Name of the Student: **S.Savithri**
Name of the Research Advisor: **Dr.V. Nandhakumar**

Ph.D. – COURSE WORK – PAPER I

Sub. Code: 15PHDCH1
Credit: 4

ENVIRONMENTAL CHEMISTRY

Unit I – CONCEPR OF ENVIRONMENTAL CHEMISTRY

Concept of environmental chemistry – Environmental pollution –Kinds of pollution – Non degradable pollutants – Industrial pollution –Soil pollution. Water pollution - definition – Types of Water pollution – Physical, Chemical, Biological and Physiological. Source of Water Pollution – Effects of Water Pollution – Industrial waste and treatment process, characteristics of industrial waste, Types of industrial waste – Treatment of effluent (organic and inorganic impurities) - Prevention and control of Water Pollution.

Unit II – INDUSTRIAL WASTE AND TREATEMENT PROCESS

Environmental problem of some industries – Fertilizers and chemical industries, Tannery, Pulp and paper industry, Distillery, Plastics, Cement, Dyeing and Coal industry. Protection of surface waters from with industrial sewage – Effluent of industrial units and their purification – Treatment of some industrial effluents – The nature of treatment of some other chemical wastes. Treatment of heavy metals – precipitation method, solvent extraction method, cementation process, electrolytic process, electro dialysis, reverse osmosis, ion exchange adsorption process.

Unit III – SURFACE CHEMISTRY

Adsorption – Difference between adsorption and absorption – Adsorbent – Adsorbate – Absorbance – characteristics of physical adsorption and chemical adsorption – Adsorption theory – Activates of carbon in Pollution Abatement of air and water – Applications of Adsorption.

Unit IV – PREPARATION OF ADSORBENTS AND ADSORBENT CHARECTERISTICS

Preparation of adsorbents –Formaldehyde treatment of plant biomass - preparation of activated carbon by physical and chemical methods (Using H_2SO_4 acid) - applications of activated carbon.

Preparation of activated carbon by Microwaves – Microwave technology – Definition and background study – Microwave major application and its working principle – Microwave assisted preparation of activated carbon – Regeneration of activated carbon.

Adsorbent characteristics – determination of carbon characteristics - Moisture content, Ash content – Bulk density - Water soluble matter – Acid soluble matter – Ion exchange capacity – Decolorizing power – pH – surface area – Ash analysis.

Unit V – KINETICS AND THERMODYNAMICS STUDIES

Kinetics - First order, second order, pseudo first order and pseudo second order kinetics. Legergren model – Ho model – Weber morrison model – Nadarajan kalaf plot – Bhattachrya and Venkobachar model – Elovich model – Adam – Bohart – Thomas model.

Thermodynamics – sorption isotherms – Freundlich, Langmuir, Temkin, Dubinin – Radushkevich, Flory – Huggins, Halsey, Brunauer – Emmett and Teller (BET), Sips, Toth, Redlich – Paterson isotherms, sorption mechanism and future work.

REFERENCES:

1. Text book of Environmental Chemistry by B.K.SHARMR.
2. Text book of Water pollution by B.K.SHARMA.
3. Text book of Environmental Chemistry by O.D.TYAGI & M.MEHRA.
4. Text book of Industrial Chemistry by V.P.KUDESIA.
5. Text book of Material Science and Engineering by V.RAGHAVAN.

Name of the Student: **S.Savithri**
Name of the Research Advisor: **Dr.V. Nandhakumar**

Ph.D. – COURSE WORK – PAPER II

Sub. Code: 15PHDCH2
Credit: 4

EXPERIMENTAL TECHNIQUES AND REVIEW OF ADSORPTION

Unit I – SPECTROSCOPY

Principle of absorption spectroscopy, UV – Visible spectroscopy – principle – instrumentation and applications.

The modes of stretching and bending – FT – IR sampling techniques – correlation tables for functional groups – Alkanes, alkenes, alkynes, aromatic rings, alcohols, carbonyl compounds – Factors that influence C=O stretching vibration – hydrogen bonding (inter, intra molecular).

Unit II – COLORIMETRIC ANALYSIS

Beers – Lambert's Law and laser and spectrophotometric method of estimation, principle and methods of visual colorimetry - Estimation of Iron and Nickel by visual colorimetry.

Unit III – NANO TECHNOLOGY

Definition – basic aspects of nano technology – CNT – types – synthesis, properties and applications of CNT – SEM analysis – Fullerene – types, properties and uses.

Unit IV – INSTRUMENTAL METHODS OF ANALYSIS

TGA – principles and application. DTA – principle and applications. AAS – instrumentation. Application – X-ray Diffraction – principle and applications.

Unit V – REVIEW OF ADSORPTION WORK

Kind of adsorbents – Clay minerals, Activated carbon, Carbon Nanotubes, Zeolites, Other materials. Effect of pH, Effect of other ions, ZPC, Determination of pH, Determination of Hg, Cu, and Cr by spectroscopy.

REFERENCES:

1. Instrumental Methods of Chemical Analysis by H.KAUR.
2. Elementary Organic Spectroscopy by Y.R SHARMA
3. Physical Methods in Inorganic Chemistry by R.S.DRAGO
4. Elements of Analytical Chemistry by R.GOPALAN, P.S.SUBRAMANIYAN & K.RENGARAJAN.
5. Nano the essentials, understanding Nano Science and technology by T.PRADEEP, Professor of IIT Chennai.
6. Advanced Physical Chemistry by PURI,SHARMA AND PATHANIYA

V.RAJASUDHA - 15CHA609 DR.R.Manikandan
(Ref.No.17540/Ph.DK2/Chemistry/FT/Oct 2015/Dt.15.7.2015)

A.V.V.M. SRI PUSHPAM COLLEGE (AUTONOMOUS), POONDI
THANJAVUR – DT

Ph.D-COURSE WORK - PAPER – I
NATURAL PRODUCT OF CHEMISTRY

Sub Code: 15PHDCH1 **Credit : 4**

UNIT: I
Alkaloids:

Classification and properties of Alkaloids. Structural elucidation of Hygrine, Papaverine, Piperidine, Nicotine, (-)-Quinine, Morphine and Ergolamine.

UNIT: II
Terpenoids:

Classification, structural elucidation, synthesis and properties of terpenoids, pinene, Phytol, Menthol, Caryophyllene and Forskolin.

UNIT: III
Steroids:

Classification and properties of steroids. Structural elucidation and synthesis of cholesterol, Lanosterol, Phytosterols, Bile acids, Oestriol and pregnanediol.

UNIT: IV
Flavanoids and Lipids:

Biological function of Lipids. Classification of Lipids, Simple Lipids, Natural fats difference between oil and fats. Production of higher fatty acids physical and chemical properties of fats. Compound- Lipids, phospholipids.

Isolation and structural elucidation of flavonoids, apigenin, quercetin, kaempherol.

UNIT: V
Advanced Medicinal Chemistry:

Applications of Molecular modelling in drug design - Docking by Energy minimization, Superimposition, Molecular dynamics, Metropolis Monte Carlo, Monte Carlo minimization, Genetic algorithm, Distance geometry, Build up approach.

Reference:

1. Unit 1,2: Gurdeep R.,Chatwal, Organic chemistry of Natural products. Chapter (3)
2. Unit 3,4 & 5:O.P Agarwal Chemistry of Organic Natural Products vol. II. Chapter (4.1 & 5).
3. I.L. Finar, Organic Chemistry, vol. II.
4. Textbook of Drug Design and Discovery, Povl Krogsgaard- Larsen, Ulf Madsen, Kristian Stromgaard, 4th Edition, 2009. Taylor and Francis

A.V.V.M. SRI PUSHPAM COLLEGE (AUTONOMOUS), POONDI

THANJAVUR – DT

Ph .D-COURSE WORK - PAPER – II

SPECTROSCOPY AND APPLICATIONS

Sub Code: 15PHDCH2 **Credit : 4**

UNIT: I

Chromatography:

Basic theory of separation, efficiency, resolution. Liquid chromatography, high performances liquid chromatography, Gas chromatography-columns and detectors, Qualitative and quantitative analysis, thin layer Chromatography.

UNIT: II

Ultraviolet and Visible Spectrophotometry:

Wood ward Scott rules for conjugated dienes and polymer, ketones, aldehydes, Unsaturated acids, esters, nitriles and amides differentiation of position isomer.

Stereo chemical factors affecting electronic spectra of biphenyls, cis and trans isomers. Angular distortion and cross conjugation. Electronic transition, spectrum, shift of bands with solvents, isolated double bonds, conjugated dienes, carbonyl compounds, aromatic and hetero aromatic compounds, application in pollution control and chemical industry.

UNIT: III

IR and Raman Spectra:

Basic theory of FTIR spectroscopy - Instrumentation and advantages of FTIR spectrophotometry, Qualitative and quantitative analysis using infrared spectrophotometry IR vibrational spectra, selection rules, oscillators, vibrational spectra of di and polyatomic molecules, rotation on polyatomic molecules. FT IR factors influencing group frequencies. Hydrogen bonding (inter molecular & intra molecular) Finger print region, identification of functional group conformational aspects in cyclic 1,2 and 1,3-diols, trans annular interaction.

UNIT: III

MASS Spectra:

Mass spectrometry-instrumentation, basic principles, parent ion peaks, base and metastable peaks, calculation of molecular formula fragmentation pattern of various classes of organic compounds and applications of GC-MS.

UNIT: V

NMR Spectra:

NMR spectroscopy multiplicity - coupling constant, First order and second order, proton spin-spin splitting, Dependence of Ion dihedral angle vicinal & germinal coupling constant, Karplus equation, long rang coupling constant, influence of stereo chemical factors on chemical shift of protons. Simplification of complex spectra, double resonance techniques shift regents, chemical spin decoupling of rapidly exchangeable protons (OH, SH, COOCH, NH, NH_2) an elementary treatment of NOE phenomenon. C^{13} NMR spectroscopy-basic theory of FT-NMR relaxation-Broad band decoupling off resonance, decoupling and chemical shift of common function groups, DEPT spectra identification of small compounds bases on NMR data techniques $_1H$-$_1H$-COSY-$_1H$-$_{13}C$ COSY-HMBC and NOESY.

REFERENE:

1. Phytochemical methods J.B. Harbone.
2. Y.R. Sharma, Organic Spectroscopy.
3. Kalsi Organic Spectroscopy

A.V.V.M. SRI PUSHPAM COLLEGE (AUTONOMOUS), POONDI THANJAVUR – DT.
DR.R.Manikandan

Subject Code	Title of the Paper	No of Credits	M.Amudha
15PHDCH1	Analytical Techniques	4	15CHA604

Unit-1: Chromatography and UV Spectra: Column, Paper, thin layer, gas-liquid, High Pressure liquid Chromatography HPLC principle and applications Woodward-scott rules for conjugated dienes and polymer, ketones, aldehydes, Unsaturated acids, esters, nitriles and amides differentiation of position isomer. Stereo chemical factors affecting electronic spectra of biphenyls, cis and trans isomers. Angular distortion and cross conjugation.

Distillation: Simple distillation, Fractional distillation, Steam distillation, Theory of distillation under reduced pressure advance of distillation.

Unit-2: IR and Raman Spectra: IR vibration spectra-selection rules-oscillators-vibration spectra of dye and polyatomic molecules-rotation on polyatomic molecules. FT IR factors influencing group frequencies both internal and external quantitative studies. Hydrogen bonding (inter molecules & intra molecules) Finger print region - identification of functional groups, conformational aspects in cyclic 1,2 and 1,3-diols, trans annular interaction.

Unit-3: NMR Spectra: NMR spectroscopy multiplicity-coupling constant-first order and second order proton spin-spin splitting-Dependence of Ion dihedral angle vicinal & germinal coupling constrant, Karplus equation, long range coupling constant, influence of stereo chemical factors on chemical shift of protons. Simplification of complex spectra, double resonance techniques, shift reagents, chemical spin decoupling of rapidly exchangeable protons (OH, SH, COOCH, NH, NH2) an elementary treatment of NOE phenomenon, C13 NMR spectroscopy, Basic theory of FT-NMR relation-Broad and decoupling off resonance decoupling and chemical shift of common function groups, Distortionless Enhancement by Polarization Transfer (DEPT) spectra identification of small compounds bases on NMR data techniques $_{1}$H-$_{1}$H-COSY-$_{1}$H-$_{13}$C COSY-HMBC and NOESY.

Unit-4: MASS Spectra: Electron Ionization, Chemical Ionization methods – base peak, isotopic peaks, meta stable peaks, parent peaks, determination of molecular formula-recognition of molecular ion peaks, Fast Atom Bombardment fragmentation, general rules-pattern of fragmentation for various classes of compounds, MClafferty rearrangement-importance of meta stable peaks. Basic principles of NQR and Massbauer spectroscopy.

Unit-5: X-ray diffraction: X-ray diffraction by single crystal-space groups-systematic absences in X-ray data and identification of lattic types, glide planes and screw axes-X ray intensities, structure factor and its relation to intensity and electron density, phase problem structure solution by Heavy atom method and direct method. Determination of absolute configuration of molecules.

