochemical studies of Indian medicinal plant : Aporusa octandra.

1. Synthesis of some novel bis spiro-indoles. 2A. a clean, benign and aqua mediated synthesis of some pharmacologically active spiro heterocycles. 2B. A Green protocol for the synthesis of 2-arylbenzimidazole. 3A. Synthesis of quinazoline and pyridine derived bioactive lead compounds. 3B. Design and synthesis of coumarin based antimicrobial agents. 4. Design and synthesis of novel fluorinated quinolines of medicinal importance. 5. Biological evaluation and phytochemical studies of Indian medicinal plant : *Aporusa octandra*. Summary. Bibliography.

121. PODDAR (Roona)
Green Approaches for Organic Compounds.
 Supervisor : Prof. M. Kidwai
Th 16632

Abstract

Searches an effective biomimetic model compound, 5-deaza-10-oxaflavin, to explore chemo-enzymatic reactions in aqueous medium, an efficient laccase-catalyzed synthesis of derivatives of 5-deaza-10-oxaflavin was investigated. This reaction also required H_2O_2 , a stoichiometric oxidant. Explores different chemoenzymatic reactions, to employ these ILs as solvents in biocatalytic reactions.

Contents

1. Laccase catalyze synthesis of substituted 5-deaza-10-oxaflavins. 2A. Transesterification of chromenes employing immobilized lipase in ionic liquids. 2B. Lipase catalyzed acylation of 7/6-hydroxy-4-methyl-2H-chromene-2-one. 3A. N-acylation of ethanolamine using chemo-selective catalyst lipase. 3B. Lipase catalyzed reactions in PEG. 4A. Laccase catalysed domino reaction for the synthesis of substituted benzopyranocoumarins. 4B. Expedient synthesis of coumarin fused 1,5-benzo thiazepines as antioxidant and cytotoxic agents. 5. Aqua mediated synthesis of substituted 2-amono-4-H-chromenes and in vitro study as antibacterial. Summary. Bibliography.

122. RATHI (Brijesh)
Synthesis, Conformational Features and Reactivity Studies of Sym N,N',N"-Triarylguanidines.
 Supervisor : Dr. N. Thirupathi
Th 16617

Abstract

Describes the results obtained from synthesis, conformational features and reactivity studies of sym N,N',N''-triarylguanidines. The new compounds prepared during the investigation have been characterized by IR, NMR (¹H and ¹³C), UV-Vis and mass spectral and microanalytical data. the structures of seven newly prepared compounds were determined by single crystal X-ray diffraction data. Describes the detailed experimental procedure for the new compounds and their characterization by analytical and spectroscopic data. the crystallographic data for the representative compounds is also presented.

Contents

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

123. SHARMA (Chetna)
Synthesis, Characterization and Applications of Silica Immobilized Metal Complexes as Sustainable Heterogeneous Catalysts for Oxidative Bromination, Esterification and Condensation Reactions.
Supervisor : Prof. R. K. Sharma
Th 16621

Abstract

Aimes at the rational design of catalysts for oxidative bromination oxidative esterification and condensation reactions. Designes, synthesizes and characterizes four silica immobilized metal complexes as heterogeneous catalysts.

Contents

1. Introduction. 2. Materials and theory of methods used. 3. Silica immobilized indium(III) acetylacetonate complex as heterogeneous catalyst for synthesis of oxindoles. 4. Copper(II) perfluorophthalocyanine immobilized silica gel catalyst for oxidative bromination reaction. 5. Synthesis of number of biologically important molecules using heterogeneous catalyst formed by covalent binding of zirconium complex to silica. 6. Manganese pyridine-2-carboxaldehyde complex covalently anchored on silica for oxidative methyl esterification of aldehydes. Summary. Bibliography.

124. SHARMA (Maneesh)
Thermal, Photochemical and Spectral Studies of Polymers and Reactive Intermediates.
Supervisor : Dr. S. V. Eswaran
Th 16611

Abstract

Discusses the preparation of “Deep UV” photoresists, thermal functionalisation of fullerene (C_{60}) and the synthesis of a new crosslinker for proteomics. These are based on new novolak resins, aryl azides and their characterization by spectral methods including 2D-NMR techniques. The highly reactive nitrene intermediate obtained by thermolysis or photolysis of the aryl azides plays a very critical role in the reactions and applications discussed. These novolak resins have been successfully derivatized, which was confirmed by 2D-NMR studies and used for formulating “Deep UV” (DUV) resists for photomicro lithography at a resolution of $5\mu\text{m}$. Thermolysis of the aryl azides with fullerene (C_{60}) has been used to solubilise it in common organic solvents. An aryl azide based heterobifunctional crosslinker has been synthesized and used to crosslink lysozyme following by mass spectrometric studies.

