

CHAPTER 9

CHEMISTRY

Doctoral Theses

069. AGGARWAL (Trapti)
Regioselective Synthesis of Polyheterocycles by the Electrophilic Iodocyclization of Alkynes and Metal-Catalyzed Diversification.
Supervisor : Dr. Akhilesh Kumar Verma
Th 19982

Contents

1. Electrophilic iodocyclization : A general introduction. 2. Synthesis of iodo-pyrano[4,3-b]quinolines via electrophilic iodocyclization of ortho-alkynyl aldehydes. 3. Iodine-mediated solvent controlled oxidative esterification followed by electrophilic Iodocyclization. 4. Structural diversification of iodopyrano[4.3-b]quinolines using palladium-catalyzed cross-coupling reactions. 5. Site-selective electrophilic cyclization and subsequent ring opening : Synthesis of pyrroloquinolines and indolizines. Summary.

070. ANSAR ANJUM
Detection and Extraction of Toxic Metal Ions (As, Sb, V) From Aqueous Media Using Naturally Occurring Clay and Their Composites.
Supervisors : Prof. Monika Datta and Dr. C. K. Seth
Th 20254

Contents

1. Introduction. 2. Analytical techniques utilized in the present work. 3. Synthesis of adsorbents. 4. Effect of adsorbents on arsenic (III) extraction. 5. Effect of adsorbents on antimony (III) extraction. 6. Effect of adsorbents on vanadium (V) extraction. 7. Comparison of adsorptive behavior of metal ions. 8. Reusability of adsorbents. 9. Summary. 10. Future prospects.

071. BEHL (Gautam)
Development of Biocompatible Nanomaterials for the Delivery of Pharmacological Agents : Synthesis, Characterization and Bioevaluation.
 Supervisor : Dr. Aruna Chhikara
Th 20198

Contents

1. Introduction. 2. Synthesis, characterization and evaluation of radical scavenging ability of ellagic acid loaded nanogels. 3. Preparation of gallic acid loaded biodegradable polymeric nanogels and study of its release kinetics. 4. Evaluation of biocompatibility and antioxidant activity of gallic acid loaded nanogels for delivery to cancer cells. 5. Synthesis of PEG supported coumarin based nanoaggregates and study of their aggregation behaviour. 6. Curcumin loaded nanoaggregates as water soluble formulation for delivery to cancer cells. Summary and addpendix.

072. BHATIA (Rohit)
Functionalized Nanocarbon Materials, Photovoltaics and Peptide Crosslinking.
 Supervisors : Dr. S. V. Eswaran and Dr. R. Nagarajan
Th 19984

Contents

1. Introduction. 2. Soluble fullerence C₆₀ for photovoltaics. 3. Functionalized single wall carbon nanotubes (SWCNTs) for photovoltaics. 4. Derivatization of multiwall carbon nanotubes (MWCNTs) for photovoltaics. 5A. Cytotoxicity studies on functionalized SWCNTs adducts. 5B. MALDI-MS studies on crosslinking of unnatural amino acid containing peptides using a heterobifunctional crosslinker. Summary and appendixes.

073. CHANDRA SHEKHAR REDDY LOKASANI
Biocatalytic Acylation Studies on Novel Sugar Precursors & UNA-U and Synthesis of 2-Alkylamino-Arabinofuranosyl Pyrimidines & 5'-Thionucleoside Disulfides.
 Supervisors : Prof. Ashok K. Prasad and Prof. V. S. Parmar
Th 20253

Contents

1. Synthesis and selective biocatalytic acylation studies on

novel carbohydrate monomers. 2. Biocatalytic acylation studies on 5'-O-(4,4'-dimethoxytrityl)-2',3'-secouridine (UNA-U). 3. Synthesis of 2-alkylamono-arabinofuranosyl pyrimidines. 4. Synthesis of 2',5'-dideoxy-5'-thionucleoside disulfides. Summary.

074. CHAUDHARY (Ankita)
Oxidations and Syntheses of N/o-Containing Heterocycles Using Ionic Liquids, Water and PEG-400 as Green Media.
 Supervisor : Prof. J. M. Khurana
Th 20026

Contents

1. N-Bromosuccinimide (NBS) in ionic liquid : A green system for rapid oxidation of 1,2-diols, α -hydroxyketones and alcohols. 2. Task specific ionic liquid mediated synthesis of 4H-pyrans, 4H-pyrano[2,3-c]pyrazoles and 4H-Benzo[g] chromenes. 3. Efficient one pot synthesis of dibenzo[a,i]xanthene-diones and evaluation of their antioxidant activity. 4. Aqua mediated indium(III) chloride catalyzed synthesis of fused pyrimidines and pyrazoles. 5. An expedient four component domino protocol for the synthesis of novel benzo[a]phenazine annulated heterocycles and their photophysical studies. 6. Summary and conclusions.