REFERENCE:

1. YR Sharma, Organic Spectroscopy, Chapter (2)

2. W. Kemp, Organic Spectroscopy, Chapter (2)
3. Robert M. Silverstein, G. Clayton Bassler, Spectrometric Identification of Organic Compound, Chapter (3&3)
4. P.S. Kalsi Organic Spectroscopy, Chapter (6)
5. Stout G.H. Jensen X-ray Structure Determination, Chapter (2)

A.V.V.M. SRI PUSHPAM COLLEGE (AUTONOMOUS), POONDI THANJAVUR – DT.

Subject Code	Title of the Paper	No of Credits	M.Amudha
15PHDCH2	Natural Products	4	15CHA604

UNIT-1:

Alkaloids: Introduction to Alkaloids, occurrence of Alkaloids, Functions of Alkaloids, Nomenclature of Alkaloids, Classification of Alkaloids, Isolation of Production of Alkaloids, Properties of Alkaloids, General Methods Employed for Determining structures of Alkaloids, Structural elucidation of papaverine, piperidine, Quinine.

UNIT-2:

Terpenoids: Classification and properties of terpenoids, Structural elucidation and synthesis of Terpenoids, Pinene, Phytol, Menthol.

UNIT-3:

Steroids: Classification and properties of steroids. Structural elucidation and synthesis of cholesterol, Lanosterol, Phytosterols, Bile acids, Oestriol and Pregnanediol.

UNIT-4:

Vitamins: Structural elucidation and synthesis of Retinol, Riboflavin, Cyanocobalamine and L-Ascorbic acid.

UNIT-5:

Lipids: Biological function of Lipids-Classification of Lipids simple Lipids-Natural fats difference between oil and fats. Production of higher fatty acids-physical chemical properties of fats. Compound Lipids-phospholipids.

REFERENCE:

1. Gurdeep R. Chatwal, Organic Chemistry of Natural Products, Chapter (3,4)

2. O.P. Agarwal, Chemistry of Organic Natural Products, Vol.II, Chapter (4,1 & 5) I.L. Final, Organic Chemistry, Vol. II.

Name of the Student: **Rajeshwari**
Name of the Research Advisor: **Dr.V. Nandhakumar**

Ph.D. – COURSE WORK – PAPER I

Sub. Code: 16PHDCH1 **Credit:4**

WATER POLLUTION AND ADSORPTION TECHNOLOGY

UNIT -I

Water pollution - Classes of water pollutants - Sources of water pollutants - industrial sources of heavy metals - Toxicity due to metals and minerals – pb,Hg, Cd, Cr, As, Co,Fe, and Zn. - Dyeing Process and Environmental impact -Effects of industrial waste and the treatment processes.- environmental problem of some industries such as fertilizers , chemical industries, Tannery, Pulp , paper industry, distillery, Plastics, Cement, and Coal industry

UNIT -II

Water quality parameters and measurement- Water purification: Treatment methods – Primary, secondary and tertiary Treatment methods) - Methods are used for large scale municipal supplies.

UNIT -III

Adsorption - Adsorbents – Different types - activated carbons - Activated carbons from agricultural wastes- preparation of activated carbons by different activation method including with the assistance of Microwaves. Determination of Characteristics of activated carbons - applications of adsorbents and activated carbons in various fields

UNIT -IV

Treatment by activated carbon - Batch equilibration method - Desorption and regeneration of activated carbon.- Column adsorption study (Bed Depth Service Time Method) - Modeling with -breakthrough curve - Bohart- Adam model

UNIT –V

Reviews on the effect of pH and ionic strength for the adsorption of Methylene blue ,Congo red ,Malachite green ,Crystal violet, Rhodamine B dyes and the metal ions Cr (VI), Ni (II) , Fe (II) , Mn (II) and Cu (II). Reviews on the desorption studies of the above adsorbates.

REFERENCES:

1. Text book of Environmental Chemistry by B.K.SHARMR.
2. Text book of Water pollution by B.K.SHARMA.
3. Text book of Environmental Chemistry by O.D.TYAGI & M.MEHRA.
4. Text book of Industrial Chemistry by V.P.KUDESIA.
5. Text book of Material Science and Engineering by V.RAGHAVAN.

Name of the Student: **Rajeshwari**
Name of the Research Advisor: **Dr.V. Nandhakumar**

Ph.D. – COURSE WORK – PAPER II

Sub. Code: 16PHDCH2 **Credit:4**

TOOLS USED IN ADSORPTION STUDY

UNIT –I

Determination of percentage of removal and quantity of adsorbate sorbed. Kinetics and mechanisms involved in adsorption –Kinetic models applied in the adsorption study such as pseudo first order, pseudo second order, modified second order, intra particle diffusion etc.

UNIT –II

Adsorption equilibrium – Apparent equilibrium constant - Isotherms - Isotherms models such as Freundlich, Langmuir, Temkin, Dubinin –Radushkevich isotherms applied in adsorption study – their significances

UNIT –III

Thermodynamics – fundamental principles – Vant Hoff's equation, Eyrings equations –Determination of enthalpy, entropy and free energy changes – significance in the adsorption study

UNIT –IV

Colorimetry – principle and applications – UV –Visible spectroscopy- Principles – instrumentation and applications. Estimation of heavy metal ions using UV –Visible spectroscopy

UNIT –V

FTIR – Principles – modes of vibrations – functional groups & their absorption range and applications of FTIR – review on the FTIR spectrums of adsorbents, activated carbon prepared from plant bio masses and adsorbents laden with metal ions and dyes.

Applications of AAS, XRD, EDOX and SEM.

REFERENCES:

1. Instrumental Methods of Chemical Analysis by H.KAUR.

2. Elements of Analytical Chemistry by R.GOPALAN, P.S.SUBRAMANIYAN & K.RENGARAJAN.
3. Advanced Physical Chemistry by PURI,SHARMA AND PATHANIYA

Name of the Student: **Karthiga**
Name of the Research Advisor: **Dr.V. Nandhakumar**

Ph.D. – COURSE WORK – PAPER I

Credit: 4

Sub. Code: 17PHDCH1A

WATER POLLUTION AND ADSORPTION STUDIES

I Water pollution

Water pollution – Definition – Types of water pollution – classification of water pollutants - Effects of water pollution – Industrial waste - types - characteristics of industrial waste and treatment processes, Heavy metal and Dye pollution– Classification of dyes-

Toxicology aspects of water pollutants: Sources and harmful effects of heavy metals such as copper, zinc, nickel, lead, chromium, manganese etc.

Sources and harmful effects of dyes such as Methylene blue, Malachite green, Rose Bengal, Rhodamine –B, Eosin, Crystal violet, Bismarck brown, Congo red etc.

Fluoride ion pollution

II Water quality and Pollution control

Overview of standards of water in relation to public health -Water quality parameters –hydrogen ion concentration - electrical conductivity - suspended solids – TDS, BOD, COD

Water treatment methods: Sewage treatment -Primary, secondary, tertiary methods.

Treatment of heavy metals: precipitation method, solvent extraction method, cementation process, electrolytic process, electro dialysis, reverse osmosis, ion exchange and adsorption process - Advantage of adsorption method.

III Surface Chemistry

Adsorption – Difference between adsorption and absorption – Adsorbent – Adsorbate – characteristics of physical adsorption and chemisorption– mechanism - Adsorption and free energy reaction relation at interfaces - physisorption and chemisorption - potential energy diagrams, - Surface area determination - Heat of adsorption, determination Adsorption from solution, Gibbs adsorption isotherm - solid - liquid interfaces - wetting and contact angle - solid gas interfaces - soluble and insoluble film.– characteristics of physical adsorption and chemical adsorption.

IV Adsorbents: Preparation and characteristics

Adsorbents –Types –Preparation of activated carbon by physical (Pyrolysis, micro wave methods) and chemical methods (formaldehyde treatment, sulfuric acid, Phosphoric acid etc., alkali treatment and phosphoric acid etc.) Mechanism of activation processes.

Adsorbent characteristics – determination of Moisture content, Ash content – Bulk density - Water soluble matter – Acid soluble matter – Ion exchange capacity – Decolorizing power – pHzpc – surface area – Ash analysis – functional groups.

Applications of adsorbents and activated carbons.

V Adsorption experiment

Experimental methods -Batch and Column mode adsorption techniques – effect of ion ions – desorption.Column adsorption experiments:Break through time - Break through curves - BDST curves Review on effect of pH, Effect of temp, Effect of other ions, Kinetics adsorption, Thermodynamics of adsorption of heavy metal ions and dyes.

REFERENCES:

1. Text book of Environmental Chemistry by B.K.SHARMI.
2. Text book of Water pollution by B.K.SHARMA.
3. Text book of Environmental Chemistry by O.D.TYAGI & M.MEHRA.
4. Text book of Industrial Chemistry by V.P.KUDESIA.
5. Text book of Material Science and Engineering by V.RAGHAVAN.

Name of the Student: **J. Princes Gracia**
Name of the Research Advisor: **Dr.V. Nandhakumar**

Ph.D. – COURSE WORK – Paper I

Structural Properties and Applications of Nanomaterials

Course Code: 17PHDCH1A
Credit: 5
Total Hours: 50 hrs
Course Outcome

At the end of the course, this scholar will be able:

1. To understand the fundamentals of nanotechnology
2. To analyse the different dimensional structures of nanomaterials
3. To highlight optical, thermal, electrical, magnetic and conducting properties of nanomaterials
4. To appreciate the applications of nanomaterials in different fields of science.

UNIT–I : Introduction to Nanomaterials

Emergence of Nano Science and Technology – Significance. Fundamentals of crystal structures – nucleation, crystal growth and material parameters – Basics of Quantum confinement

UNIT– II: Different Dimensional Nano Structures

Types and strategies for synthesis of Nanomaterials depending on end applications.

Zero-Dimensional Nanostructure: Nanoparticles: Introduction, different strategies for synthesis of 0D Nanomaterials and their technology applications.

One-Dimensional Nanostructure: Introduction, different strategies for synthesis of 1D Nanomaterials and their technological applications.

Two-Dimensional Nanostructure: Introduction, different strategies for synthesis of 2D Nanomaterials and their technological applications.

Three-Dimensional Nanostructure: Introduction, different strategies for synthesis of 3D Nanomaterials and their technological applications.

UNIT – III: Special Nano Structures

Special Nanomaterials and Applications: Introduction, different strategies for synthesis of special Nanomaterials (e.g. CNTs, Mesoporous, zeolites, core-shell structures, hybrid nanomaterials etc. and their technological applications)

UNIT– IV: Properties of Nanomaterials

Mechanical-Morphological – Optical – Thermal – Electrical and Magnetic – Semiconducting and Super Conducting Properties of Nanomaterials.

UNIT– V: Applications of Nanomaterials

Applications of Nanotechnology in Renewable energy, solar energy, fuel cells etc. – Biomedical science, diagnostics, etc. – Applications of Nanotechnology in Analytical, Pharma, Environmental sciences and Marine Nanotechnology – Computers, electronics and communication – Biosciences (Nano Biosciences - Biotechnology) – Agriculture, food, textile and cosmetics.

References

1. J.R.Friedman, V.Patel, W.Chen, S.K.Tolpygo, J.E.Lukens. "Quantum superposition of distinct macroscopic states, (Nature, 406, 43 2000)
2. B.E.Kane, "A silicon-based nuclear spin quantum computer", (Nature 393, (133) 1998).
3. A.Roosen and H.Hausner, "Cermanic Powders",(Elsevier, Amserdam, 1983).
4. J.Eckert, J.C.Halzer, and C,E.Krill III, J.Appl.Phys.73, 2794 (1993).
5. Christian Brosseau, James Ben, Youssef, Philippe Tallot, Anne-Marie Konn, Nanometer versus Micrometer – Sized Particles – Appl. Physics Vol.93, (2003).
6. S.K.Ma and J.T.Lue, Solid State Commun. 97, 979 (1996).
7. W.Stober, A.Fink, and E.J.Bohn, J.Colloid Interf. Sci. 26, 62 (1968).
8. C.P. Poole Jr.and F.J. Owens, Introduction to Nanotechnology, Wiley Interscience.
9. W.A. Goddard, D.W. Brenner and G.J.Iafrate, Handbook of Nanoscience, Engineering and Technology, (CRC Press, 2003).
10. M.F.Ashby, Paulo J.S.G. Ferreira, Daniel L.Schodek, Nanomaterial, Nanotechnology and Design, An Introduction for Engineers and Architects, (World Scientific Publishing Private Ltd., Singapore. 2009).

Name of the Student: **J. Princes Gracia**
Name of the Research Advisor: **Dr.V. Nandhakumar**

Ph.D. – COURSE WORK – Paper II

Nanomaterials Synthesis and their Characterisation Techniques

Course Code: 17PHDCH2A

Credit: 5

Total Hours: 50 hrs

Course Outcomes

At the end of the course, this scholar will be able:

1. To synthesis nanomaterials.
2. To apply spectral techniques for the characterization of nanomaterials.
3. To characterize nanomaterials by XRD, SEM, TEM and thermal analysis.
4. To apply computational techniques for the characteisation of nanomaterials.

UNIT-I Synthesis-Physical Approaches

Vapor deposition and different types of epitaxial growth techniques (CVD, MOCVD, MBE, ALD)- pulsed laser deposition, Magnetron sputtering - lithography : Photo/UV/EB/FIB techniques, Dip pen nanolithography, Etching process :Dry and Wet etching, micro contact printing.