Contents

1. Introduction. 2. Synthesis of novolak resins. 3. Derivatization of novolak resins. 4. Synthesis of new aryl azides. 5. “Deep UV” microlithography. 6. Derivatization of fullerene (C_{60}). 7. MALDI-MS investigations of the crosslinking of a new heterobifunctional crosslinker with lysozyme. 8. Summary. Bibliography and appendices.

125. SHARMA (Mukul)
Synthesis and Characterization of Biologically Relevant Natural Product Analogues and Nitrogen Heterocycles.
Supervisor : Dr. Diwan S. Rawat
Th 16837

Abstract

Synthesizes 13-membered cyclic and acyclic enediyne esters by multistep synthetic protocol. Develops an improved synthesis of this naturally occurring ester and yield was improved by two fold amount in comparison to previously reported method. Synthesized seventeen examples of

1,2-dihydro-naphtho[1,2-e][1,3]oxazin-3-ones with 50-94% yield with electron rich and deficient benzaldehydes.

Contents

1. Synthesis of bromhexine analogues as antibacterial agents.
 2. Design, synthesis and characterization of cyclic and acyclic enediynes.
 3. Design, synthesis and characterization of sintonin analogues.
 - 4A. Sulphamic acid catalyzed three component one pot synthesis of 1,4-dihydropyridines.
 - 4B. Iodine catalyzed three-component, one pot synthesis of 1,2-dihydro-1-ary l-naphtho[1,2-e]oxazine-3-ones.
126. SHARMA (Prmod K.)
Synthesis and Anti-Inflammatory Activity Evaluation of 4-Methylcoumarylcarboxamides, Triazolylisatins and Pegylated Methylcoumarins.
 Supervisor : Prof. V. S. Parmar
Th 16610

Abstract

describes the design, synthesis and inhibitory activity of novel 4-methylcoumarylcarboxamides on TNF- α induced expression of intercellular adhesion molecule-1 (ICAM-1) on human umbilical vein endothelial cells. Describes the synthesis of novel 4-methylcoumarylcarboxamides. The 5-hydroxy-4-methyl-2-oxo-2H-chromene-7-carboxylic acid, 7-hydroxy-4-methyl-2-oxo-2H-chromene-6-carboxylic acid and 7-hydroxy-4-methyl-2-oxo-2H-chromene-8-carboxylic acid were synthesized in quantitative yields by the Pechmann condensation reaction of 3,5-dihydroxybenzoic acid, 2,4-dihydroxybenzoic acid and 2,6-dihydroxybenzoic acid, respectively with ethyl acetoacetate in the presence of concentrated sulphuric acid at room temperature. Synthesizes a series of novel triazolylisatin derivatives and evaluated their anti-inflammatory activities. Further synthesized nanomicellar copolymers of pluronic and 4-methylcoumarin & 4,8-dimethylcoumarin which have been used for encapsulation of curcumin. for this purpose, a low molecular weight pluronic (BASF Pluronic L44 NF, Mn 2200) was enzymatically copolymerized with various linkers to observe the effect of linkers on the encapsulation properties of the pluronic. Immobilized *Candida antarctica* lipase [also known as Novozyme 435 (CAL-B)] was used as the biocatalyst in the presence of molecular sieves (4A) under solventless reaction conditions. the linkers used were 3-(2-ethoxycarbonyl_ethyl-1-7-