075. CHAUHAN (Ritika)
Studies in Green Chemistry Innovations.
 Supervisor : Prof. M. Kidwai
Th 20258

Contents

1. A rapid and an efficient route to the one-pot, multicomponent synthesis of 1H-pyrazolo[1,2-b]phthalazine-5,10-dione ring systems. 2A. Efficient CAN catalyzed synthesis of 1H-Indazolo[1,2-b]phthalazine-1,6,11-triones : An eco-friendly protocol. 2B. Amberlyst-15 in PEG : A novel catalytic system for the facile and efficient one-pot synthesis of benzothiazolo [2,3-b]quinazolinone derivatives. 3. Nafion-H catalyzed efficient one-pot synthesis of triazolo[5,1-b]quinazolinones and triazolo[1,5-a]pyrimidines : A green strategy. 4A. Nafion-H catalyzed synthesis of polyhydroquinolines via the hantzsch multi-component reaction. 4B. Eco-friendly synthesis of 2-aminothiazoles using nafion-H as a recyclable catalyst in

PEG-water solvent system. 5. Sulfamic acid : An efficient, cost-effective and recyclable catalyst for the synthesis of triazolo [1,2-a] indazoletrione derivatives. 6A. Potassium carbonate catalyzed green and rapid access to 2-amino-3,5-dicarbonitrile-6-thio-pyridines. 6B. Catalyst-free synthesis of betti bases in a mannich-type reaction. Summary.

076. CHHABRA (Pranshu)
Development of Novel Materials with Photocatalytic Effect for Effluent Treatment.
 Supervisors : Dr. R. K. Khandal and Dr. R. Nagarajan
Th 19983

Contents

1. Introduction. 2. Literature review. 3. Objectives of the study. 4. Materials. 5. Methods. 6. Characterization techniques. 7. Modification of titanium dioxide. 8. Photoactivity of titanium dioxide : Ultraviolet region to visible region. 9. Development of solar active materials based on titanium dioxide. 10. Dye degradation studies : Photocatalytic device-I. 11 Dye degradation studies : Photocatalytic device-II. 12. Conclusion, annexures, references and publications.

077. DEEPAK KUMAR
Library of Aryls, Alkyl Aryls and Heteroaryls As Biodynamic Agents.
 Supervisor : Prof. Diwan S. Rawat
Th 20251

Contents

1. Synthesis, antimicrobial activity and 3D-QSAR study of cyclohexane diamine derivatives. 2. Synthesis and antituberculosis activity evaluation of isoniazid derivatives. 3A. Synthesis, antioxidant and antituberculosis activity evaluation of thymol and carvacrol based schiff bases. 3B. Synthesis and anticancer activity evaluation of resveratrol-chalcone conjugates. 4. Synthesis of aminoquinoline-pyrimidine and triazine-pyrimidine conjugates as antimalarial agents. Summary and publications.

078. DEWAN (Manika)
Applications of Ionic Liquids and Ionic Liquid Stabilized Nanoparticles in Organic Transformations.
 Supervisor : Dr. Subho Mozumdar
Th 19998

Contents

1. Introduction and literature review. 2. Instrumentation. 3. Application of ionic liquids as solvents. 4. Applications of ionic liquids as catalyst. 5. Synthesis of stabilized transition metal nanoparticles using ionic liquids. 6. Application of ionic liquid stabilized nanoparticles in catalysis. 7. Application of ionic liquid stabilized nanoparticles in catalysis. Summary.

079. DHAMANDE (Vaishali)
Removal of Toxic Metals and Organic Derivatives from Wastewater Using Different Chitosans and Its Crosslinked Derivatives.
Supervisor : Dr. P. S. Jassal
Th 20020

Contents

1. Introduction. 2. Review of previous work. 3. Scope and object of present work. 4. Materials and methods. 5. Adsorption of Cr(VI) on chitosan and crosslinked derivatives : Langmuir isotherm studies. 6. Adsorption of Cd(II) by chitosan : langmuir isotherm studies. 7. Adsorption study of Pb(II) ion different types of chitosans and cross-linked derivatives. 8. Adsorption study of crystal violet using chitosan and cross-linked chitosan derivatives. Summary and references.

080. GARG (Seema)
Development of Nano-Particulate Systems for their Applications in Biomedical Area.
Supervisor : Dr. Subho Mozumdar
Th 20201

Contents

1. Introduction. 2. Review of the literature. 3. Instrumentation. 4. Development and optimization of a reverse micellar system for the synthesis of Nano-particulate matter. 5. Synthesis, cytotoxicity assessment and in vitro protein interaction studies of gold based nano-vehicle for bio-molecule immobilization. 6. Immobilization of the model enzyme urease on the surface of the gold based nano-vehicle and its bio-activity studies. 7. Synthesis of a novel fluorescent gold nano-vehicle for liver specific drug-delivery and its glutathione mediated release studies. 8. Synthesis, characterization and in vitro release kinetics of PNIPAAm based SMART co-polymeric hydrogels. Summary and conclusions.