UNIT-II Synthesis-Chemical Approaches

Sol gel processing-Solvothermal, Hydrothermal, Precipitation, Spray pyrolysis, Electro spraying and spin coating routes, Self-assembly, Self-Assembled Monolayers (SAMs). Langmuir-Blodgett (LB) films, micro emulsion polymerization- templated synthesis, pulsed electrochemical deposition.

UNIT – III Characterization of Nanomaterials using Spectroscopy

Nanomaterials Characterization using molecular spectroscopy - atomic, UV-visible spectroscopy, FT-IR spectroscopy - ESR Spectroscopy –NMR Photoluminescence.

UNIT - IV Advanced Characterizaiton techniques of Nanomaterials

X-ray diffraction (XRD-Power/Single crystal), Small angle X-ray scattering (SAXS), scanning electron microscopy (SEM), transmission electron microscopy (TEM), energy dispersive X-ray analysis (EDAX), Low Energy Electron Diffraction (LEED), Scanning Probe Microscopy (SPM) – Principle of operation, instrumentation and probes, Atomic force microscopy (AFM), Optical spectroscopy (UPS), XPS, ESCA, Auger, Thermal Analysis methods etc.

UNIT - V Computation Techniques

Basics of Origin, JCPDS method, Simulation technique, Statistical Analysis tools - analysis of variance (ANOVA)

References:

5. Joshi Mj & Viswanathan V, J Appl Polym Sci, 102, (3) 2164 (2006).
6. Joshi M, Butola B S, Simon G & Kukalevab N, Macromolecules, 39, 1839 (2006).
7. Kalajn R, Bishop K J M, Fialkowski M, Paszewski M, Campbell Chris J.C, Gray TP & Grzybowski A B, Science, 316, (5822) 261 (2007).
8. Dr.Siddharth Vaidya, Nanotechnology Research and Perspectives, (Pearl Books2007).
9. Michael L. Roukes, "Understanding Nanotechnology" (Scientific American, Inc, and Byron Press Visual Publications, 2002).
10. Guozhong Cao, Nanostructures and Nanomaterials Synthesis, Properties and Applications (World Scientific Publishing Private Ltd., Singapore, 2004)
11. Dougles A. Skoog, F. James Holler and Timothy A. Nieman, Principle of Instrumental Analysis, Visual Publication, 1998.
12. Joseph I. Goldstein, Dale E. Scanning Electron Microscope and X-ray Micro Analysis, (Newbury Academic/Plenum Publishers, Newyork, 2003).
13. Tseung – Yuen, Tseng and Hari Singh Nalwa, Handbook of Nanoceramics and their Based Nano Devices (Vol.2), (American Scientific Publishing 2008).
14. 'William .H. Press, Brian P. Flannery, Saul A. Teukolsly, and William T.Vetter-ling, "Numerical Recipes – The Art of Scientific Computing", (Cambridge University Press, 1986).

student Name : Gr. Balu Mahendran Guide : Dr. S. Jothi Ramalingam

Sub. Code: 17PHDCH1 **Ph.D. - Course work - Paper I** **Credit: 4**

GRAPHENE MATERIALS

UNIT I

Graphene: Introduction of graphene, Graphite, Definition and structure of graphene, Types of graphene: stacking AA, BB, AB dispersion relation, Single layer, Bi-layer, Few layer, Properties of graphene; Optical: thickness dependency, optical conductivity, electric filed tunable transparency, plasmons and polaritons, carrier multiplication. Electrical: Boltzmann equation, ambipolar conduction, density of states and doping (electrostatic and chemical), quantum hall effect, Klein tunneling, diamagnetism, magnetoresistance and spin current, thermal conductivity. Mechanical, Surface phenomenon.

Characterization of graphene: Transmission electron microscopy (TEM), Scanning tunneling microscopy (STM), Raman Spectroscopy, Electrical measurements: electric field effect, temperature dependent resistivity measurement.

UNIT II

Preparation and Characterization of graphene: Epitaxial growth of graphene on Silicon carbide, Chemical deposition (CVD) growth of graphene films, Chemically drived graphene, Synthesis of graphene oxide: Hummer's method, Modified Hummer's method, Reduction of graphene oxide: Chemical methods, Physical methods, Electrochemical exfoliation, Nanotube slicing, from solid state carbon sources.

UNIT III

Applications of graphene: Graphene in the energy application: Li-ion batteries, Supercapacitors, Photovoltaic, Radio-frequency transistor, Photodetector, Modulator, Mode locked lasers, Other applications of graphene: Anti-corroison coating, Anti- bacterial coating, catalyst, Sensors, Transparent Conductors

UNIT IV

Carbon Nanotubes: Introduction of Carbon Nanotube (CNT): Introduction and definition of CNT, Bonding of carbon atoms, SP3, SP2, Deformed SP2 , Structure of Carbon Natotubes, Chiral Vector, Armchair, Zig-Zag and Chiral tubes, Properties of Carbon Nanotubes: Electronic, Optical and Optoelectronic, Mechanical, Chemical and Electrochemical, Opening, wetting and filling, doping, intercalation, Thermal and Thermoelectric.

UNIT V

Carbon Nanotubes: Synthesis Methods and Growth Mechanisms: High temperature method, Arc discharge, General technical features of the production process, Growth Mechanism, Laser Ablation of Graphite, Low temperature method, Chemical Vapor deposition (CVD) process, Vapor liquid solid model, Catalytic role. Purification and functionalization: Methods of Purification, Methods of Functionalization (Chemical and Physical), Advantage of purification and functionalization, Separation of cnts: based on chirality, semiconducting, metallic, Applications of Carbon nanotube, Field emission, Li-ion battery, Supercapacitor, Sensors, Solar cell , CNT-polymer composite and avionics EM shielding

Reference Books:

1) Graphene: Carbon in Two Dimensions, by Mikhail I. Katsnelson
2) Physics of Graphene, Editors: Aoki, Hideo, S. Dresselhaus, Mildred (Eds.)
3) Graphene: Synthesis, Properties, and Phenomena, by C. N. R. Rao (Editor), Ajay K. Sood (Editor),
4) Graphene Nanoelectronics, Metrology, Synthesis, Properties and Applications, Editors: Raza, Hassan (Ed.)
5) Graphene Nanoelectronics: From Materials to Circuits, Editors: Murali, Raghu (Ed.)
6) Carbon Nanotube and Graphene Device Physics, by H.-S. Philip Wong (Author), Deji Akinwande (Author)
7) Carbon Nanotube Electronics (Integrated Circuits and Systems) by Ali Javey (Editor), Jing Kong (Editor),
8) Polymer-Graphene Nanocomposites, Editor(s): Vikas Mittal
9) Physics and Chemistry of Graphene: Graphene to Nanographene, Toshiaki Enoki, Tsuneya Ando

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Dr. K. Ravichandran Ph.D.,
Head, Department of Physics
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Tamilnadu, India.

student name: Dr. Balu Mahendran Guide: Dr. S. Jothi Ramalingam

Code: 17PHDCH2 **Ph.D. - Course work - Paper II** **Credit: 4**

CHARACTERISATON OF MATERIALS

UNIT : I

THERMAL ANALYSIS

Introduction – thermogravimetric analysis (TGA) – instrumentation – determination of weight loss and decomposition products – differential thermal analysis (DTA)- cooling curves - differential scanning calorimetry (DSC) – instrumentation – specific heat capacity measurements – determination of thermomechanical parameters .

UNIT : II

MICROSCOPIC METHODS

Optical Microscopy: optical microscopy techniques – Bright field – Dark field optical microscopy – phase contrast microscopy -differential interference contrast microscopy - fluorescence microscopy - confocal microscopy - Metallurgicalmicroscope.

UNIT : III

ELECTRON MICROSCOPY AND SCANNING PROBE MICROSCOPY

SEM- FESEM- EDAX,- HRTEM: working principle and Instrumentation – sample preparation – scanning probe microscopy - STM – AFM - working principle, Instrumentation and modes of operation.

UNIT : IV

ELECTRICAL AND OPTICAL METHODS OFCHARACTERISATION

Two probe and four probe methods- van der Pauw method – Hall probe and measurement – scattering mechanism – C-V, I-V characteristics – Schottky barrier capacitance – impurity concentration – electrochemical C-V profiling – limitations - Photoluminescence – light – matter interaction – instrumentation – electroluminescence – instrumentation – Applications.

UNIT : V

SPECTROSCOPY

Principles and instrumentation for UV-Vis-IR, FTIR spectroscopy, Raman spectroscopy, ESR, NMR, NQR, ESCA and SIMS- proton induced X-ray Emission spectroscopy (PIXE) – application – mass spectroscopy.

REFERENCES:

1. R.A.Stradling and P.C.Klipstain. Growth and Characterization of semiconductors. Adam Hilger, Bristol, 1990.
2. J.A.Belk. Electron Microscopy and Microanalysis of Crystalline Materials. Applied Science Publishers, London, 1979.
3. L. E.Murr. Electron and Ion microscopy and Microanalysis principles and Applications. Marcel Dekker Inc., New York, 1991.
4. D.Kealey & P.J.Haines, Analytical Chemistry, Viva Books Private Limited, New Delhi, 2002.
5. Banwell, Fundamentals of Molecular Spectroscopy, McGraw-Hill Education, Pvt. Ltd., 2013.

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Tamilnadu, India

Department of chemistry - Ph.D Course work

Scholar name: **M.Vetriselvan** Guide name**: M.Pramesh**

Sub code: 17PHDCH1 Synthetic organic chemistryCredit: 4

UNIT-I: Heterocyclic compounds

Synthesis and reactivity of the following heterocyclic compounds and their derivatives- pyrazole, oxazole, imadazol, thiazole, pyridazine and pyrazine,pyrrole, pyridine,furan, Quinoline, isoquinoline and indole.

UNIT-II: Reagents in organic synthesis

$LiAlH_4$,$NaBH_4$, tri- tertiarybutoxy aluminium hydride, $NaCNBH_3$ and tri n-butyl tin hydride, Wilkinson catalyst, Lithium dimethyl cuprate, lithium di-isopropylamide, DCC, 1,3-dithane,trimethyl silyl iodide, DDQ, SeO_2, OsO_4 ,$KMnO_4$ HIO_4 Lead tetra acetate, H_2O_2,Pyridinium Chlorochromate (PCC) ,Peracids, Phenyl Selenium Chloride (PhSeCl),phase transfer catalysis, crown ethers.

UNIT-III: Organic name reactions

Stork enamine reaction,Michael addition, mannich reaction,nef reaction, sharpless asymmetric epoxidation, barton reaction, Hoffman-loffler-freytag reaction, bombard-stevens reaction, Shapiro reaction, reformatsky, reimer-tiemann.gattermann,gattermann coach, vilsmeir hack reaction, stobbe,dieckmann,aldol and darzen's, condensation.

UNIT-IV:Molecular Rearrangements

Mechanism and applications of Bayer villager, favorski, stevens, neber,dienone-phenone, Beckman, fries, claisen, cope, demyanov rearrangements.

UNIT-V: Stereochemistry

Optical activity and criteria for chirality – Enantiotopic, diastereotopic and Prochiral centres- threo and erythro configurations-Fischer, newman and sawhorse projection formulae and inter conversions - RS notataion – Atropisomerism – Geometrical isomerism - EZ notations. Stereo selective, stereo specific and diastereoselective reactions.

References

1. J. March, Advanced Organic Chemistry: Reactions, Mechanisms and structure, 5thed. Wiley, 2000
2. Clayden, Greeves,. Warren and Wothers, Organic chemistry, 2nded. Oxford University press.
3. Francis A. Carey and Richard J. Sundberg, Advanced organic chemistry part A: Structure and Mechanisms.5th ed.springer
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5. Peter Sykes, A Guide book to Mechanism in organic chemistry, 6th editionLongman, 1986
6. P.S.Kalsi, Stereochemistry Conformation and mechanism, 5th edition New Age international
7. V.K.Ahluwalia and R.K.Parashar, Organic reaction mechanisms.3rd edition, Alpha Science Int'l Ltd
8. S.M.Mukherji and S.P.Singh, Reaction mechanism in organic chemistry.3rd edition Macmillan India Limited.
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Department of chemistry

Scholar name: **M.Vetriselvan** Guide name**: M.Pramesh**

Ph.D Course work

Sub code: 17PHDCH2Credit: 4

Applications of spectroscopy in synthetic organic chemistry

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Unit II: UV-Visible Spectroscopy

Introduction –principle-Sampling techniques - Woodward–Fieser and Scott rules for conjucated dienes and polymers, ketones, aldehydes, α,β-unsaturated acids, esters,nitriles, and amides. Differentiation of geometrical isomers and positional isomers – Disubstituted benzene derivatives - Study of steric effect in aromaticity.

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Introduction - Instrumentation, Sampling techniques, factors influencing group frequencies –. Hydrogen bonding – intermolecular and intramolecular -important functional group region.

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Unit V: Chromatography

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References

1. R.M. Silverstein,G.C. Bassler F. X. Webster, Spectroscopic Identification of Organic Compounds, 6th ed.,Wiley 1998.
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3. J.R. Dyer, Applications of Absorption Spectroscopy of Organic Compounds, Prentice Hall, 1965.
4. Y.R. Sharma, Elementary Organic Spectroscopy – Principles and Chemical applications, S.Chand, 1992.
5. P.S.Kalsi, Spectroscopy of Organic Compounds, Wiley eastern limited.
6. Jag Mohan, Organic spectroscopy, Principles and applications, 2nd edn., Narosa publication.