ethoxycarbonylmethoxy-4-methylcoumarin or 3-(2-ethoxycarbonyl)ethyl-7-ethoxycarbonyl-methoxy-4,8-dimethylcoumarin and dimethyl 5-hydroxyisophthalate or dimethyl 5-amino-isophthalate. Furthermore studies the drug encapsulation potential of our novel polymeric systems by attempting the encapsulation of antitumor hydrophobic drug "curcumin". the copolymers and the hydrophobic drug curcumin were dissolved in acetonitrile, in a 1:2drug/polymer w/w ratio, and mixed for 15 minutes. the organic solvent was then evaporated under vacuum at 40 °C. the viscous reaction mixture of drug and polymer was then dissolved in water with extensive vortexing. Non-incorporated curcumin was filtered off the nanoparticle suspension through a 0.2 μ filter. As seen by UV-spectroscopy, the polymers have no UV absorption above 400 nm, while curcumin showed λ_{max} at 425 nm. The concentration of curcumin in the filtrate was determined by measuring absorbance at 425 nm and using a plotted calibration curve with known concentrations of curcumin in methanol. the percentage solubilization/encapsulation of curcumin was found to be in the range of 2.7-5.7 % wrt the weight of the different polymers. thus, it can be concluded that changing the linker on pluronics based polymers changes the percentage of encapsulation of curcumin.

Contents

1. Synthesis and anti-inflammatory activity evaluation of 4-methylcoumarylcarboxamides.
2. Synthesis and anti-inflammatory activity evaluation of triazolylisatins.
3. synthesis and anti-inflammatory activity evaluation of PEGylated methylcoumarins.
4. Summary. Bibliography.

127. SHARMA (Vineet)
Studies on Plant Ureases : Purification of Pumpkin Urease, Newer Assays for the Enzyme, Kinetic and Structural Studies on Free and Immobilized Urease.
 Supervisors : Prof. J. M. Khurana and Prof. K. Muralidhar
Th 16623

Abstract

Presents purification, characterization and immobilization of pumpkin urease along with development of new assay system for this enzyme. Describes the development of a new in-gel activity staining methods for urease. Employment of thiol-nitroprusside reagent for activity staining of urease offers

distinct advantages over previously reported methods. Thiol-nitroprusside based activity staining has been used for screening different plant sources for the presence of urease. Also describes physio-chemical and biochemical characterization of pumpkin urease. Purified pumpkin urease has been subjected to different biochemical characterization by exposing the enzyme towards the change of pHs, temperature, buffers, substrate, inhibitors, active site modifying reagents, additives and heavy metals. Pumpkin urease has been analyzed for its chemical interactions towards solid supports of different chromatographies.

Contents

1. Review of literature. 2. In-Gel detection of urease activity by a newly developed thiol-nitroprusside reagent and application of zymogram methods for screening of sources of urease. 3. Development of a new solution based biochemical assay by using bispyrazolone reagent. 4. Purification of urease from dehusked seeds of pumpkin (*Cucurbita maxima*). 5. Physico-chemical and biochemical characterization of pumpkin seed urease. 6. Immobilization of pumpkin urease in agarose and demonstration of its use as biosensor. 7. Summary and conclusions. Bibliography.
128. SHARMA (Yogesh Kumar)
Studies on the Synthesis of ABO_3 Oxides ($A=Mn^{2+}, Fe^{2+}, Co^{2+}, Ni^{2+}, Cd^{2+}$; $B=Ti^{4+}$) By Wet Chemical Method, Their Characterization and Applications.
 Supervisor : Dr. R. Nagarajan
Th 16627

Abstract

Describes the experimental studies carried out on the synthesis and characterization of precursor for ilmenite structured transition metal containing titanates of the formula $MTiO_3$ and their applications. Deals with the basic principles of various analytical techniques which have been extensively used at various stages of characterization. Describes the efforts to obtain a single source precursor by the reaction of divalent transition metal chlorides with $K_2TiO(C_2O_4)_2 \cdot 2H_2O$ under various conditions are reported in Mn^{2+} , Fe^{2+} , Co^{2+} , Ni^{2+} and Cd^{2+} ions were chosen for the study. Presents a detailed discussion on dielectric spectroscopic investigations of $MnTiO_3$ obtained by the mixed metal oxalate method together with its application as a sensor material for ethanol and magnetic properties are

described. The photocatalytic screening tests for NiTiO_3 and FeTiO_3 are also reported. It is for the first time that the dielectric properties of pure phase ilmenite MnTiO_3 above room temperature have been reported.