081. GAUTAM (Manish Kumar)
Study of Some Triazoles as Corrosion Inhibitors for Mild Steel in Acidic Medium.
 Supervisor : Prof. Gurmeet Singh
Th 19995

Contents

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

082. GIRIJESH KUMAR
Coordination Complexes Appended with Pyridine or Arylcarboxylic Acid Groups : Extended Ensembles and Functional Materials.
 Supervisor : Dr. Rajeev Gupta
Th 19986

Contents

1. Introduction to metalloligands as the building blocks and their role in hydrogen-bonded and coordination-based self-assembly. 2. Synthesis, structures, and heterogeneous catalytic application of $\{Co^{3+}-Eu^{3+}\}$ and $\{Co^{3+}-Tb^{3+}\}$ heterobimetallic coordination polymers. 3. Novel Co^{3+} -based asymmetrical metalloligands : Heterobimetallic metallacycles versus coordination networks. 4. Cobalt complexes appended with para- and meta- arylcarboxylic acids : Hydrogen-bonded assemblies. 5. Part A : Synthesis and characterization of $\{Co^{3+}-Zn^{2+}\}$ and $\{Co^{3+}-Cd^{2+}\}$ heterobimetallic networks using Co^{3+} -based metalloligands appended with para- and meta- arylcarboxylic acids. 5. Part B. Regio-; chemo-; and size-selective heterogeneous catalysis of $\{Co^{3+}-Zn^{2+}\}$ and $\{Co^{3+}-Cd^{2+}\}$ heterobimetallic networks. Summary and list of publications.

083. GULATI (Shikha)
Synthesis, Characterization and Investigation of Catalytic Activity of Metallophthalocyanines Anchored on Silica Gel for Various Organic Transformations.
 Supervisor : Prof. R. K. Sharma
Th 19999

Contents

1. Introduction. 2. Instrumentation & theory of the techniques used. 3. Nickel tetrasulfophthalocyanine complex anchored on silica : Novel efficeint and recyclable silica based, orgnic-inorganic hybrid catalyst for degradation of dye pollutants. 4. Manganese phthalocyanine immobilized on silica gel : Efficient and recyclable catalyst for single step oxidative esterification of aldehydes with alcohols. 5. Polyfluorinated zinc(II) phthalocyanine complex immibilized on silica : A novel, highly selective and recyclable inorganic-organic hybrid catalyst for the synthesis of biologically important 1,5-benzodiazepines. 6. Silica-supported CO^{2+} - tetrachlorophthalocyanine ($\text{COPCCL-APTES@SIO}_2$) : A novel and recyclable organic-inorganic hybrid catalyst for eco-friendly oxidation of secondary alcohols. Conclusion, references and summary.

084. GUPTA (Nikesh)
Synthesis of Inorganic Nanoparticles and Their Applications in Cancer Therapy and as Antibacterial Agents.
 Supervisor : Dr. Rakesh Kumar Sharma
Th 20025

Contents

1. Introduction. 2. Literature review. 3. Experimental and characterization techniques. 4. Silica nanoparticles co-encapsulating gadolinium oxide and horse radish peroxidase for imaging and therapeutic applications. 5. Synthesis, characterization and enzymatic activity of horse radish peroxidase encapsulated in hollow gold nanoparticles. 6. Peroxidase entrapped in hollow gold nanoparticles can be used for induction of oxidative stress to kill cancer cells. 7. Green approach for the synthesis of silver nanoparticles and their antibacterial activity against multi-drug resistance human pathogens. 8. Conclusion.

085. GUPTA (Shweta)
Preparation & characterization of Palladium Nanoparticles Using Organic Molecules.
 Supervisor : Dr. Dhanraj T. Masram
Th 19996

Contents

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of PEG12K-Pd nanoparticles and their characterization. 4. Preparation of quercetin-Pd nanoparticles and their characterization. Summary and list of publications.

086. ISSAR (Upasana)
In Silico Studies of DNA Interactions With Minor Groove Binders Based On the Hoechst Family.
 Supervisor : Prof. Rita Kakkar
Th 20256

Contents

1. DNA minor groove binder hoechst 33258 and its analogues : A review. 2. Computational techniques. 3. Theoretical study of the DNA minor groove binder hoechst 33258 in gas phase and in aqueous solution. 4. Docking studies of hoechst 33258 and its rotameric, tautomeric and ionization states into the minor groove of B-DNA : A thorough investigation. 5. Assessment of molecular binding of hoechst 33258 analogues into DNA using docking and MM/GBSA approach. 6. Pharmacophore modelling and atom-based 3D-QSAR on bis-benzimidazoles and ter-benzimidazoles as topoisomerase I poisons and antitumor agents. 7. Conclusions and perspectives. Summary.