Department of chemistry

Scholar name: **S.Helen Perci**Guide name**: M.Pramesh**

Ph.D Course work

Sub code: 17PHDCH1 Synthetic organic chemistryCredit: 4

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Ph.D Course work

Sub code: 17PHDCH2Credit: 4

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Department of chemistry

Scholar name:**K.Gunasundari** Guide name**: M.Pramesh**

Ph.D Course work

Sub code: 17PHDCH1 Synthetic organic chemistryCredit: 4

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Synthesis and reactivity of the following heterocyclic compounds and their derivatives- pyrazole, oxazole, imadazol, thiazole, pyridazine and pyrazine,pyrrole, pyridine,furan, Quinoline, isoquinoline and indole.

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Ph.D Course work

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6. Jag Mohan, Organic spectroscopy, Principles and applications, 2nd edn., Narosa publication.

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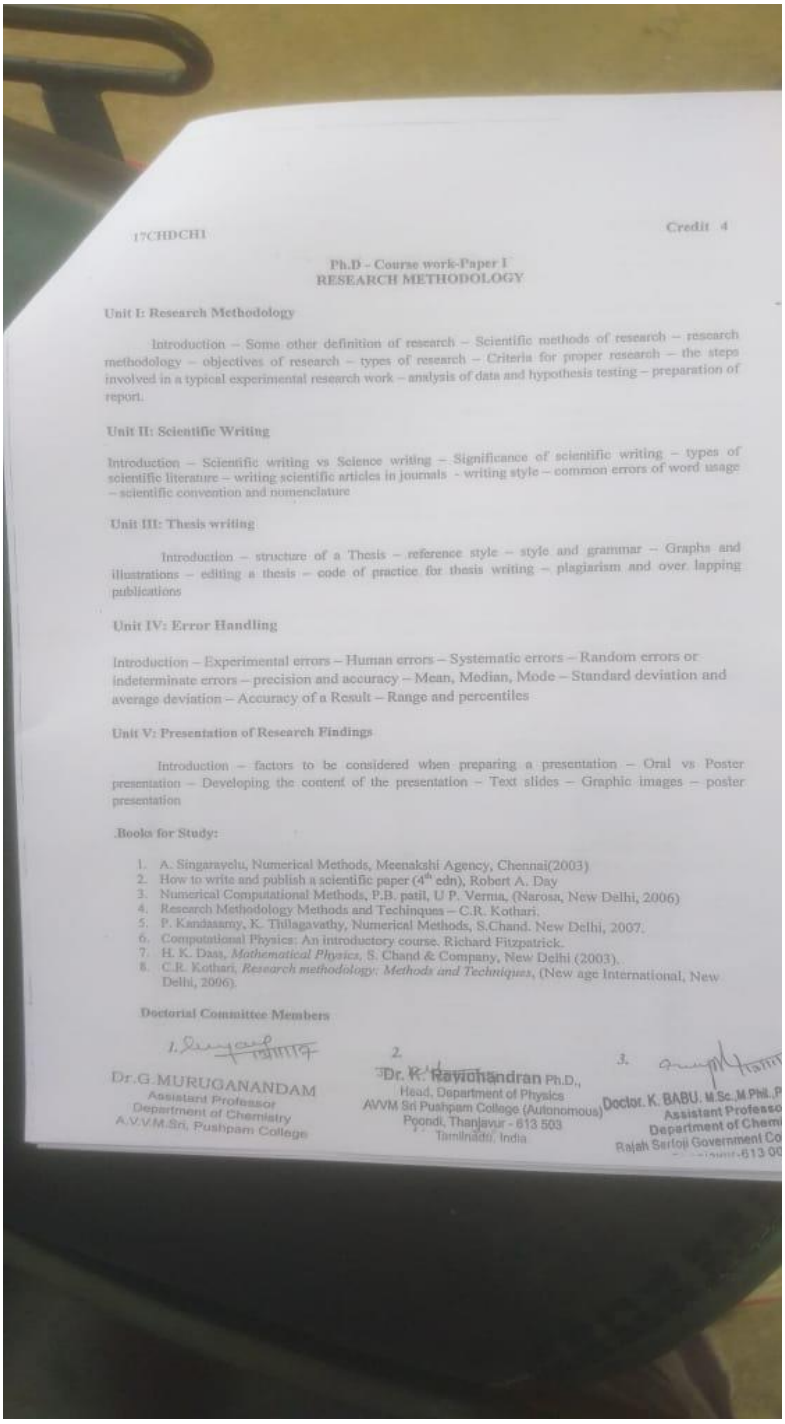

17CHDCH1 Credit 4

Ph.D - Course work-Paper I
RESEARCH METHODOLOGY

Unit I: Research Methodology

Introduction – Some other definition of research – Scientific methods of research – research methodology – objectives of research – types of research – Criteria for proper research – the steps involved in a typical experimental research work – analysis of data and hypothesis testing – preparation of report.

Unit II: Scientific Writing

Introduction – Scientific writing vs Science writing – Significance of scientific writing – types of scientific literature – writing scientific articles in journals - writing style – common errors of word usage – scientific convention and nomenclature

Unit III: Thesis writing

Introduction – structure of a Thesis – reference style – style and grammar – Graphs and illustrations – editing a thesis – code of practice for thesis writing – plagiarism and over lapping publications

Unit IV: Error Handling

Introduction – Experimental errors – Human errors – Systematic errors – Random errors or indeterminate errors – precision and accuracy – Mean, Median, Mode – Standard deviation and average deviation – Accuracy of a Result – Range and percentiles

Unit V: Presentation of Research Findings

Introduction – factors to be considered when preparing a presentation – Oral vs Poster presentation – Developing the content of the presentation – Text slides – Graphic images – poster presentation

Books for Study:

1. A. Singaravelu, Numerical Methods, Meenakshi Agency, Chennai(2003)
2. How to write and publish a scientific paper (4th edn), Robert A. Day
3. Numerical Computational Methods, P.B. patil, U P. Verma, (Narosa, New Delhi, 2006)
4. Research Methodology Methods and Techinques – C.R. Kothari.
5. P. Kandasamy, K. Thilagavathy, Numerical Methods, S.Chand. New Delhi, 2007.
6. Computational Physics: An introductory course. Richard Fitzpatrick.
7. H. K. Dass, *Mathematical Physics*, S. Chand & Company, New Delhi (2003).
8. C.R. Kothari, *Research methodology: Methods and Techniques*, (New age International, New Delhi, 2006).

Doctorial Committee Members

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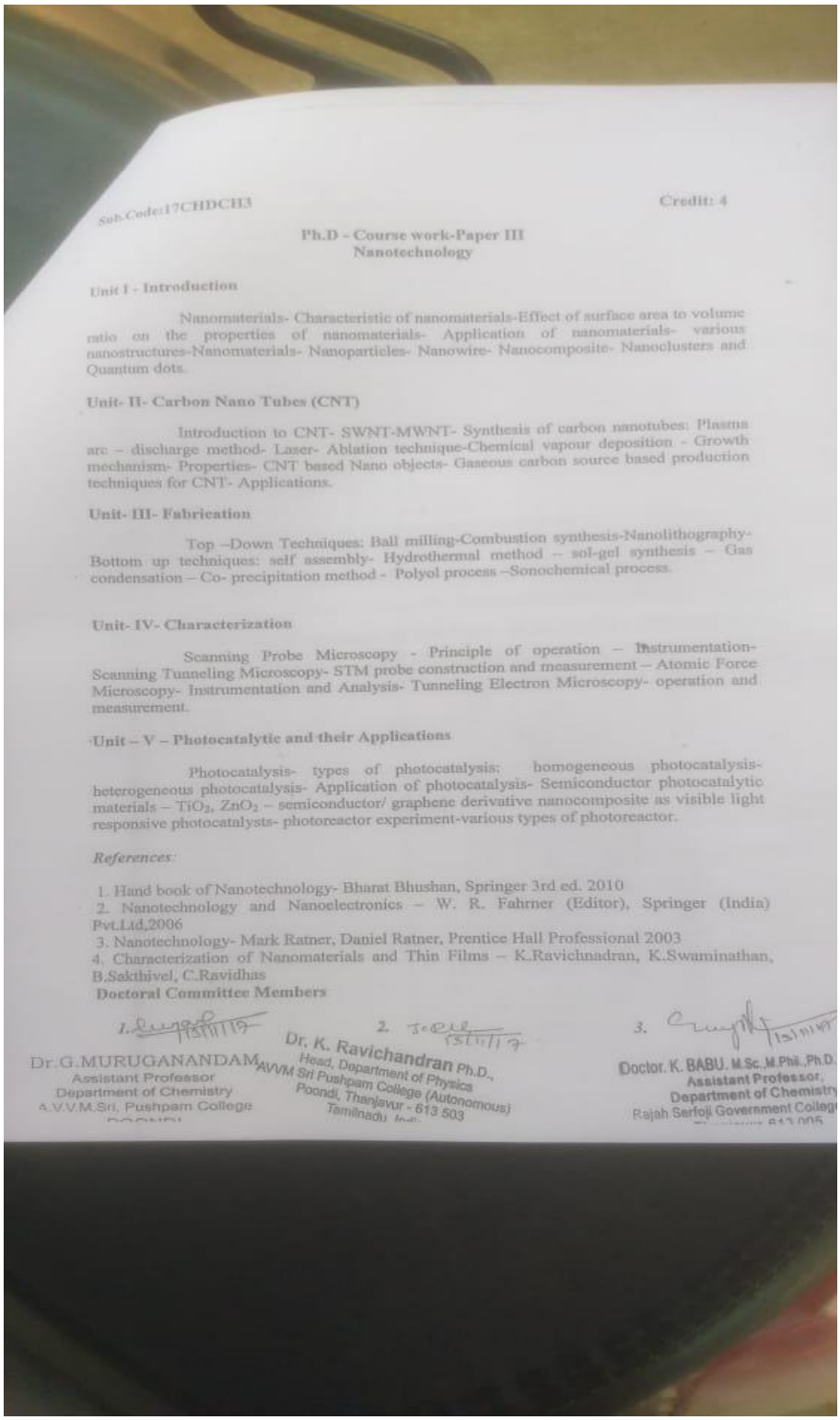
Scholar name:**M.Prasanth** Guide name**: G.Muruganadham**



Sub.Code:17CHDCH3 Credit: 4

Ph.D – Course work-Paper III
Nanotechnology

Unit I - Introduction

Nanomaterials- Characteristic of nanomaterials-Effect of surface area to volume ratio on the properties of nanomaterials- Application of nanomaterials- various nanostructures-Nanomaterials- Nanoparticles- Nanowire- Nanocomposite- Nanoclusters and Quantum dots.

Unit- II- Carbon Nano Tubes (CNT)

Introduction to CNT- SWNT-MWNT- Synthesis of carbon nanotubes: Plasma arc – discharge method- Laser- Ablation technique-Chemical vapour deposition - Growth mechanism- Properties- CNT based Nano objects- Gaseous carbon source based production techniques for CNT- Applications.

Unit- III- Fabrication

Top –Down Techniques: Ball milling-Combustion synthesis-Nanolithography- Bottom up techniques: self assembly- Hydrothermal method – sol-gel synthesis – Gas condensation – Co- precipitation method - Polyol process –Sonochemical process.

Unit- IV- Characterization

Scanning Probe Microscopy - Principle of operation – Instrumentation- Scanning Tunneling Microscopy- STM probe construction and measurement – Atomic Force Microscopy- Instrumentation and Analysis- Tunneling Electron Microscopy- operation and measurement.

Unit – V – Photocatalytic and their Applications

Photocatalysis- types of photocatalysis: homogeneous photocatalysis- heterogeneous photocatalysis- Application of photocatalysis- Semiconductor photocatalytic materials – TiO_2, ZnO_2 – semiconductor/ graphene derivative nanocomposite as visible light responsive photocatalysts- photoreactor experiment-various types of photoreactor.

References:

1. Hand book of Nanotechnology- Bharat Bhushan, Springer 3rd ed. 2010
2. Nanotechnology and Nanoelectronics – W. R. Fahrner (Editor), Springer (India) Pvt.Ltd,2006
3. Nanotechnology- Mark Ratner, Daniel Ratner, Prentice Hall Professional 2003
4. Characterization of Nanomaterials and Thin Films – K.Ravichnadran, K.Swaminathan, B.Sakthivel, C.Ravidhas

Doctoral Committee Members

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DR.R.Manikandan

A.V.V.M. SRI PUSHPAM COLLEGE (AUTONOMOUS), POONDI THANJAVUR – DT.

Subject Code	Title of the Paper	No of Credits	R.Shyamala
17PHDCH1	Analytical Techniques	4	15CHA605

Unit-1: Chromatography and UV Spectra: Column, Paper, thinlayer, gas-liquid, High Pressure liquid Chromatography HPLC principle and applications Woodward-scott rules for conjugated dienes and polymer, ketones, aldehydes, Unsaturated acids, esters, nitriles and amides differentiation of position isomer. Stereo chemical factors affecting electronic spectra of biphenyls, cis and trans isomers. Angular distortion and cross conjugation.