Contents

1. Introduction. 2. Characterization techniques. 3. Experimental. 4. Applications.

129. SINGH (Amit Pratap)
Development of Coordination Complexes as Building Blocks for the Generation of Novel Heterobimetallic Complexes.
 Supervisor : Dr. Rajeev Gupta
Th 16625

Abstract

Attempts to provide an alternate synthetic procedure for the synthesis of the desired heterobimetallic complexes and networks where a coordination complex has been used as the building block. Two tridentate pyridine-amide based ligands H2L^1 , H2L^2 , or H2L^3 (general formula : $\text{N,N}'\text{-bis(X-pyridyl)pyridine-2,6-dicarboxamide}$, where $\text{X}=2, 3$ or 4) selectively coordinate a central/primary metal ion through deprotonated N_{amide} and $\text{N}_{\text{pyridine}}$ atoms to create an octahedral geometry around the central metal ion. Interestingly, this coordination mode of the ligand leaves two pyridine rings uncoordinated or hanging. these hanging pyridine rings act as the peripheral functional groups or secondary binding site and coordinate a secondary metal ion to afford heterobimetallic complexes and/or networks. Ligands H2L^1 , H2L^2 , or H2L^3 have been used for the synthesis and characterization of Co^{3+} and Fe^{3+} complexes as the building blocks for the preparation of discrete as well as extended $\{\text{M}_2\text{-M}_1\text{-M}_2\}$ complexes or networks.

Contents

1. Introduction to Metallo-ligand as building blocks and their role in self - assembly and supramolecular organization. 2. Synthesis and characterization of Co^{3+} and Fe^{3+} complexes and their role as the building blocks. 3. Synthesis and characterization of $\{\text{M}^{3+}=\text{Cu}^+\}$ heterobimetallic complexes using Co^{3+} and Fe^{3+} complexes as the building blocks. 5. Synthesis and characterization of $\{\text{Co}^{3+}\text{-Cd}^{2+}\}$ heterobimetallic networks using Co^{3+} complexes as the building blocks. Bibliography.

130. SINGH (Parul)
Vibrational Spectroscopic Studies to Evaluate the Stability of Some Antiretroviral and Anticancer Drugs.
 Supervisors : Prof. A. K. Bakhshi and Dr. Ranjana Mehrotra
Th 16618

Abstract

Conclude that stability is one of the important quality attributes of any pharmaceutical product and any deviation from the defined limits might affects the safety and efficacy of the product and renders it unsuitable for the intended purpose. Establishing the stability profile of pharmaceutical is a key development activity that involves a number of systematic studies. It therefore becomes important to develop a simple, fast and accurate methods to determine the stability of drug substance under different stress conditions. the rapid testing by spectroscopic techniques at all stages of the manufacturing processes can reduce manufacturing time and provide assurance at each step of the process that the product quality is maintained.

Contents

1. Introduction. 2. Instrumentation and methodology. 3. Evaluation of stability of indinavir sulphate as per ICH guidelines. 4. Stress degradation studies on nelfinavir mesylate. 5. Stability studies of 5-flurouracil under different stress conditions. 6. Development and validation of an infrared spectroscopy based method for the analysis of moisture content in 5-flurouracil. 7. Summary and conclusions.

131. SINGH (Sunil Kumar)
Chemo-enzymatic Synthesis of Nucleosides and Triazole-& Thioacetamido-linked LNA Based Nonionic Nucleoside Dimers of Biological Importance.
 Supervisor : Prof. Ashok K. Prasad
Th 16614

Abstract

Synthesizes therapeutically suitable and commercially viable nucleic acid analogues. Oligonucleotide-based antisense strategies represent a unique paradigm for the treatment of wide variety of human diseases states. The novel utility of these agents resides in their ability to selectively prevent the expression of a particular disease-associated gene in a sequence specific manner. Describes, (a) the selective biocatalytic

deacylation studies on modified peracylated 4'-hydroxymethyl nucleosides for the synthesis of xylo-configured locked nucleic acid monomers and selective biocatalytic deacylation studies on the mixture of peracylated N-9 & N-7 guanine nucleosides with an aim to develop an efficient and easy methods for their separation and (b) synthesis of phosphate backbone modified triazole- & thioacetamido-linked locked nucleic acid based nucleoside dimers.

Contents

1. Chemoenzymatic synthesis of xylo-LNA monomers. 2. Efficient enzymatic separation of N-7 & N-9 guanine nucleosides. 3. Synthesis of nonionic triazole-linked nucleoside dimers of biological importance. 4. Synthesis of nonionic thioacetamido-linked nucleoside dimers of biological importance. 5. Summary. Bibliography.