087. JAIN (Arti)
Role of ZN[L-Proline]₂ Laccase, Iron Oxide-Nanoparticles and Iodine in Organic Transformations.
 Supervisor : Prof. M. Kidwai
Th 19989

Contents

1A. 1,4-addition of terminal alkynes of conjugated enones in water using green catalyst Bis(L)prolinato-N,O]Zn - An environmentally benign protocol. 1B. Regioselective synthesis of 1,4-disubstituted triazoles using Bis[(L)prolinato-N,O]Zn complex as an efficient catalyst in water as a sole solvent. 2. Magnetic nanoparticles catalyzed synthesis of diverse N-heterocycles. 3A. Eco-friendly approach for detection of phenols in water using laccase from different fungi. 3B. First time reported enzymatic synthesis of new series of quinoxalines-A green approach. 3C. Laccase- a natural source for the synthesis of benzofuro[2,3-c]pyrazole. 4A. Bis[(L)prolinato-N,O]Zn in acetic acid/water : A novel catalytic system for the synthesis of β -amino carbonyls via Mannich reaction at room temperature. 4B. Zn[(L)Proline]₂ in water : A new easily accessible and recyclable catalytic

system for the synthesis of pyrazoles. 5. Efficient entry to diversely functionalized spirooxindoles from isatin and their biological activity. Summary.

088. JOSHI (Rini)
Studies on Protein Acetyltransferase Function of Calreticulin.
 Supervisor : Prof. Diwan S. Rawat
Th 20021

Contents

1. Introduction. 2A. 7,8-diacetoxy-4-methylcoumarin (DAMC) mediated activation of nitric oxide synthase (NOS) and other receptor proteins in rat tracheal smooth muscle cells (TSMC) ex vivo : Possible role of Calreticulin tranacetylase (CRTAase). 2B. Studies on the comparison of expression of TSMC CRTAase and its activity in hypoxia exposed rat and normoxic rats. 3. Calreticulin transacetylase mediated upregulation of thioredoxin by 7,8-diacetoxy-4-methyl coumarin enhances the expression of Vascular endothelial growth factor in peripheral blood mono nuclear cell. 4. Site-directed mutagenesis of P-domain of human placental calreticulin to elucidate the possible active site residue of calreticulin transacetylase. Summary and conclusions and appendices.

089. JOSHI (Seema)
Antimicrobial Peptides : Design, Synthesis and Biological Evaluation.
 Supervisors : Prof. Diwan S. Rawat and Dr. Santosh Pasha
Th 20000

Contents

1. Antibiotics and cationic antimicrobial peptides : An overview. 2. Design, synthesis and characterization of antimicrobial peptides based on template and hybrid peptide approach. 3. Antimicrobial activity and interaction studies of novel cell selective peptides with model membranes and bacterial cells. 4. Design, synthesis and mode of action of novel linoleic acid tagged di-peptide spermidine conjugates. 5. Design, synthesis and interaction studies of novel, Trp-Arg rich nanovesicles with antimicrobial activity and cell selectivity. Summary and list of publications.

090. KOHLI (Esha)
**Conformers and Complexes of Isatin-3-thiosemicarbazone :
 A DFT Study.**
 Supervisor : Prof. Rita Kakkar
Th 20029

Contents

1. Introduction. 2. Computational techniques. 3. Stability of tautomers and conformers of Isatin- β -thiosemicarbazone. 4. Tautomerization and E-Z isomerisation in Isatin- β -semicarbazone (IBS) and Isatin- β -thiosemicarbazone (IBT). 5. Group VIII transition metal complexes of IBS and IBT. 6. Metal Ion selectivity of isatin- β -thiosemicarbazone (IBT). 7. Concluding remarks. 8. Bibliography.

091. KULDEEP
**Synthesis, Structural, spectral and Catalytic Studies of Some
 Copper(II) Metallatriangle Complexes of a New Bis-Benzimidazolyl
 Diamide Ligand with a Biphenyl Spacer and its N-substituted
 Derivatives.**
 Supervisor : Prof. Pavan Mathur
Th 19991

Contents

1. Introduction. 2. Theory of techniques utilized in the identification of diamide ligands and their copper(II) metallatriangles. 3. Synthesis, structural and spectral characterization of bis-benzimidazolyl diamide ligands. 4. Synthesis, structural, spectral, magnetic and electrochemical studies of copper(II) metallatriangles. 5. Detection of copper(II), iron(III), lead(II) and silver(I) ions using bis-benzimidazolyl diamide ligands by fluorescence spectroscopy. 6. Catalytic oxidation of some substituted benzyl alcohols, phenols and hydrocarbon homogeneously and heterogeneously. Summary and appendix.