Distillation: Simple distillation, Fractional distillation, Steam distillation, Theory of distillation under reduced pressure advance of distillation.

Unit-2: IR and Raman Spectra: IR vibration spectra-selection rules-oscillators-vibration spectra of dye and polyatomic molecules-rotation on polyatomic molecules. FT IR factors influencing group frequencies both internal and external quantitative studies. Hydrogen bonding (inter molecules & intra molecules) Finger print region - identification of functional groups, conformational aspects in cyclic 1,2 and 1,3-diols, trans annular interaction.

Unit-3: NMR Spectra: NMR spectroscopy multiplicity-coupling constant-first order and second order proton spin-spin splitting-Dependence of Ion dihedral angle vicinal &

germinal coupling constrant, Karplus equation, long range coupling constant, influence of stereo chemical factors on chemical shift of protons. Simplification of complex spectra, double resonance techniques, shift reagents, chemical spin decoupling of rapidly exchangeable protons (OH, SH, COOCH, NH, NH2) an elementary treatment of NOE phenomenon, C13 NMR spectroscopy, Basic theory of FT-NMR relation-Broad and decoupling off resonance decoupling and chemical shift of common function groups, Distortionless Enhancement by Polarization Transfer (DEPT) spectra identification of small compounds bases on NMR data techniques $_{1}H$-$_{1}H$-COSY-$_{1}H$-$_{13}C$ COSY-HMBC and NOESY.

Unit-4: MASS Spectra: Electron Ionization, Chemical Ionization methods – base peak, isotopic peaks, meta stable peaks, parent peaks, determination of molecular formula-recognition of molecular ion peaks, Fast Atom Bombardment fragmentation, general rules-pattern of fragmentation for various classes of compounds, MClafferty rearrangement-importance of meta stable peaks. Basic principles of NQR and Massbauer spectroscopy.

Unit-5: X-ray diffraction: X-ray diffraction by single crystal-space groups-systematic absences in X-ray data and identification of lattic types, glide planes and screw axes-X ray intensities, structure factor and its relation to intensity and electron density, phase problem structure solution by Heavy atom method and direct method. Determination of absoluteconfiguration of molecules.

REFERENCE:

1. YR Sharma, Organic Spectroscopy, Chapter (2)
2. W. Kemp, Organic Spectroscopy, Chapter (2)
3. Robert M. Silverstein, G. Clayton Bassler, Spectrometric Identification of Organic Compound, Chapter (3&3)
4. P.S. Kalsi Organic Spectroscopy, Chapter (6)
5. Stout G.H. Jensen X-ray Structure Determination, Chapter (2)

A.V.V.M. SRI PUSHPAM COLLEGE (AUTONOMOUS), POONDI THANJAVUR – DT.

Subject Code	Title of the Paper	No of Credits
17PHDCH2	Natural Products	4

UNIT-1:

Alkaloids: Introduction to Alkaloids, occurrence of Alkaloids, Functions of Alkaloids, Nomenclature of Alkaloids, Classification of Alkaloids, Isolation of Production of Alkaloids, Properties of Alkaloids, General Methods Employed for Determining structures of Alkaloids, Structural elucidation of papaverine, piperidine, Quinine.

UNIT-2:

Terpenoids: Classification and properties of terpenoids, Structural elucidation and synthesis of Terpenoids, Pinene, Phytol, Menthol.

UNIT-3:

Steroids: Classification and properties of steroids. Structural elucidation and synthesis of cholesterol, Lanosterol, Phytosterols, Bile acids, Oestriol and Pregnanediol.

UNIT-4:

Vitamins: Structural elucidation and synthesis of Retinol, Riboflavin, Cyanocobalamine and L-Ascorbic acid.

UNIT-5:

Lipids: Biological function of Lipids-Classification of Lipids simple Lipids-Natural fats difference between oil and fats. Production of higher fatty acids-physical chemical properties of fats. Compound Lipids-phospholipids.

REFERENCE:

1. Gurdeep R.Chatwal, Organic Chemistry of Natural Products, Chapter (3,4)

2. O.P. Agarwal, Chemistry of Organic Natural Products, Vol.II, Chapter (4,1 & 5) I.L. Final, Organic Chemistry, Vol. II.

Department of chemistry

Scholar name:**B.Pradhiba Priyadharshini**
Guide name**: G.Muruganadham**

Sub.Code:17CHDCHI

Credit: 4

B.PRADHIBA PRIYADHARSHINI
17CHA611

Ph.D - Course work-Paper I
Thin Films and their Applications

Unit I - Introduction

Thin films an overview – Film growth stages- Nucleation stage - Island structure stage- Coalescence stage- Channel stage and continuous film stage -crystal structure –crystal lattice and unit cell – Crystal planes and Miller indices – Crystal system and symmetry- Interplaner spacing.

Unit II -Fabrication

Physical vapour deposition –Thermal evaporation – Electron beam evaporation- Molecular beam epitaxy – Sputtering techniques – Pulsed laser deposition - Chemical vapour deposition: – Spray pyrolysis – Chemical bath deposition - Electro chemical deposition – Sol–gel technique – Spin coating- SILAR method.

Unit – III Structural and Electrical studies

X-ray diffraction- Powder diffraction technique for polycrystalline thin films-Structural parameters.

Electrical resistivity- Sheet resistance - Valde's formula for sheet resistance Four probe method- Hot probe method for the determination of type of conductivity - Hall probe method to find mobility, Carrier concentration and resistivity.

Unit –IV Optical, Surface and Magnetic studies

UV-vis-NIR spectrophotometer- Transmission and absorption spectra of thin films- Optical band gap - absorption co-efficient-SEM- AFM-TEM- EDS–XPS- PL spectra- Thickness measurement- Weight gain method- surface profilometer- optical interference method – multiple beam interferometry – ellipsometry-Fizeau method- Magnetic properties of thin films- VSM-SQUID.

Unit –V Applications

Discrete resistive components- Thermistor, Varistor, Strain gauge element- Capacitor- Hall probe element- Active devices- Micro electronics, Integrated circuits and other applications- Interference filters- Anti -reflection coatings- Thin film gas sensors- Solar cell- photocatalytic and antibacterial applications.

References:

1.Thin film fundamentals- A. Goswami,New Age international pvt .Ltd, New Delhi 1996
2. Materials science process technology series- Rointan F. Bunshah, Noyes publications USA 1994
3. Elements of X-ray diffraction- B. D. Cullity,Addition – Wesley Publishing Company, Inc. USA,1956
4.Introduction to thin films- K. Ravichandran, K. Swaminathan, B. Sakthivel, Research India Publications, New Delhi, 2013

Doctoral Committee Members

1. *2.* *3.*

Scholar name:**B.Pradhiba Priyadharshini**
Guide name**: G.Muruganadham**

B. PRADHIBA PRIYADHARSHINI
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Sub.Code:17CHDCH2 Credit: 4

Ph.D - Course work-Paper II
Nanotechnology

Unit I - Introduction

Nanomaterials- Characteristic of nanomaterials-Effect of surface area to volume ratio on the properties of nanomaterials- Application of nanomaterials- various nanostructures-Nanomaterials-Nanoparticles- Nanowire- Nanocomposite- Nanoclusters and Quantum dots.

Unit- II- Carbon Nano Tubes (CNT)

Introduction to CNT- SWNT-MWNT- Synthesis of carbon nanotubes: Plasma arc – discharge method- Laser- Ablation technique-Chemical vapour deposition - Growth mechanism-Properties- CNT based Nano objects- Gaseous carbon source based production techniques for CNT-Applications.

Unit- III- Fabrication

Top –Down Techniques: Ball milling-Combustion synthesis-Nanolithography- Bottom up techniques: self assembly- Hydrothermal method – sol-gel synthesis – Gas condensation – Co-precipitation method - Polyol process –Sonochemical process.

Unit- IV- Characterization

Scanning Probe Microscopy - Principle of operation – Instrumentation- Scanning Tunneling Microscopy- STM probe construction and measurement – Atomic Force Microscopy-Instrumentation and Analysis- Tunneling Electron Microscopy- operation and measurement.

Unit – V – Photocatalytic and their Applications

Photocatalysis- types of photocatalysis: homogeneous photocatalysis- heterogeneous photocatalysis- Application of photocatalysis- Semiconductor photocatalytic materials – TiO_2, ZnO_2 – semiconductor/ graphene derivative nanocomposite as visible light responsive photocatalysts-photoreactor experiment-various types of photoreactor.

References:

1. Hand book of Nanotechnology- Bharat Bhushan, Springer 3rd ed. 2010
2. Nanotechnology and Nanoelectronics – W. R. Fahrner (Editor), Springer (India) Pvt.Ltd,2006
3. Nanotechnology- Mark Ratner, Daniel Ratner, Prentice Hall Professional 2003
4. Characterization of Nanomaterials and Thin Films – K.Ravichnadran, K.Swaminathan, B.Sakthivel, C.Ravidhas

Doctoral Committee Members

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Name	**:**	S. Karthika
Guide Name	**:**	Dr. N. Mani
Course work held on	**:**	03.04.2019
Ref. No.	**:**	Ref.No.26303/Ph.D.K2/Chemistry/PartTime /January.2018/ Date: 22.12.2017

Sub. Code: 18PHDCH1 **Ph.D. - Course work - Paper I** **Credit: 4**

PHYTOCHEMISTRY

UNIT – I

Natural Products: Definition – classification of metabolites – primary metabolites and secondary metabolites – Green chemistry in natural products. Primary Metabolites - Protein – definition – characteristic features – classification – properties. Isoelectric point denaturation – test for proteins – structure of proteins.Aminoacids – definition – classification – preparation – properties – inner salt – peptide linkage.

UNIT – II

Carbohydrates and Vitamins: Carbohydrates – definition – classification – preparation, properties and structural elucidation of glucose and sucrose.Polysaccharides – starch and cellulose.Vitamins – definition – classification – source – structural elucidation of ascorbic acid.

UNIT – III

Secondary Metabolites: Terpenoids – definition – Isolation and separation – classification – Isoprene rule – special isoprene rule – Biosynthesis of terpenoids – Zingiberene and squalene. Steriods – Introduction – definition – classification – Nomenclature – synthesis of cholesterol.Alkaloids – Nomenclature – Classification – Isolation – properties – detection of alkaloids – structure of morphine.

UNIT – IV

Isolation Techniques: General protocol for isolating phytochemical – choice of solvents for extraction.Chromatography – definition – types – column, TLC, paper chromatography, Ion – exchange, Gas chromatography and HPLC – principles and applications – Gel electrophoresis.

UNIT – V

Nanochemistry: Introduction – Nonomaterials – types – approaches – properties – applications. Techniques – SEM (Scanning Electron Microscope) – TEM (Transmission

Electron Microscope) – STEM (Scanning Transmission Electron Microscope) – difference between an optical microscope and electron microscopes (SEM, TEM, STEM)

References

1. Chemistry of Natural Product by A.P. Rajalakshmi.
2. Bio – Organic Chemistry by P. Sharma
3. Nanostructure and Nano Materials by Y. S. Raghavan.
4. Instrumental Methods of Chemical Analysis by H. Kaur
5. Nano the essential, understanding Nano science and Nano technology by T. Pradeep.

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Course work held on	**:**	03.04.2019
Ref. No.	**:**	Ref.No.26303/Ph.D.K2/Chemistry/PartTime /January.2018/ Date: 22.12.2017

Sub. Code: 18PHDCH2 **Ph.D. - Course work - Paper II** **Credit: 4**

ANALYTICAL TECHNIQUES IN CHEMISTRY

UNIT – I

Electronic configuration, terms, and micro states. Derivation of term symbols (p2, d2) and arranging the various terms according to their energies. Spectroscopy terms – effect of inter electronic repulsion and spin – orbit coupling, j-j coupling. Selection rule – group theoretical explanation. Oh and Td systems – the corresponding energy level diagrams – mixing of orbitals of orgel diagram – characteristic – presentation and assignment of transition for d^n cases.

UNIT – II

Principles of Spectroscopy: Electromagnetic radiation (emr) interaction of emr with matter. Uncertainity relation – natural line width, Transition probability.

Microwave Spectroscopy: the rotation of molecules – selection rule – stark effect, molecular rotation – Nuclear spin coupling. Rotational energy of symmetric top molecules – selection rule and spectra of asymmetric top molecules – Isotopic mass and inter nuclear distance from microwave spectral studies.

UNIT – III

NMR Spectroscopy : Magnetic and Non – magnetic nuclei condition – principle of NMR – ring current effect – shielding mechanism – chemical shift – Number of signals – spin – spin coupling constant(J) – splitting of signals. NMR paramagnetic molecules – isotropic shifts, contact shifts and pseudo contact shifts – Lanthanide shift reagents – FT – NMR - off resonance decoupling. Identification of structure based on NMR data – problems. **ESR Spectroscopy:** Basic concept ESR spectroscopy – theory – comparison between NMR and ESR – Hyperfine splitting – determination of g Value – factors affecting g values - McConnel equation - Application.

UNIT – IV

UV – Visible spectroscopy : Various electronic transition (185 – 800nm) Beer – Lambert law, effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, Dienes, conjugated dienes and carbonyl compounds, Ultraviolet spectra of Aromatic and Heterocyclic compounds.