132. SINGHAL (Anchal)
Biomimetic Oxygenation, Polymerization and Synthetic Models for Photosynthesis with Metalloporphyrins and Chemical Studies of Calix[4]pyrins.
 Supervisor : Prof. S. M. S. Chauhan
Th 16622

Abstract

Deals with the biomimetic oxygenation of α , β -unsaturated compounds such as guggulsterone, cyclopentenone and related compounds with hydrogen peroxide catalysed by iron(III)porphyrins. Also deals with the biomimetic polymerization of the selected functional olefins with different monooxygen donors catalyzed by lipid soluble metalloporphyrins in organic media and ionic liquids. Further deals with the copolymerization of selected monomers with monooxygen donors catalyzed by metalloporphyrins. The reaction of calix[4]pyrins with $\text{Zn}(\text{OAc})_2 \cdot 2\text{H}_2\text{O}$ in chloroform : methanol at room temperature gave Zn-metalated calix[4]pyrins. The insertion of Zn metal inside the cavity of macrocycle has been confirmed by ^1H NMR, ESI-MS and UV-Vis spectra. In the ^1H NMR spectra, the absence of peak at δ 13-14 ppm region due to NH protons confirms the formation of Zn(II)calix[4]pyrin. The bathochromic shift in the Soret band was observed in the UV-Vis spectra of zinc metalated calix[4]pyrins. β , β' substituted dipyrromethane and diketone moiety as strap has been synthesized by using multi-step procedure. The reaction of β , β' substituted dipyrromethane and

diketone in the presence of trichloroacetic acid followed by oxidation with DDQ gave strapped calix[4]phyrin. the formation of product has been confirmed by ESI-MS and UV-Vis spectrophotometer.

Contents

1. Biomimetic oxygenation of α , β -unsaturated compounds with H_2O_2 catalyzed by iron(III)porphyrins in organic media and ionic. 2A. Biomimetic polymerization of selected functional olefins with different monooxygen donors catalyzed by lipid soluble iron(III)porphyrins in organic media and ionic liquids. 2B. Synthetic biomaterials by copolymerization of selected monomers with different monooxygen donors catalyzed by lipid soluble iron(III)porphyrins in organic media and ionic liquids. 3. Synthesis and chemical models of photosynthesis in the presence of palladium reagents. 4. Synthesis and chemical studies of functional bis-porphyrins using $AgPF_6$ and related reagents. 5. Synthesis and chemical studies of calix[4]phyrins. Bibliography.

133. SNEHLATA
Designing, Synthesis and Biological Screening of Peptidomimics as ACE Inhibitors.
 Supervisors : Dr. Parbati Biswas and Dr. Santosh Pasha
Th 16838

Abstract

Focuses on the lesser bioavailability. In order to increase the bioavailability of these ACE inhibitors, concept of peptidomimics was used wherein one of peptide moiety present in a known inhibitor was replaced by a suitable non-peptidic residue to have a peptidomimic. Designes and synthesized library of tripeptidomimics. In-vitro results were further complemented by using some computational methodologies. Describes the effect of TOP on different makers associated with the hypertension in the different tissues isolated after the chronic treatment for 7 days. Also explains the differential mRNA and protein expression of the various genes involved in hypertension. Illustrates the organ bath studies of TOP and discusses mechanistic approach.

Contents

1. Introduction : An overview of hypertension and ACE inhibitors. 2. Designing, synthesis, purification & characterization

of peptidomimics. 3. In-vitro studies of peptidomimics and ACE inhibitors. 4. Computational studies of peptidomimics as ACE inhibitors. 5. In-vivo studies of peptidomimics as ACE inhibitors.

134. SRIVASTAVA (Amit Kumar)
Design and Synthesis of Untenine-B, Its Structure Modification for the Bioactive Lead Molecules and Phytochemical Investigation of Some Medicinally Important Plants.
 Supervisor : Prof. S. C. Jain
Th 16630

Abstract

Deals with the first total synthesis of a novel natural product Untenine-B isolated from marine sponge, with the synthesis of some novel 3-alkylpyridines containing heterocyclic secondary amines at the end of the aliphatic chain viz. morpholine, thiomorpholine, N-methylpiperazine, piperidine, pyrrolidine and some aliphatic amines like methoxyamine, methoxymethylamine, N, O-dimethylamine, N,N-dimethylamine etc. Deals with the phytochemical investigation of aerial roots of Ficus bengalensis and with the phytochemical investigation of Strobilanthes auriculatus.