092. MALIK (Pragati)
**II-VI Quantum Dots As Chemical and Bio-Sensors and Core/
 Shell Quantum Dots : A DFT Study.**
 Supervisor : Prof. Rita Kakkar
Th 20257

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1. Quantum dots : A brief introduction. 2. Computational

techniques. 3. Effect of increasing number of rings on ion sensing ability of CdSe quantum dots. 4. Interaction of $(\text{CdSe})_3$ quantum dots with nucleobases. 5. DFT study of II-VI core/shell quantum dots. 6. Transition metal doped CdS/SzS core-shell quantum dots. 7. Concluding remarks. Bibliography

093. MATHUR (Divya)
Synthesis and Selective Biocatalytic Acylation/Deacylation Studies on 4-C-Hydroxymethylated xylo-Furanosides, Triazolynucleosides, coumarins and Dihydrocoumarins of Medicinal Importance.
 Supervisor : Prof. Ashok K. Prasad
Th 20027

Contents

1. Synthesis and selective biocatalytic acylation/deacylation studies on 4-C-hydroxymethylated xylo-furanosides. 2. Synthesis of novel 2'-substituted triazolynucleosides. 3. Synthesis and antimicrobial activity of novel 1,2,3-triazole conjugated coumarins. 4. Diels-alder synthesis of 3,3-dialkyl-4-morpholino-3,4-dihydrocoumarins from 2-(Dimorpholinomethyl)-phenols.

094. MISHRA (Sweta)
Chemically modified graphenes and fullerenes in the synthesis of porphyrinoids, nanocomposites and their non-covalent interactions.
 Supervisor : Prof. S. M. S. Chauhan
Th 20030

Contents

1. Alkali and transition metal intercalation in graphite layers and their applications in selected organic transformations. 2. Synthesis of graphene oxides and reduced graphene oxides and their application in acid catalyzed transformation. 3. Sulfonated graphene and sulfonated graphene oxide in the synthesis of porphyrinoids and related macrocycles. 4. Synthesis of modified graphenes and their role in base catalyzed organic transformations. 5. Synthesis of nanocomposites of graphene oxide with selected porphyrinoids and biopolymers. 6. functionalization of carbon materials and their non-covalent interactions with porphyrinoids.

095. MONDAL (Prakash Chandra)
Surface-Confined Assembly of Iron, Ruthenium & Osmium Terpyridine Complexes.
 Supervisor : Dr. Tarkeshwar Gupta
Th 20033

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1. Introduction - A Brief Overview of Surface-Confined Assemblies. 2. Preparation of molecular Building blocks. 3. Covalent-Assembled homoleptic and heteroleptic monolayers. 4. Surface-confined homo- and hetero-metallic molecular dyads and triads. 5. Bottom-up assembly of multicomponent coordination-based oligomers.

096. PANDEY (Amit)
Synthesis, Characterization and Applications of Silica Based Organic-Inorganic Hybrid Materials as Chelating Resins for Metal Ion Extraction and Catalysts for Various Organic Transformations.
 Supervisor : Prof. R. K. Sharma
Th 19994

Contents

1. Introduction. 2. Theory of instrumental techniques. 3. Silica modified with diphenyldiketone-monothiosemicarbazone : A highly selective chelating resin for preconcentration, determination and on-line recovery of palladium. 4. Silica-supported palladium complex : An efficient, highly selective and reusable organic-inorganic hybrid catalyst for the synthesis of e-stilbenes. 5. Silica modified with 2,6-diacetylpyridine monosalicyloylhydrazone : A novel and selective organic-inorganic sorbent for separation of molybdenum ions in a newly designed reactor. 6. Silica-supported molybdenum complex : A novel, selective and reusable organic-ionorganic hybrid catalyst for eco-friendly oxidation of sulfides and olefins. References and summary.

097. PRADEEP KUMAR
Metal Nanoparticles Using Plant Extract : Synthesis and Their Biological Applications.
 Supervisor : Dr. Subho Mazumdar
Th 20255

Contents

1. Introduction & review of literature. 2. Material, methods and characterization techniques. 3. Phytochemical characterization of plant extract. 4. Biological synthesis of metal nanoparticles using leaf aqueous extract of callistemon viminalis. 5. Spectroscopic investigations on interactions between metal nanoparticles and biomolecules. 6. Antimicrobial and free radical scavenging activities of plant extract and metal nanoparticles. 7. Cell viability assay and in-vitro antidiabetic activities of plant extract and metal nanoparticles. 8. Conclusions and summary. Appendix.

098. RAWAT (Nidhi)
Statistical Analysis of the Physico-chemical Properties of Proteins, Nucleic Acid and their Complexes.
 Supervisor : Dr. Parbhathi Biswas
Th 19988

Contents

1. Introduction. 2. Size, shape, and flexibility of proteins and DNA. 3. Shape, flexibility and packing of proteins and nucleic acids in complexes. 4. Hydrophobic moments, shape and packing in disordered proteins. 5. Molecular dynamics simulations of hydrophobic moments and hydrogen bonds in intrinsically disordered proteins. Bibliography.

099. REDDY (P. Madhusudhana)
Exploring the Polymer Behaviour in Phase Separated Systems.
 Supervisor : Dr. P. Venkatesu
Th 20019

Contents

1. Introduction and review of literature. 2. Materials and experimental techniques. 3. Exploring the poly(ethylene oxide) behaviour in isobutyric acid and water. 4. Exploring the poly(N-isopropylacrylamide) behaviour in water containing ionic liquid, osmolyte or denaturant. 5. Exploring the poly(N-isopropylacrylamide) behaviour in water containing hofmeister series of anions of ILs. 6. Exploring the PEG-PPG-PEG behaviour in water containing hofmeister series of anions of ILs. 7. Conclusions.