IR Spectroscopy: Introduction – principle – theory – molecular vibration, vibrational frequency – number of fundamental vibrations. Selection rule – factors influencing vibrational frequency

UNIT – V

Mass Spectroscopy: Basic principles – Theory – Instrumentation – Resolution: EI and CI methods – mass spectrum: base peak, isotopic peak, parent peak, meta stable peak. Determination of molecular formula – FAB –fragmentation - general rules – pattern of fragmentation for various classes of compounds. McLafferty rearrangement. Nitrogen rule – important features of the mass spectra of hydrocarbons: Alkenes, Alkynes, Cycloalkanes, Aromatic compounds.

References

1. C.N. Banwell, Fundamentals of Molecular spectroscopy, Tata McGraw Hill.
2. R.S. Drago, Physical Methods for Chemistry, Saunders Company.
3. Y.R. Sharma, “Elementary Organic Spectroscopy Principle and Applications”, S. Chand and Company Ltd.,
4. J.R. Dyer, “Applications of Spectroscopy of Organic Compounds”, Prentice Hall.
5. R. Chang, “Basic Principles of spectroscopy”, McGraw Hills.

Name	**:**	B. Latha Maheswari
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Sub. Code: 18PHDCH1 **Ph.D. - Course work - Paper I** **Credit: 4**

PHYTOCHEMISTRY

UNIT – I

Natural Products: Definition – classification of metabolites – primary metabolites and secondary metabolites – Green chemistry in natural products. Primary Metabolites - Protein – definition – characteristic features – classification – properties. Isoelectric point denaturation – test for proteins – structure of proteins.Aminoacids – definition – classification – preparation – properties – inner salt – peptide linkage.

UNIT – II

Carbohydrates and Vitamins: Carbohydrates – definition – classification – preparation, properties and structural elucidation of glucose and sucrose.Polysaccharides – starch and cellulose.Vitamins – definition – classification – source – structural elucidation of ascorbic acid.

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UNIT – IV

Isolation Techniques: General protocol for isolating phytochemical – choice of solvents for extraction.Chromatography – definition – types – column, TLC, paper chromatography, Ion – exchange, Gas chromatography and HPLC – principles and applications – Gel electrophoresis.

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Nanochemistry: Introduction – Nonomaterials – types – approaches – properties – applications. Techniques – SEM (Scanning Electron Microscope) – TEM (Transmission

Electron Microscope) – STEM (Scanning Transmission Electron Microscope) – difference between an optical microscope and electron microscopes (SEM, TEM, STEM)

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1. Chemistry of Natural Product by A.P. Rajalakshmi.
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Sub. Code: 18PHDCH2 Ph.D. - Course work - Paper II Credit: 4

SPECTROSCOPY TECHNIQUES IN CHEMISTRY

UNIT – I

Electronic configuration, terms, and micro states. Derivation of term symbols (p2, d2) and arranging the various terms according to their energies. Spectroscopy terms – effect of inter electronic repulsion and spin – orbit coupling, j-j coupling. Selection rule – group theoretical explanation. Oh and Td systems – the corresponding energy level diagrams – mixing of orbitals of orgel diagram – characteristic – presentation and assignment of transition for d^n cases.

UNIT – II

Principles of Spectroscopy: Electromagnetic radiation (emr) interaction of emr with matter. Uncertainity relation – natural line width, Transition probability.**Microwave Spectroscopy:** the rotation of molecules – selection rule – stark effect, molecular rotation – Nuclear spin coupling. Rotational energy of symmetric top molecules – selection rule and spectra of asymmetric top molecules – Isotopic mass and inter nuclear distance from microwave spectral studies.

UNIT – III

NMR Spectroscopy : Magnetic and Non – magnetic nuclei condition – principle of NMR – ring current effect – shielding mechanism – chemical shift – Number of signals – spin – spin coupling constant(J) – splitting of signals. NMR paramagnetic molecules – isotropic shifts, contact shifts and pseudo contact shifts – Lanthanide shift reagents – FT – NMR - off resonance decoupling. Identification of structure based on NMR data – problems. **ESR Spectroscopy:** Basic concept ESR spectroscopy – theory – comparison between NMR and ESR – Hyperfine splitting – determination of g Value – factors affecting g values - McConnel equation - Application.

UNIT – IV

UV – Visible spectroscopy : Various electronic transition (185 – 800nm) Beer – Lambert law, effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, Dienes, conjugated dienes and carbonyl compounds, Ultraviolet spectra of Aromatic and Heterocyclic compounds.

IR Spectroscopy: Introduction – principle – theory – molecular vibration, vibrational frequency – number of fundamental vibrations. Selection rule – factors influencing vibrational frequency

UNIT – V

Mass Spectroscopy: Basic principles – Theory – Instrumentation – Resolution: EI and CI methods – mass spectrum: base peak, isotopic peak, parent peak, meta stable peak. Determination of molecular formula – FAB –fragmentation - general rules – pattern of fragmentation for various classes of compounds. McLafferty rearrangement. Nitrogen rule –

important features of the mass spectra of hydrocarbons: Alkenes, Alkynes, Cycloalkanes, Aromatic compounds.

References

1. C.N. Banwell, Fundamentals of Molecular spectroscopy, Tata McGraw Hill.
2. R.S. Drago, Physical Methods for Chemistry, Saunders Company.
3. Y.R. Sharma, "Elementary Organic Spectroscopy Principle and Applications", S. Chand and Company Ltd.,
4. J.R. Dyer, "Applications of Spectroscopy of Organic Compounds", Prentice Hall.
5. R. Chang, "Basic Principles of spectroscopy", McGraw Hills.

Scholar name:**N.Kavikala** Guide name**: S.Shankar**

Sub. Code: 18PHDPC1 **Ph.D. - Course work - Paper I** **Credit: 4**

PHYTOCHEMISTRY

Unit I

NATURAL PRODUCTS: Extraction- principles of extraction methods, types of extraction. Spot tests, colour reactions, chromatographic behaviour-Spectrometric identification of phenolics, plant acids sugar alcohols and nitrogen compounds. Chemical derivatization techniques like Acetylation ,Methylation ,Ethylation and Degradative techniques.

Unit II

GENERAL METHODS OF SCREENING NATURAL PRODUCTS:

General methods of screening natural products for the following biological activity.

i. Antioxidant activity
ii. Anti-inflammatory activity
iii. Anti microbial activity
iv. Anti Obesity
v. Hypo glycemic activity
vi. Cardiac activity

Unit III

PHENOLIC COMPOUNDS AND TERPENOIDS: Methods of separation, isolatio identification and classification of –phenolic- phenyl propanoids, Anthocyanins, Flavonoids chemical conversion of these compounds. Introduction- definition – classification- Nomenclature –source-importance-structural elucidation of citral, menthol, Geraniol and zingiberene- and isoprene rule.

Unit IV

ALKALOIDS: Introduction- definition-classification- Nomenclature-source-imporatnce-structural elucidation of quinine ,morphine and coniine.

FLAVONOIDS: Detailed chemical account of rutinn and quercetin.

STEROIDS: Introduction –definition- classification – Nomenclature- source Importance –structural elucidation of cholestrol, progesterone-structure and function of amino acids and protein

Unit V

GAS CHROMATOGRAPHY: Instrumentation-Packed and open tabular column, column efficiency parameters, the van Demeter equation , resolution liquid stationary phases, Derivatization methods of GC including acylation, perfluoroacylation, alkylation and esterificationn.

LIQUID CHROMATOGRAPHY: Comparison of GC and HPLC Instrumentation in HPLC, analytical, analytical preparative and microborecolums, normal and reserved phse packaging materials. Reverse phase HPCL, detectors in HPLC. Comparision of sensitivity and selectivity and application of detectors.

References:

1. Introduction to Chromatography Theory and Practice, V.K.Srivastava and KK Srivastava, S.Chand and Company Ltd., New Delhi,1987.
2. Analytical Chemistry, R.Gobalan, S.Chand and Company Ltd., New Delhi,1987.
3. Chemistry of Natural Products ,O.P Agarwal, Vol.Goel Publishing House ,1997
4. Natural Products Isolation , Richard JP Cannell Vol IV- Humana Press,Jan 1998.
5. Phytochemical Methods , JB Harborne Vol 37 Springer-Verlag, Sep 1985
6. Natural Products, Raphaellkan, A laboratory Guide , Jerusalem, Israel University Press.

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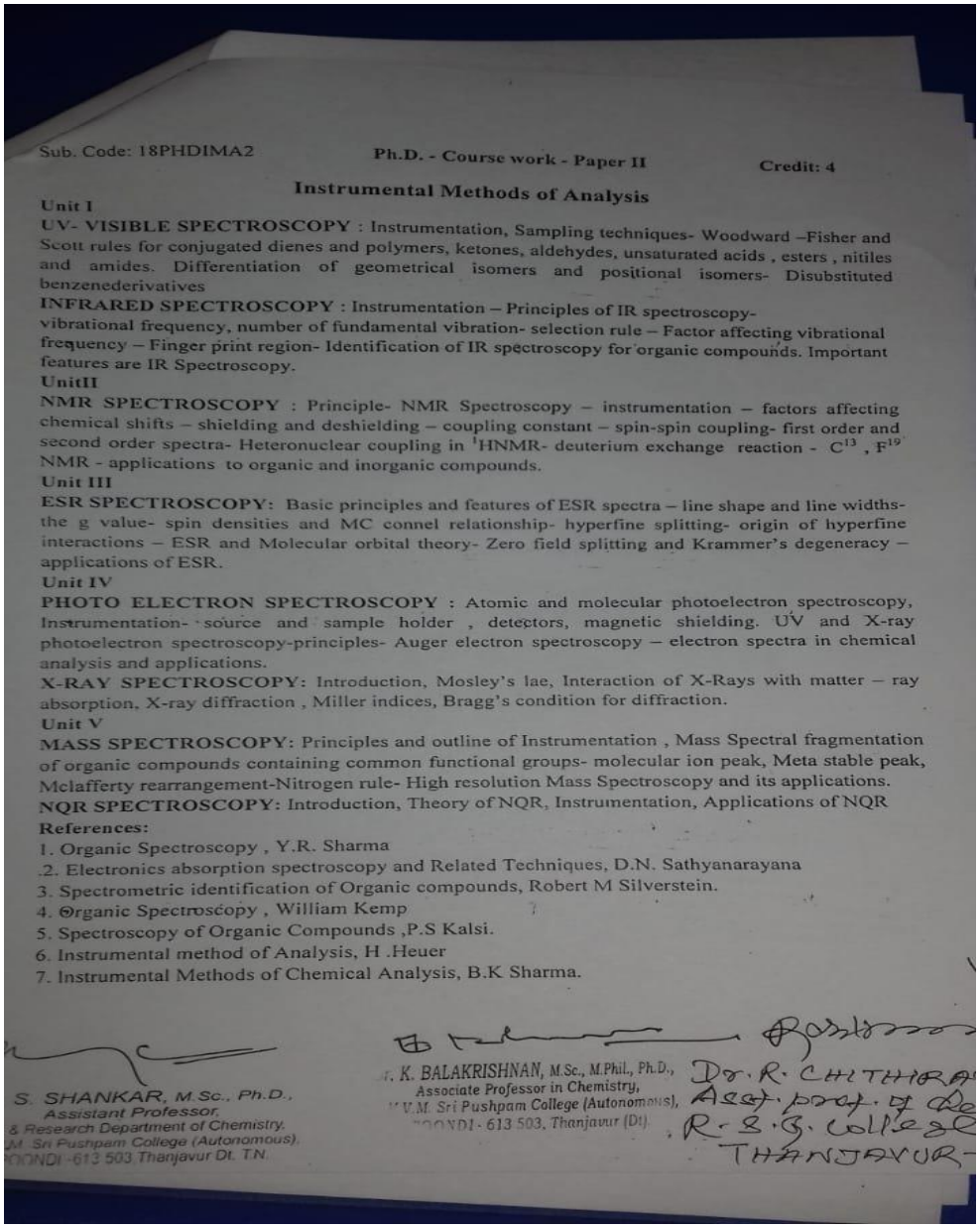

Sub. Code: 18PHDIMA2 **Ph.D. - Course work - Paper II** **Credit: 4**

Instrumental Methods of Analysis

Unit I

UV- VISIBLE SPECTROSCOPY : Instrumentation, Sampling techniques- Woodward –Fisher and Scott rules for conjugated dienes and polymers, ketones, aldehydes, unsaturated acids , esters , nitiles and amides. Differentiation of geometrical isomers and positional isomers- Disubstituted benzenederivatives

INFRARED SPECTROSCOPY : Instrumentation – Principles of IR spectroscopy- vibrational frequency, number of fundamental vibration- selection rule – Factor affecting vibrational frequency – Finger print region- Identification of IR spectroscopy for organic compounds. Important features are IR Spectroscopy.

UnitII

NMR SPECTROSCOPY : Principle- NMR Spectroscopy – instrumentation – factors affecting chemical shifts – shielding and deshielding – coupling constant – spin-spin coupling- first order and second order spectra- Heteronuclear coupling in ^{1}HNMR- deuterium exchange reaction - C^{13} , F^{19} NMR - applications to organic and inorganic compounds.

Unit III

ESR SPECTROSCOPY: Basic principles and features of ESR spectra – line shape and line widths- the g value- spin densities and MC connel relationship- hyperfine splitting- origin of hyperfine interactions – ESR and Molecular orbital theory- Zero field splitting and Krammer's degeneracy – applications of ESR.