Contents

1. Total synthesis of a novel natural product of Marine sponge : Untenine B, 2. Synthesis of some bioactive lead molecules by structural modification of a marine alkaloid. 3. Phytochemical investigation of the aerial roots of Ficus bengalensis. 4. Phytochemical investigation of Strobilanthes auriculatus. 5. Summary. Bibliography.

135. SUSHMA
Synthesis and Characterization of Lanthanide Complex With Heterocyclic Compound as Ligand.
 Supervisor : Dr. Man Singh
Th 16634

Abstract

Synthesizes the novel "Lanthanide(III) complexes" with newly synthesized and different combination of ligands having an effective coordinating donor atoms to bind with an effective site on the cations and to carry out their spectroscopic characterization in order to highlight their stable molecular structures.

1. Introduction. 2. Literature review. 3. Synthesis and characterization of lanthanide(III) complexes series with new azo dye: N,N-Dimethylazoglycine. 4. Synthesis and characterization of praseodymium(III) complex with new azo dye: N,N-dimethylazoleucine. 5. Synthesis and spectral studies of 4(f) metals with mixed ligands : Schiff base, acetylglycinebenzoic anhydride, 1,10 phenanthroline. 6. Synthesis and spectral studies of neodymium metal with mixed ligands : Schiff base, acetylleucinebenzoic anhydride, 1,10 phenanthroline. 7. Synthesis and spectroscopic characterizations of rare earth metals complexes with newly synthesized supramolecule and heterocyclic adducts. 8. Summary. Bibliography.
136. THAREJA (Rakhi)
Quantum Chemistry in Action - Applications and Properties of II-VI Quantum Dots.
Supervisor : Prof. Rita Kakkar
Th 16640

Abstract

Deals with a computational study on the structural and electronic properties of a special class of artificial atoms, also known as quantum dots. Quantum dots are semiconductors with unique optical and electronic properties and have gained increasing attention of scientists and have been widely used in biological applications, such as biosensing, biolabelling, bioimaging, and so on. The quantum dots considered in this thesis belong to the II-VI class/group of semiconductors. II-VI semiconductors are of great interest due to their wide band gap, possession of large excitonic binding energies, unique optical and electronic properties for device applications, since they provide zero dimensional structures with delta function density of states. This impelled out research work by beginning with a comparison of these quantum dots with their bulk counterparts and then to study the effect of doping them with an isovalent species. II-VI wide band gap materials have been used in the optical device applications, such as Quantum Dot Lasers, and in fundamental physics, chemical sensing, and biomedical labelling, etc. Amongst these, the size, shape and surface passivation of semiconductor CdSe nanocrystals have been topics of great interest in both theoretical and experimental investigations. Owing to their unique properties, CdSe quantum dots are the ideal candidates for biological applications,

laser media, light emitting diodes, non linear optics, and photovoltaics. CdSe quantum dots have size-dependent fluorescence, tunable across the visible spectrum and so have become the most extensively investigated quantum dots. The importance of CdSe quantum dots has led us to study their interactions with various organic molecules as well as biomolecules to check if they can play an effective role as biosensors for the latter.

Contents

1. Introduction. 2. Computational techniques. 3. Comparison of II-VI quantum dots with their bulk counterparts using various core treatments. 4. Structural and electronic properties of oxygen doped charged II-VI quantum dots. 5. Interaction of CdSe quantum dots with some aliphatic and aromatic diamines. 6. CdSe quantum dot as a sensor for urea. 7. Concluding remarks. Bibliography and appendices.

137. TOMAR (Nobel)
Synthesis, Structure and Applications of Silver Containing Mixed Metal Oxides.
 Supervisor : Dr. R. Nagarajan
Th 16638

Abstract

Describes the experimental studies carried out on the silver containing mixed metal oxides. Synthesizes copper containing delafossite oxide containing Al^{3+} as the B cation in ABO_2 through alkoxide approach. Towards this end, a double alkoxide containing copper in +1 oxidation state has been synthesized and investigated, the details of which has been summarized in Appendix 1. The effect of the steric hindrance in the aluminium phenoxide has been investigated with the help of FTIR, ^{27}Al MAS NMR, TG/DTA and powder X-ray diffraction techniques which revealed three types of aluminium coordination (4, 5 and 6) in aluminium phenoxide which yielded disordered $\gamma-Al_2O_3$ on decomposition unlike the hydrolysed one in which $\gamma-Al_2O_3$ was the dehydrated product.