100. RUSTAGI (Vineeta)
Ag(I)-Catalyzed Regioselective Tandem Synthesis of Fused Heterocycles from ortho-Alkynylaldehydes.
 Supervisor : Dr. Akhilesh Kumar Verma
Th 20023

Contents

1. Tandem reactions : A general introduction. 2A. Ag(I)-catalyzed regioselective tandem synthesis of fused pyrroloquinoxalines. 2B. Ag (I) Catalyzed regioselective tandem synthesis of fused indoloquinoxalines. 3. Ag(I)-catalyzed regioselective tandem synthesis of fused benzimidazoles. 4. Ag(I)-catalyzed regioselective tandem synthesis of fused isoquinolinones. Summary.

101. SHAHZAD AHMAD
Studies on the Synthesis of Some Novel Fluoride Host Lattices, Fluorid Doped Oxides and Their Applications.
 Supervisor : Dr. r. Nagarajan
Th 20259

Contents

1. Introduction. 2. Characterization techniques. 3. Investigation into the synthesis of rare earth doped cubic KLaF_4 and its optical and magnetic properties. 4. Investigation into the phase controlled synthesis of hexagonally ordered KLaF_4 and its properties as a luminescence host. 5. RbGdF_4 : Synthesis, structure, optical and magnetic properties. 6. Studies on the synthesis, structure, optical, catalytic and photocatalytic properties of CeO_2 and $\text{CeO}_2:\text{F}$ nanocrystals. 7. Synthesis, characterization, optical and photocatalytic properties of nanocrystals of $\text{ZnO}_2:\text{F}$, $\text{ZnO}:\text{F}$ and $\text{Zn}(\text{OH})\text{F}$ using a single source precursor approach. 8. Cubic CdO_2 : Synthesis, photo catalytic activities, catalytic oxidation activities and optical studies.

102. SHANKAR (B.)
Cyclic and Acyclic Rhenium(I)-Based Complexes.
 Supervisor : Dr. M. Sathiyendiran
Th 19990

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1. Introduction. 2. Synthesis, characterization and photophysical studies of neutral rhenium-based tetragonal prisms. 3. Synthesis,

characterization and photophysical studies of flexible chelating ligands and their cyclic complexes. 4. Synthesis and characterization of mixed-ligands metallacycles constructed from flexible tritopic nitrogen donor and rigid anionic linkers. 5. Synthesis, characterization and photophysical studies of acyclic molecule containing spatially arranged four light-emitting rhenium complexes.

103. SHARMA (Neha)
Adsorption of Chemical Warfare Agents and Their Simulants on Metal Oxides and Mixed Metal Oxide Nanoparticles.
 Supervisor : Prof. Rita Kakkar
Th 20024

Contents

1. Recent advancements of warfare agents/metal oxides surface chemistry and their simulants study. 2. Computational techniques. 3. Destructive decomposition of sarin on mixed metal oxide MgAl_2O_4 nanoparticles. 4. Comparative study of the adsorption of paraoxon on alkaline Earth metal (Mg, Ca, Sr, Ba) and transition metal (Co, Ni, Cu) aluminate nanoparticles. 5. Adsorption of sarin on MgO nanotubes : Role of doped and defect sites. 6. Adsorption of some chemical warfare agent simulants on MgO nanotubes. Effect of doping and surface hydroxylation on adsorption parameters. 7. Conclusions and bibliography.

104. SHUKLA (Satya Prakash)
Iodine-Mediated and Metal-Catalyzed Synthesis of Heterocycles Via Electrophilic 6-endo-dig Ring Closure of Alkynes.
 Supervisor : Dr. Akhilesh Kumar Verma
Th 19981

Contents

1. A general introduction. 2. Iodine-mediated synthesis of 5-iodopyrrolo [1,2-a]quinolines. 3. Palladium-catalyzed synthesis of indolo[1,2-a]quinolines and pyrrolo[1,2-a]quinolines. 4. Silver-catalyzed synthesis of acridines, quinolines and naphthalenes. Summary.