Unit IV

PHOTO ELECTRON SPECTROSCOPY : Atomic and molecular photoelectron spectroscopy, Instrumentation- source and sample holder , detectors, magnetic shielding. UV and X-ray photoelectron spectroscopy-principles- Auger electron spectroscopy – electron spectra in chemical analysis and applications.

X-RAY SPECTROSCOPY: Introduction, Mosley's lae, Interaction of X-Rays with matter – ray absorption, X-ray diffraction , Miller indices, Bragg's condition for diffraction.

Unit V

MASS SPECTROSCOPY: Principles and outline of Instrumentation , Mass Spectral fragmentation of organic compounds containing common functional groups- molecular ion peak, Meta stable peak, Mclafferty rearrangement-Nitrogen rule- High resolution Mass Spectroscopy and its applications.

NQR SPECTROSCOPY: Introduction, Theory of NQR, Instrumentation, Applications of NQR

References:

1. Organic Spectroscopy , Y.R. Sharma
.2. Electronics absorption spectroscopy and Related Techniques, D.N. Sathyanarayana
3. Spectrometric identification of Organic compounds, Robert M Silverstein.
4. Organic Spectroscopy , William Kemp
5. Spectroscopy of Organic Compounds ,P.S Kalsi.
6. Instrumental method of Analysis, H .Heuer
7. Instrumental Methods of Chemical Analysis, B.K Sharma.

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Ph.D., - COURSE WORK – PAPER –I

ELECTRO ORGANIC CHEMISTRY

Department of chemistry

Scholar name:**G.Malathi** Guide name**: C.Thillaiyadivalliyammai**

Sub. Code : 19PHDCH1 **Credit : 4**

UNIT I

Basic concepts of electro organic synthesis

Introduction – Fundamental aspects of electro transfer reaction: Oxidation, reduction reaction vs electron transfer reaction in organic chemistry and electrochemistry – standard potentials; Mechanism and theory of outer sphere electron transfer reaction – Fundamental aspects of electrode phenomena, monitoring a half – reaction general view of an electrode reaction, adsorption phenomena - Mass transfer in electro chemistry, fundamental aspects, steady state electro chemical methods, transient chemical methods

UNIT II

Electro Kinetic Phenomena:

Theories of electrical double layer – Theory of multiple layers at electrode electrolyte interface - electro kinetic phenomena processes at electrodes – the rate of charge transfer – current density – Bulter – Volmer equation – taft equation, Electro chemical corrosion – construction and use of Pourbaix and evans diagram – prevents of corrosion – electro chemical oxidation and reduction

UNIT III

Anodic oxidation of organic compounds:

Introduction, general mechanistic consideration, direct anodic oxidation, indirect anodic oxidation, Anodic oxidation of hydrocarbons, nitrogen containing compounds.

Electro synthesis of Bioactive materials: Introduction, simple Kolbe oxidation : application to synthesis of (+) α onxerin and (+) – penta Cyclosqalene, Kolbe cyclization and Tandem cyclization.

UNIT IV

Cathodic reductions:

Introduction, formation of radical anions,dianions and polyanions, experimental aspects, thermodynamics kinetics, addittion of electrophillic reagents and

related reaction dimerization, Electrical reduction of halogenated compounds, mono halogenated alkanes, halogenated aromatic compounds, cathodic reduction of nitro and related compounds. Electro chemical reduction of carbonyl compounds, general aspects.

UNIT V

Special topic in electro organic synthesis:

Paired electro organic synthesis, simple examples, General aspects of indirect electron exchange, pure redox catalysis (general use) – of indirect electro chemical reaction in synthesis, oxidation, reduction reactions – Electro generated superoxides. Electro chemical partial flurination of aromatic compounds, olefins, carbonyl compounds heterocylic compounds.

REFERENCES

1. Organic electro chemistry by Henning Lund & Ole Hammerich , 4th edition, Marcel Dekker, inc, New York.
2. Electrolytic synthesis and reactions of organometallic compounds by William J. Settineri and L. Dennis Mc Keever.
3. Technique of Electro organic synthesis Edited by Norman L. Weinberg A. wiley-Interscience Publications John wiley & sons.
4. March J, Advanced Organic chemistry, Fourth Edition, John – Wiley and sons, New York
5. Gould E S, Mechanism and structure in Organic chemistry, Holt – Reinhart and Winston, New York (1959)

Ph.D., - COURSE WORK – PAPER –II

INSTRUMENTAL METHODS OF CHEMICAL ANALYSIS

Scholar name:**G.Malathi** Guide name**: C.Thillaiyadivalliyammai**

Sub. Code : 19PHDCH1 **Credit : 4**

UNIT I

UV – Visible and IR Spectroscopy:

Introduction – Instrumentation, Sampling techniques Differentitation of geometrical isomers and positional isomers – bisubstituted derivatives.

Infrared Spectroscopy: Introduction - Instrumentation Sampling techniques, factors influencing group frequencies – Both internal and external – quantitative studies. Hydrogen bonding – (intermolecular and intramolecular)

UNIT II

NMR Spectroscopy:

^{1}H NMR Spectroscopy – Multiplicity- Coupling constant – First order and second order proton, Spin – Spin spilitting – Dependence of J on dihedral angle – vicinal and geminal coupling constants – karplus equation. C^{13} NMR Spectroscopy – Basic theory of FT – NMR, Relaxation broad band decoupling, Off resonance decoupling and chemical shifts of common functional groups,2D techniques : ^{1}H - ^{1}H COSY, ^{1}H - C^{13} COSY –HMBC and NOESY.

UNIT III

Chromatography:

Solvent extraction - Principles of ion exchange, paper, thin layer and column chromatography, gas chromatographyntechniques – columns, adsorbents,methods,R values, Mc Reynold's constants and their uses –HPTLC, HPLC techniques – absobents, column,detection methods,stimations, preparative column – GC – MS techniques - methods, principles and uses.

UNIT IV

Electro analytical metods:

Introduction, liners sweep voltametry and cyclic voltametry , Experimental setup, simple electro transfer reaction, electro transfer reaction followed by chemical reaction

and solution,limiting experimental factors – potential step and current setp method, chronoamperometry, chronocoulometry, chrono potentiometry – polarography – methods for determine of number of electrons.

UNIT V

Nano Chemistry:

Introduction – discovery of CNT, preparation of CNT, preparation of nano materials by micro wave synthesis – sol –gel method – chemical co- operation – hydrothermal and solvothermal methods. Preparation and uses of TiO_2 and ZnO. Implications of nano science and nano technology on society. Nano shells and their applications.

REFERENCES

1. C.N. Banwell, Fundamentals of molecular spectroscopy, 3rd ed., TMH, New Delhi, 1983.
2. P.M. Silverstein, F.X. Wester, Spectroscopic Identificationb of Organic Compouinds, 6th ed.,Wiley 1998.
3. Y.R. Sharma, Elementary Organic Spectroscopy – Principles and Chemical applications. S. Chand 1992.,
4. A. K. Srivastava and P.C. Jain, Instrumental approach to chemical analysis, S. chand company ltd. Fourth revised edition – 2009.
5. Grudeep. R. Chatwal, Sham. K Anand Instrumentals methods of chemical analysis, Himalaya publishing house pvt ltd., Mumbai reprint 2008.
6. Principles of Nanoscience and Nanotechnology, M.A. Shah and Tokeer Ahamed (Unit - I)
7. T. Pradeep, Nano The Essentials in Understanding Nanoscience and Nanotechnology, Tata McGraw Hill, New Delhi 2007 (Unit I & Unit II)

Name of the Student: **G. Suganya**
Name of the Research Advisor: **Dr.V. Nandhakumar**

Ph. D - Course work - Paper I

Sub code: 20PHDCH1 **Credit: 4**

Nanotechnologyand Its Applications

Unit –I – Green Chemistry

Principles and concepts of green chemistry-photochemicaldegradation-oxidation and reduction process –eco friendly approach of waste treatments-photochemical principles – homo and heterogeneous –photo catalysis-applications

Unit - II – Nanomaterials

Nanomaterials – characteristic of nanomaterials – effect of surface area to volume ratio on the properties of nanomaterials – application of nanomaterials – various nanostructures – nanomaterials – nanoparticles – nanowire – nanocomposite –nanoclusters and quantum dots.

Unit – III – carbon nanotubes (CNT)

Introduction to CNT – SWNT – MWNT – Synthesis of carbon nanotubes: plasma are – discharge method – laser – ablation technique – chemical vapour deposition – growth mechanism – properties – CNT based nano objects – gaseous carbon source based production techniques for CNT – Application.

Unit – IV –Nanomaterials fabrication methods

Top – down techniques: ball milling – combustion synthesis – nanolithography – bottom up techniques: self assembly – hydrothermal method – sol-gel synthesis – gas condensation – co-precipitation method – polyol process – sonochemical process.

Unit – V – Nanomaterials application

Photocatalysis – type of photocatalysis: homogeneous photocatalysis – heterogeneous photocatalysis – application of photocatalysis – semiconductor photocatalytic materials- TiO2 ,ZnO , SnCl2- semiconductor

/ grapheme derivative nanocomposite as visible light responsive photocatalysts – photoreactor experiment – various types of photoreactor – Adsorption – super capacitor – sensors application – antimicrobial activity.

References:

1. Green chemistry by M.M.SRIVASTA and RASHMI SANGHI
2. Green Chemistry – Designing Chemistry for the Environment – edited by
   Paul T. Anastas& Tracy C. Williamson. Second Edition, (1998).
3. C.P. Poole, Jr: F.J. Owens, Introduction to Nanotechnology Wiley Interscience, New Jersey, 2003
4. C.N.R. Rao, A. Muller, A.K. Cheetam (Eds), The Chemistry of Nanomaterials, Vol.1, 2, Wiley – VCH, Weinheim, 2004.

Name of the Student: **G. Suganya**
Name of the Research Advisor: **Dr.V. Nandhakumar**

Ph. D - Course work - Paper II

Sub code: 20PHDCH2 **Credit: 4**

INSTRUMENTALMETHODS

Unit – I - UV-Visible Spectroscopy

Introduction - Instrumentation, Sampling techniques - Woodward–Fieser and Scott rules for conjucated dienes and polymers, ketones, aldehydes, ∝,β-unsaturated acids, esters, nitriles, and amides. Differentiation of geometrical isomers and positional isomers – Disubstituted benzene derivatives - Study of steric effect in aromaticity.

Unit –II- Infrared Spectroscopy

Introduction - Instrumentation, Sampling techniques, factors influencing group frequencies –.Hydrogen bonding – intermolecular and intramolecular -important functional group region – FT-IR spectroscopy.

Unit – III- X-ray diffraction

X-ray diffraction by single crystal – Space groups –Systematic absences in X-ray data and identification of lattice types , glide planes and screw axes.X-ray intensities, structure factor and its relation to intensity and electron density , phase problem. Structure solution by Heavy atom method and direct method. Determination of absolute configuration of molecules. A brief account of Cambridge Structural Database (CSD) and Protein Data Bank (PDB).

Unit – IV- Thermal Analytical methods and others

Photoluminescence, particle size analyses, fluorescence spectroscopy. AAS – instrumentation, principle and applications.TGA – principles and application. DTA – principle and applications.

Unit – V- Instruments for morphological Analysis

Scanning Tunneling Microscopy (SEM) - Transmission electron microscopy (TEM)- Atomic force microscopy (AFM)- and scanning transition electron microscopy (STEM) - principles and applications. Scanning ion conductance microscope, scanning thermal microscope, scanning probe microscopes and surface Plasmon spectroscopy.

References:

1. Elementary Organic Spectroscopy by Y.R. SHARMA.
2. W.Kemp, Organic Spectroscopy, 3rd Ed., MacMillon, 1994
3. Jag Mohan, Organic Spectroscopy – Principles and Application, 2nd edn., Narosa publication.
4. Elements of Analytical Chemistry by R. GOPALAN, P.S SUBRAMANIAN & K.RENGARAJAN.
5. Hand book of Nanotechnology- Bharat Bhushan, Springer 3rd ed. 2010.

Student Name: B. CERIL JEOFFREY Guide: Dr. S Jothi Ramalingam

Sub. Code: 20PHDCH1 **Ph.D. - Course work - Paper I** Credit: 4

Graphene and Carbon materials

UNIT I

Graphene: Introduction of graphene, Graphite, Definition and structure of graphene. Types of graphene: stacking AA, BB, AB dispersion relation, Single layer, Bi-layer, Few layer, Properties of graphene; Optical: thickness dependency, optical conductivity, electric filed tunable transparency, plasmons and polaritons, carrier multiplication. Electrical: Boltzmann equation, ambipolar conduction, density of states and doping (electrostatic and chemical), quantum hall effect, Klein tunneling, diamagnetism, magnetoresistance and spin current, thermal conductivity. Mechanical, Surface phenomenon.

UNIT II

Preparation of Graphene: Epitaxial growth of graphene on Silicon carbide, Chemical deposition (CVD) growth of graphene films, Chemically drived graphene, Synthesis of graphene oxide: Hummer's method, Modified Hummer's method, Reduction of graphene oxide. Chemical methods, Physical methods, Electrochemical exfoliation, Nanotube slicing, from solid state carbon sources.