Contents

1. Introduction. 2. Characterization techniques. 3. Synthesis of silver containing oxides $AgMO_2$ (M=Fe, Ga) by ultrasonication. 4. Synthesis and silver ion exchange studies of $LiM'_{0.75}Te_{0.25}O_2$ (M' = Mg, Ni, Co and Zn), $LiCu_{0.67}Sb_{0.33}O_2$, $NaCu_{0.67}Sb_{0.33}O_2$,

$\text{Na}_2\text{Ti}_6\text{O}_{13}$ and $\text{Na}_2\text{W}_4\text{O}_{13}$. 5. Synthesis of 'A' site deficit delafossites by leaching ($\text{AgFeO}_2, \text{AgCrC}_2$). 6. Synthesis of silver containing oxides by precipitation having formula $\text{Ag}_2\text{M}_2(\text{C}_2\text{O}_4)_3$ ($\text{M}=\text{Co}, \text{Cu}, \text{Ni}$), $\text{AgM}_{0.5}\text{M}'_{0.5}(\text{C}_2\text{O}_4)_2$ ($\text{M}=\text{Co}; \text{M}'=\text{Fe}$) and Ag (Onine anthranilate). Bibliograohy and appendices.

138. TOMAR (Shilpi)
Greener Approaches Towards Synthesis of Bioactive Compounds.
 Supervisor : Prof. V. S. Parmar
Th 16636

Abstract

Synthesizes coumarin derivatives by three different methods, i.e. Pechmann condensation, Wittig reaction and Knoevenagel condensation in different ionic liquids. The reactions went smoothly in all the ionic liquids studied giving the coumarin derivatives in good yield, significantly better than those obtained under conventional conditions.

Contents

1.A. Biocatalytic synthesis of optically enriched novel antimicrobial fluconazole analogs. 1B. Synthesis and anti-inflammatory activity of novel dimethylchromanyl acrylates. 1C. Synthesis and anti-inflammatory activity of Novel 2-(5-Phenylpyrazoly)ethyl cinnamates. 2. Efficient synthesis of coumarins in ionic liquids. Summary. Bibliography.

139. UMESH KUMAR
Investigation of the Reactions of Zinc(II) Carboxylates with Pyridine/Substituted Pyridine and their Implications in Coordination and Materials Chemistry.
 Supervisor : Dr. N. Thirupathi
Th 16620

Abstract

Describes the results obtained from investigation of the reactions of zinc(II) carboxylates with pyridine/substituted pyridine and their implications in coordination and materials chemistry. The new compounds prepared during the investigation have been characterized by microanalytical, IR, TGA/DTA, solution (^1H and ^{13}C) and solid-state CPMAS ^{13}C NMR spectroscopic techniques. The crystal and molecular structures of seventeen newly prepared compounds were determined by single crystal X-ray

diffraction data. Describes the detailed experimental procedure for the new compounds and their characterization by microanalytical, IR, TGA/DTA, solution (^1H and ^{13}C) and solid-state CPMAS ^{13}C NMR spectroscopic techniques. the crystallographic data of newly prepared Lewins base coordinated zinc(II) carboxylate complexes is also presented.

Contents

1. Introduction. 2. Results and discussion. 3. Experimental. Bibliography and Appendix.

140. YADAV (Shramila)
Corrosion Inhibition on Mild Steel by Some Green Inhibitors in Acidic Medium.
 Supervisor : Prof. Gurmeet Singh
Th 16836

Abstract

Explains the theoretical & mathematical details of galvanostatic polarization studies. It also describes the latest research being carried out using this technique. Also explains the effect of temperature on Adsorption processes. It studies the various Adsorption Isotherms (Langmuir, Temkin, Freundlich, Frumkin, El-awady and Flory-hyggins), their theoretical details and the calculations of various thermodynamic parameters. Further explains the theoretical, experimental details and graphical interpretation of electrochemical impedance technique. It proposes mechanistic details of corrosion inhibition process and also gives the latest research carried out using this technique. Delas with anodic dissolution of mild steel in 5%, 4%, 3% and 1% inhibitor solution at 298K. It describes the theoretical concepts of this technique and present latest studies on this technique. Attempts to correlate the quantitative corrosion inhibition studies with the surface analysis done by SEM. AFM gives three dimensional surface topography on a scale from angstroms to 100 microns. This technique was used in non-contact mode. This section includes a comparison between AFM and SEM studies. The roughness of metal surface was calculated by using average area analysis method.