105. SINGH (Maibam Birla)
Mathematical Modeling of Electric Double Layer Phenomena in Nanostructured and Rough Interfaces.
 Supervisor : Prof. Rama Kant
Th 20022

Contents

1. Electric double layer phenomena : A review on models and problems. 2. Electronic screening model for the capacitance and dielectric and arbitrary shaped nanostructured materials. 3. Generalization of gouy-chapman-stern model of electric double layer for morphologically complex electrode : Deterministic and stochastic morphology. 4. Theory of morphology dependent free energy of electric double layer. 5. Debye-falkenhagen dynamics of electric double layer on partially blocking heterogeneous electrode. 6. Theory of electric double layer admittance of partially blocking heterogeneous rough electrode. 7. Dynamics of electric double layer at partially blocking arbitrary shaped nanostructured and porous electrodes with surface heterogeneities. 8. Theory of generalized randles-ershler admittance of rough and finite fractal electrode. 9. Summary and conclusions.
106. SINGH (Niraj)
Design, Synthesis and Biological Evaluation of 1-(2-Methoxyphenyl)Piperazine Analogues as Spect and Pet Imaging Agent.
 Supervisors : Prof. Shrikant Kukreti and Dr. Anil K. Mishra
Th 19993

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1. Molecular imaging : Introduction and review of literature. 2. Synthesis and preclinical evaluation of multimodal imaging agent based on DO3A-butyl-MPP for serotonin 5HT1A neuroreceptor imaging. 3. Synthesis of pet radiopharmaceuticals based on MPP. 4. Bivalent ligand approach to synthesise MPP based spect imaging agent. 5. Summary. 6. Materials and instrumentation.
107. SINGH (Shailja)
Crystallographic, Spectroscopic and Antimalarial Activity of 4-Aminoquinoline Derivatives.
 Supervisor : Dr. Satish Kumar Awasthi
Th 19992

Contents

1. Design, synthesis and antimalarial activity of 4-aminoquinoline derivatives. 2A. An outlook on the tenacity of H-bonding pattern in antimalarial 4-aminoquinoline derivatives. 2B. Evidence of halogen...halogen interactions in 4-

aminoquinoline derivatives. 3. A steady-state fluorescence and circular dichroism study on the binding of (7-chloroquinolin-4-yl)-(2,5-dimethoxyphenyl)-amine hydrochloride dihydrate to bovine and human serum albumin. 4. Comparative study of the binding mode of 4-aminoquinoline derivatives of calf thymus DNA. Summary and list of publications.

108. SINGH (Suneeti)
On-Line Preconcentration and Determination by Faas of Cadmium and Lead Using Modified Amberlite Xad based chelating resins.
 Supervisor : Dr. Reena Saxena
Th 20031

Contents

1. Introduction. 2. Materials and methods. 3. Synthesis and characterization of amberlite XAD based chelating resins. 4. On-line preconcentration and determination of cadmium by flow injection-flame atomic absorption spectroscopy using modified chelating resins. 5. On-line preconcentration and determination of lead by flow injection-flame atomic absorption spectroscopy using modified chelating resins. Summary and List of publications.

109. SNEHA
Applications of Ni/Ag Nanoparticles and [BMIM]BF₄ in the Syntheses of N/O-Containing Heterocycles.
 Supervisor : Prof. J. M. Khurana
Th 19987

Contents

1. Ni nanoparticles : Mild and efficient catalyst for the (i) chemoselective synthesis of 2-arylbenzimidazoles, 2-arylbenzothiazoles and schiff's bases. 2. PEG-stabilized Ni nanoparticles : A proficient catalyst for synthesis of biologically important spiropyrans. 3. Chemselective N-benylation of 2-thiohydantoin and 2-thiobarbituric acids catalyzed by PEG-stabilised Ni nanoparticles and their anti-microbial activities. 4. Cinnamomum tamala leaf extract mediated green synthesis of Ag nanoparticles and its application in the synthesis of pyranopyrazoles. 5. An efficient synthesis of novel 2/3-hydroxy-12-arylbenzo[a]xanthen-11-ones and 5,13-diarylxantheno[2,1-a]xanthene-4,12 (1H,5H)-diones using pTSA in [bmim] BF₄. 6. Summary and conclusions.

110. SRIVASTAVA (Shruti)
Physico-Chemical Studies of Encapsulated Enzyme HRP in 'Reverse Micelles' and 'Magnetic Nanomaterials' Applied as 'In Vitro Prodrug Activation'.
 Supervisors : Dr. Rakesh Kumar Sharma and Dr. Surender Kumar Sharma
Th 19980

Contents

1. Introduction. 2. Literature review. 3. Experimental. 4. Comparative study on the enzymatic activity of HRP encapsulated in reverse micelles of 'Anionic', 'Cationic' and 'Non-Ionic' surfactant systems. 5. Superparamagnetic iron-oxide nanoparticles encapsulating enzyme HRP, its stability studies and effect of agglomeration on cytotoxicity. 6. Physico-chemical studies of enzyme HRP encapsulated in manganese phosphate nanoparticles and comparative cytotoxic studies of manganese phosphate with iron-oxide NPs. 7. Enzyme 'HRP' encapsulated magnetic nanoparticles applied as in vitro prodrug activation by enzyme HRP. 8. Conclusion.