Characterization of Graphene: Transmission electron microscopy (TEM), Scanning tunneling microscopy (STM), Raman Spectroscopy, Electrical measurements: electric field effect, temperature dependent resistivity measurement.

UNIT III

Graphene in the energy application: Li-ion batteries, Supercapacitors, Photovoltaic, Radio-frequency transistor, Photodetector, Modulator, Mode locked lasers, Other applications of graphene: Anti-corroison coating, Anti-bacterial coating, catalyst, Sensors, Transparent Conductors

UNIT IV

Carbon Nanotubes I : Introduction of Carbon Nanotube (CNT): Introduction and definition of CNT, Bonding of carbon atoms, sp3, sp2, Deformed sp2 , Structure of Carbon Natotubes, Chiral Vector, Armchair, Zig-Zag and Chiral tubes, Properties of Carbon Nanotubes: Electronic, Optical and Optoelectronic, Mechanical, Chemical and Electrochemical. Opening, wetting and filling, doping, intercalation, Thermal and Thermoelectric.

UNIT V

Carbon Nanotubes II: Synthesis Methods and Growth Mechanisms: High temperature method, Arc discharge, General technical features of the production process, Growth Mechanism, Laser Ablation of Graphite, Low temperature method, Chemical Vapor deposition (CVD) process, Vapor liquid solid model, Catalytic role. Purification and functionalization: Methods of Purification, Methods of Functionalization (Chemical and Physical), Advantage of purification and functionalization, Separation of cnts: based on chirality, semiconducting, metallic, Applications of Carbon nanotube, Field emission, Li-ion battery, Supercapacitor, Sensors, Solar cell , CNT-polymer composite and avionics EM shielding

References :

1) Graphene: Carbon in Two Dimensions, by Mikhail I. Katsnelson
2) Physics of Graphene, Editors: Aoki, Hideo, S. Dresselhaus, Mildred (Eds.)
3) Graphene: Synthesis, Properties, and Phenomena, by C. N. R. Rao (Editor), Ajay K. Sood (Editor),
4) Graphene Nanoelectronics, Metrology, Synthesis, Properties and Applications, Editors: Raza, Hassan (Ed.)
5) Graphene Nanoelectronics: From Materials to Circuits, Editors: Murali, Raghu (Ed.)
6) Carbon Nanotube and Graphene Device Physics, by H.-S. Philip Wong (Author), Deji Akinwande (Author)
7) Carbon Nanotube Electronics (Integrated Circuits and Systems) by Ali Javey (Editor), Jing Kong (Editor),
8) Polymer-Graphene Nanocomposites, Editor(s): Vikas Mittal
9) Physics and Chemistry of Graphene: Graphene to Nanographene, Toshiaki Enoki, Tsuneya Ando.

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Student Name: A. CERIL JEOFFREY Guide: Dr. S Jothi Ramalingam

Code: 20PHDCH2 **Ph.D. - Course work - Paper II** **Credit: 4**

ANALYTICAL TECHNIQUES

UNIT : I

SPECTROSCOPY

Principles and instrumentation for UV-Vis-IR, FTIR spectroscopy, Raman spectroscopy, ESR, NMR, NQR, ESCA and SIMS- proton induced X-ray Emission spectroscopy (PIXE) – application – mass spectroscopy

UNIT : II

MICROSCOPIC METHODS

Optical Microscopy: optical microscopy techniques – Bright field – Dark field optical microscopy – phase contrast microscopy -differential interference contrast microscopy - fluorescence microscopy - confocal microscopy - Metallurgical microscope.

UNIT : III

ELECTRON MICROSCOPY AND SCANNING PROBE MICROSCOPY

SEM- FESEM- EDAX,- HRTEM: working principle and Instrumentation – sample preparation – scanning probe microscopy - STM – AFM - working principle, Instrumentation and modes of operation.

UNIT : IV

ELECTRICAL AND OPTICAL METHODS OFCHARACTERISATION

Two probe and four probe methods- van der Pauw method – Hall probe and measurement – scattering mechanism – C-V, I-V characteristics – Schottky barrier capacitance – impurity concentration – electrochemical C-V profiling – limitations - Photoluminescence – light – matter interaction – instrumentation – electroluminescence – instrumentation – Applications.

UNIT : V

. THERMAL ANALYSIS

Introduction – thermogravimetric analysis (TGA) – instrumentation – determination of weight loss and decomposition products – differential thermal analysis (DTA)- cooling curves - differential scanning calorimetry (DSC) – instrumentation – specific heat capacity measurements – determination of thermomechanical parameters .

REFERENCES:

1. R.A.Stradling and P.C.Klipstain. Growth and Characterization of semiconductors. Adam Hilger, Bristol, 1990.
2. J.A.Belk. Electron Microscopy and Microanalysis of Crystalline Materials. Applied Science Publishers, London, 1979.
3. L. E.Murr. Electron and Ion microscopy and Microanalysis principles and Applications. Marcel Dekker Inc., New York, 1991.
4. D.Kealey & P.J.Haines, Analytical Chemistry, Viva Books Private Limited, New Delhi, 2002.
5. Banwell, Fundamentals of Molecular Spectroscopy, McGraw-Hill Education, Pvt. Ltd., 2013.

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Scholar name:**P.Monisha** Guide name**: M.Pramesh**

Ph.D Course work

Sub code: 19PHDCH1 Synthetic organic chemistryCredit: 4

UNIT-I: Heterocyclic compounds

Synthesis and reactivity of the following heterocyclic compounds and their derivatives- pyrazole, oxazole, imadazol, thiazole, pyridazine and pyrazine,pyrrole, pyridine,furan, Quinoline, isoquinoline and indole.

UNIT-II: Reagents in organic synthesis

$LiAlH_4$,$NaBH_4$, tri- tertiarybutoxyaluminium hydride, $NaCNBH_3$ and tri n-butyl tin hydride, Wilkinson catalyst, Lithium dimethyl cuprate, lithium di-isopropylamide, DCC, 1,3-dithane,trimethyl silyl iodide, DDQ, SeO_2, OsO_4 ,$KMnO_4$ HIO_4 Lead tetra acetate, H_2O_2,Pyridinium Chlorochromate (PCC) ,Peracids, Phenyl Selenium Chloride (PhSeCl),phase transfer catalysis, crown ethers.

UNIT-III: Organic name reactions

Stork enamine reaction,Michael addition, mannichreaction,nef reaction, sharpless asymmetric epoxidation, barton reaction, Hoffman-loffler-freytag reaction, bombard-stevens reaction, Shapiro reaction, reformatsky, reimer-tiemann.gattermann,gattermann coach, vilsmeir hack reaction, stobbe,dieckmann,aldol and darzen's, condensation.

UNIT-IV:Molecular Rearrangements

Mechanism and applications of Bayer villager, favorski, stevens, neber,dienone-phenone, Beckman, fries, claisen, cope, demyanov rearrangements.

UNIT-V: Stereochemistry

Optical activity and criteria for chirality – Enantiotopic, diastereotopic and Prochiral centres- threo and erythro configurations-Fischer, newman and sawhorse projection formulae and inter conversions - RS notataion – Atropisomerism – Geometrical isomerism - EZ notations. Stereo selective, stereo specific and diastereoselective reactions.

References

1. J. March, Advanced Organic Chemistry: Reactions, Mechanisms and structure, 5thed. Wiley, 2000
2. Clayden, Greeves,. Warren and Wothers, Organic chemistry, 2nded. Oxford University press.
3. Francis A. Carey and Richard J. Sundberg, Advanced organic chemistry part A: Structure and Mechanisms.5thed.springer
4. Francis A. Carey and Richard J. Sundberg, Advanced organic chemistry part B. 5thed.springer
5. Peter Sykes, A Guide book to Mechanism in organic chemistry, 6theditionLongman, 1986
6. P.S.Kalsi, Stereochemistry Conformation and mechanism, 5th edition New Age international
7. V.K.Ahluwalia and R.K.Parashar, Organic reaction mechanisms.3rd edition, Alpha Science Int'l Ltd
8. S.M.Mukherji and S.P.Singh, Reaction mechanism in organic chemistry.3rd edition Macmillan India Limited.
9. I.L. Finar, Organic Chemistry, Vol.II, 5th ed., ELBS 1975.

Scholar name:**P.Monisha** Guide name**: M.Pramesh**

Ph.D Course work

Sub code: 19PHDCH2Credit: 4

Applications of spectroscopy in synthetic organic chemistry

Unit I: Nuclear magnetic resonance spectroscopy

^{1}H NMR Spectroscopy –solvents-reference-chemical shift, Multiplicity – Coupling constant — Vicinal and geminal coupling constants – Influence of stereochemical factors on chemical shift of protons. An elementary treatment of NOE phenomenon. **^{13}CNMR Spectroscopy** – Basic theory of FT – NMR, Relaxation – Broad band decoupling. Off resonance decoupling and chemical shifts of common functional groups.

Unit II: UV-Visible Spectroscopy

Introduction –principle-Sampling techniques - Woodward–Fieser and Scott rules for conjucated dienes and polymers, ketones, aldehydes, α,β-unsaturated acids, esters,nitriles, and amides. Differentiation of geometrical isomers and positional isomers – Disubstituted benzene derivatives - Study of steric effect in aromaticity.

Unit III: Infrared Spectroscopy

Introduction - Instrumentation, Sampling techniques, factors influencing group frequencies –. Hydrogen bonding – intermolecular and intramolecular -important functional group region.

Unit IV: Mass Spectrometry

Principle, EI and CI methods – Base peak, isotopic peaks, metastable peak, parent peak, determination and use of molecular formula, recognition of molecular ion peak – Fragmentation – General rules – Pattern of fragmentation for various classes of compounds, McLafferty rearrangement, Importance of metastable peaks.

Unit V: Chromatography

Principles of thin layer and column Chromatography techniques – Columns, adsorbents, methods, Rf values and their uses –HPLC techniques – Adsorbents, columns, preparative column – GC-MS techniques: methods, principles and applications.

References

1. R.M. Silverstein,G.C.Bassler F. X. Webster, Spectroscopic Identification of Organic Compounds, 6th ed.,Wiley 1998.
2. W. Kemp, Organic Spectroscopy, 3rd Ed., MacMillon, 1994.
3. J.R. Dyer, Applications of Absorption Spectroscopy of Organic Compounds, Prentice Hall, 1965.
4. Y.R. Sharma, Elementary Organic Spectroscopy – Principles and Chemical applications,S.Chand, 1992.
5. P.S.Kalsi, Spectroscopy of Organic Compounds, Wiley eastern limited.
6. Jag Mohan, Organic spectroscopy, Principles and applications, 2ndedn., Narosa publication.

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Sub code:19PHDCH3 **Credit:4**

RESEARCH METHODOLOGY

UNIT- I Literature survey

1. Source of information –primary, secondary, Tertiary source -Journals-abstracts-current titles-Review Monographs-Dictionaries-information retrievals using Internet and other electronic medias (preparing a review article related to problem of research of the student).

2. E-Journals, search engines-Google, Yahoo search, Wikipedia.

3. Reports of research work-laboratory observation- preparation of records-Manuscripts-Research paper formats in Indian J. chemistry., J. Indian chem. Soc., J. Am. Chem. Soc., Tetrahedron. Ana., chem. Education, Etc., writing of the project reports of thesis.

UNIT-II Error Analysis

Types of Error- Minimization of error-Accuracy, precision, significant figures, use of calculus in the estimation of errors- Frequency distributions, the binominal distribution and normal distribution- mean, and standard deviation varcence Q-test, t-test- chi-square test- F-test- Analysis of variance(ANOVA)-s correlation and Regression- curve fitting.

UNIT-III Digital

Web resources, E-Journals, journal access, TOC alerts. Hot articles: Citation index, UGC infonet, E-books, search engines- Google scholar, chemical industry, Wiki-databases, chemspider, ScienceDirect, SciFinder, Scopus, Field studies, planning of research- The planning process- selection of a problem for research, formulation of the selected problems, hypothesis formation, measurement, research design/plan.

UNIT-IV Research Problem

Identification, statement of research problems, objectives, design and execution of experiments, collection and interpretation of experimental data, arriving at conclusions, reporting the results of research- style and format, title, abstract and the text, references, tables, figures, elucidations, quotations and footnote. Writing of monographs, review articles and dissertations.

UNIT-V Basic knowledge of computer system

Software's -system software and application software, programming languages-machine language, assembly language and high-level languages. Interpreter and compiler, flow charts and algorithms, general awareness of software packages and other scientific applications. Application and uses of common softwares in chemistry-origin, chemsketch, chemdraw, basic ideas on the use of internet in chemistry education.

REFERENCES:-

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3.http://www.springerlink.com

4.http://www.rsc.org

5.http://www.pubs.acs.org

6.http:/dspace.bdu.ac.in

7.D.B. Hibbert and J.J. Gooding, Data analysis for chemistry, Oxford University press,2006.

8.J. Topping, Errors of Observation and their Treatment, Fourth Edition, chapman Hall, London,1984.

9.H.E. Solbers, Inaccracies in computer calculation of standard Deviation, Anal. Chem.55, 1611(1983).

10.Kothari, C.R., 1990.Research methodology: Methods and techniques, New age International.,

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12. Ramesh Kumar, computers and their applications to chemistry, 2nd edition., Alpha Sci.