Contents

1. Introduction. 2. Literature survey. 3. Experimental procedure. 4. Galvanostatic polarization studies. 5. Temperature kinetics.

6. Electrochemical impedance spectroscopy. 7. Potentiostatic polarization studies. 8. Scanning electron microscopy. 9. Atomic force microscopy. 10. Conclusion. Bibliography.

M.Phil Dissertations

141. ANURADHA
DNA-Drug Interactions.
Supervisor : Prof. Shrikant Kukreti
142. ARORA (Jyoti)
Synthesis of 2-Aminoalkylamino-1(1'- α -L-Ribofuranosyl) Thymine & 2-Aminoalkylamino-1-(1'- β -D-Arabinofuranosyl) Thymine.
Supervisor : Prof. Ashok K. Prasad
143. ARUN LAL
Synthesis and Characterization of Some Amino Acids Dithiocarbamate Ligands and Their Cobalt, Nickle and Copper Complexes.
Supervisor : Prof. N. K. Kaushik
144. AWANISH KUMAR
Influence of Polyols and Denaturants on the Folding/Unfolding Transition States of α -Chymotrypsin.
Supervisor : Dr. P. Venkatesu
145. CHAUHAN (Arun)
Probing the Basicity of Lewis Bases Upon the Aggregation/ Nuclearity and Acetate Coordination Modes of Zinc(II) Acetate Complexes.
Supervisor : Dr. N. Thirupathi
146. DEBNATH (Anamika)
Adsorption Behaviour of Acid Orange-7 and Acid Orange-10 on Smectite Group of Clays.
Supervisor : Prof. Monika Datta
147. GAUTAM (Seema)
Synthesis and Application of 2, 2'-Dipyridyl Ketone (DPK) Immobilized Silica Gel for Analysis of Copper (II) Metal Ion.
Supervisor : Prof. R. K. Sharma

148. GROVER (Ruchi)
Effect of Nano Zinc Oxide Particles on Corrosion Resistance of Solgel Coatings.
Supervisor : Prof. Gurmeet Singh
149. GUPTA (Deepak)
Synthesis and Characterization of Re(I) Based Functionalized Metalloprisms.
Supervisor : Dr. M. Sathiyendiran
150. JAGMINDER SINGH
Corrosion Inhibition of Brass by Pyridine 2-Aldehyde in Nitric Acid.
Supervisor : Prof. Gurmeet Singh
151. KASHYAP (Jyoti)
Chemical Studies of Chlorophylls and Related Natural Porphyrins.
Supervisor : Prof. S. M. S. Chauhan
152. MANOHAR LAL
Green Methodology for the Aza-Markonikov Addition.
Supervisor : Prof. M. Kidwai
153. NEETA AZAD
AZ12 Based Design of PDHK Inhibitors.
Supervisor : Prof. Rita Kakkar
154. PANDEY (Archana)
Aqua Mediated Green Approach for the Synthesis of 12-Ary 1-8,9,10,12-Tetrahydrobenzo[a]Xanthenes-11-Ones.
Supervisor : Prof. J. M. Khurana
155. PRASHANT KUMAR
Synthesis and Characterization of Iron Sulfides Using Soft Chemical Method.
Supervisor : Dr. R. Nagarajan
156. RATHI (Sonika)
UV Spectroscopic Studies on 5-Chlorouracil in Aqueous and Non-Aqueous Phase.
Supervisor : Dr. Harish Chandra

157. ROY (Bhupesh Kumar)
Templates in the Synthesis of Porphyrins and Multiporphyrins.
Supervisor : Prof. S. M. S. Chauhan
158. SHARMA (Kanika)
Solventless One-Pot Synthesis of Cobalt and copper Carboxy Amide Phthalocyanine Complexes.
Supervisor : Prof. R.K.Sharma
159. SHARMA (Raj Kumar)
Synthesis of Framework Alumino Silicates form Flyash.
Supervisor : Prof. Monika Datta
160. SHYAM LAL
Self-Assembly of Re(1) -based Metallocyclic Chairs.
Supervisor : Dr. M. Sathiyendiran
161. SINGH (Sarita)
Metal Ion Selectivity of Kojate Complexes.
Supervisor : Prof. Rita Kakkar
162. VAISHALI
Lipase Catalysed Substituted Coumarines with Antioxidant Activity.
Supervisor : Prof. M.Kidwai