111. SUNNY MANOHAR
Design, Synthesis and Biological Activity Evaluation of Hybrid Molecules Based on 4-Aminoquinoline, Curcumin, Chalcone and Cyclohexanediamine.
 Supervisor : Prof. Diwan S. Rawat
Th 20028

Contents

1. Synthesis and antimalarial activity evaluation of 4-aminoquinoline-triazine and 4-aminoquinoline-pyrimidine hybrids. 2. Synthesis of 4-aminoquinoline-triazole and 4-aminoquinoline-triazole-triazine hybrids via click chemistry and evaluation of their antimalarial activity. 3. Synthesis of symmetrical and unsymmetrical monocarbonyl analogues of curcumin as potential anticancer and antimalarial agents. 4A. Synthesis, characterization and anticancer activity evaluation of chalcone derivatives. 4B. Synthesis of stereochemically pure cyclohexane-1,2-diamine derivatives and evaluation of their antibacterial activity. Summary and list of publications.

112. SUSHIL KUMAR
Studies on Selected Transition Metal Complexes of Amide-Based Ligands : Evaluating the Role of E-Withdrawing and E-Donating Substituents on Ligand.
Supervisor : Dr. Rajeev Gupta
Th 20032

Contents

1. Introduction : A synopsis of coordination chemistry of amidebased macrocyclic ligand including relevant biological and literature examples. 2. Copper complexes of amide-based macrocyclic ligands : Effects of electronic substituents on redox properties. 3. Synthesis and properties of dinuclear - μ -oxodiiron(III) complexes of amide-based macrocyclic ligands. 4. Cobalt complexes of amide-based macrocyclic ligands : Synthesis, structures and catalytic properties. 5. Palladium complexes of amide-based macrocyclic ligands : Understanding catalysis through electrochemistry. Summary and List of publications.

113. TRIPTI
Studies on Modification of Certain Optical Plastics by Incorporating Biopolymers to Improve Biochompatibility.
Supervisors : Dr. R. K. Khandal and Dr. Sulekh Chandra
Th 19997

Contents

1. Introduction. 2. Literature survey. 3. Plan of work. 4. Materials used. 5. Characterization techniques. 6. Designing of hydrophobic optical plastic materials. 7. Designing biocompatible optical plastic material with improved hydrophilicity. 8. Maneuvering of hydrophilicity/hydrophobicity while designing optical plastic material. 9. Incorporation of biopolymers for improved biocompatibility. 10. Biosafety evaluation of optical plastic compositions developed. 11. Conclusion.

114. TRIPTI KUMARI
In Silico Studies of Peptide Deformylase Inhibitors.
Supervisor : Prof. Rita Kakkar
Th 20252

Contents

1. Peptide deformylase inhibitors for addressing the issue of bacterial resistance. 2. Computational techniques. 3. Docking

modes of BB-3497 into the PDF active site-A comparison of the pure MM and QM/MM based docking strategies. 4. Pharmacophore modeling, atom-based 3D-QSAR and docking studies on non-peptidic PDF inhibitors. 5. 3D pharmacophore based virtual screening and molecular docking studies for the identification of chemically diverse and novel peptide deformylase inhibitors. 6. Effect of variation in peptide deformylase active site metal ion on the binding affinity and coordination mode of ligands followed by an analysis of ligands for their activity spectrum. 7. Concluding remarks. Bibliography.

115. TYAGI (Abhilash)
Synthesis of Novel Potentially Bioactive Coumarinyldihydropyrimidin-2-thiones, Aryl-2-oxo-1,3-thiazines and bis-Coumarinylmethylenecycloalkanones.
 Supervisors : Prof. Ashok K. Prasad and Dr. Rajpal Singh
Th 19985

Contents

1. Synthesis of Novel Coumarinyldihydropyrimidin-2-thiones. 2. Synthesis of novel biginelli type 6-Aryl-2-oxo-1,3-thiazin-5-carboxylates. 3. Synthesis of novel bis-coumarinylmethylenecycloalkanones. Summary

116. TYAGI (Jyoti)
Adsorption of Disinfection By-Products on Intrinsic and Doped Graphene : A DFT Study.
 Supervisor : Prof. Rita Kakkar
Th 20199

Contents

1. Graphene, its applications, and interactions with a variety of molecules : A review. 2. Computational techniques. 3. Graphene and doped graphene : A comparative DFT study. 4. A first principles comparative study of adsorption of chloroacetic acid on the intrinsic and doped graphene. 5. Theoretical study of adsorption of monohaloacetic acids on Pt-doped graphene in gas phase and aqueous solution. 6. Adsorption of cyanogen chloride on intrinsic and Pt-doped graphene and carbon nanotubes. 7. Conclusions and perspectives. Bibliography.

117. YADAV (Ram Jeewan)

Complex Oxides for Dielectric Resonator Applications.

Supervisor : Dr. M. Thirumal

Th 20200

Contents

1. Introduction. 2. Influence of processing condition on the properties of $\text{BaZn}_{1/3}\text{Ta}_{2/3}\text{O}_3$ ceramic. 3. Molten salt synthesis of $\text{Ba}(\text{Zn}_{1/3}\text{Nb}_{2/3})\text{O}_3$ and $\text{Ba}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3$ perovskites. 4. Soli solutions and composites involving 8-layered perovskite structure.