H.H. THE RAJAH'S COLLEGE

(AUTONOMOUS)

PUDUKKOTTAI - 622 001

PG & RESEARCH DEPARTMENT OF CHEMISTRY

M.Sc., CHEMISTRY COURSE

STRUCTURE UNDER CBCS

FOR THE STUDENTS ADMITTED FROM THE ACADEMIC YEAR2021 – 2022 ONWARDS

M.Sc., CHEMISTRY - SYLLABUS

2021-2022

THE VISION AND MISSION OF THE DEPARTMENT

VISION
We provide society with people serving, skilled and problem solving professionals in chemical sciences

MISSION
Provide our society with high quality professionals having a strong education and technical skills in chemistry; with rich cultural, ethical, environmental, and social sensitivities; capacity for critical thinking; and the entrepreneurial skills to solve industrial and environmental problems

PROGRAM SPECIFIC OUTCOMES for **M. Sc. Chemistry** program	
After Successful completion of the Degree, students can	
PSO1	Get solid foundation in different fields of chemistry which are required to solve chemical, technical and environmental problems.
PSO2	Develop the skills to select, design and apply appropriate techniques, resources and tools to complex research activities with an understanding of the limitations.
PSO3	Comprehend and write effective reports and documentation, make effective presentations.
PSO4	Communicate effectively on complex activities with the scientific community and with society.
PSO5	preparation and ability to engage in independent and life-long learning in the context of scientific and technological change.

PROGRAM OUTCOMES for **M. Sc. Chemistry** program	
After Successful completion of the Degree	
PO1	Students acquire the advanced knowledge in different branches of chemistry and understand all the theories, essential facts, core concepts, principles and postulates relating to the chemistry.
PO2	Students can identify, formulate, analyse and solve complex problems using the basic principles of chemistry.
PO3	Students understand the role of chemistry in day to day life
PO4	Students can apply the knowledge and ability to synthesize, separate and characterize compounds using laboratory and instrumentation techniques.
PO5	Equipping students to develop analytical and problem skills to articulate the scientific and technical information to enterinto industries, higher research program and the job market.
PO6	Creating awareness of the impact of chemistry on the environment, society and to contribute present and future perspectives of scientific community
PO7	Acquire the knowledge towards the role of chemistry in industries and to create passion to become entrepreneur.

COURSE STRUCTURE

COURSES	NO. OF PAPERS	CREDIT
CORE COURSES	14	70
ELECTIVE COURSES	3	15
EDC	1	05
TOTAL	18	90

SEMESTER-WISE DISTRIBUTION OF COURSES AND CREDITS

PART	CODE	COURSE	TITLE	HRS	MARKS		TOTAL	CREDIT
					Int.	Ext.		
I SEMESTER								
III	21PCH1	CC-I	Organic Chemistry-I	6	25	75	100	5
III	21PCH2	CC-II	Inorganic Chemistry-I	6	25	75	100	5
III	21PCH3P	CP-III	Inorganic Practical-I*	6				
III	21PCH4P	CP-IV	Organic Practical-I*	6				
III	21PCHE1 A/B/C	EC-I	Photochemistry and Pericyclic Reaction (OR) Chemistry of Macromolecules (OR) Advanced Pharmaceutical Chemistry	6	25	75	100	5
			Total	30			300	15
II SEMESTER								
III	21PCH5	CC-V	Physical Chemistry-I	6	25	75	100	5
III	21PCH6	CC-VI	Inorganic chemistry-II	6	25	75	100	5
III	21PCH3P	CP-III	Inorganic Practical-I	6	40	60	100	5
III	21PCH4P	CP-IV	Organic Practical-I	6	40	60	100	5
III	21PCHE2 A/B/C	EC-II	Nanomaterials and Green Chemistry (OR) Drug design and discovery (OR) Sensors and Transducers	3	25	75	100	5
III	21PCHEDI	EDC-I	Supramolecular Chemistry	3	25	75	100	5
			Total	30			600	30

PART	CODE	COURSE	TITLE	HRS	MARKS		TOTAL	CREDIT
					Int.	Ext.		
III SEMESTER								
III	21PCH7	CC-VII	Organic Chemistry-II	6	25	75	100	5
III	21PCH8	CC-VIII	Physical Chemistry-II	6	25	75	100	5
III	21PCH9	CC-IX	Inorganic Chemistry-III – Bioinorganic Chemistry	6	25	75	100	5
III	21PCH13P	CP-XIII	Physical chemistry practical-I*	6				
III	21PCHE3 A/B/C	EC-III	Physical methods in chemistry (OR) Food chemistry and Adulteration (OR) Catalysis and Catalytic Processes	6	25	75	100	5
			Total	30			400	20
IV SEMESTER								
III	21PCH10	CC-X	Organic chemistry-III	6	25	75	100	5
III	21PCH11	CC-XI	Physical chemistry-III	6	25	75	100	5
III	21PCH12	CC-XII	Organic Spectroscopy	6	25	75	100	5
III	21PCH13P	CP-XIII	Physical chemistry practical-I	6	40	60	100	5
III	21PCH14	PW-I	Project work	6			100	5
			Total	30			500	25

Finalized (for the I to IV Semester) in the

BOARD OF STUDIES MEETING HELD ON ----------
&
APPROVED BY THE ACADEMIC COUNCIL ON _____

SEMESTER – I

CC - I: ORGANIC CHEMISTRY – I

SEMESTER: I **SUBJECT CODE: 21PCH1**

CREDITS: 5 **TOTAL HOURS: 6**

Objectives

1. *To understand the naming of aliphatic, aromatic, hetero aromatic and alicyclic systems.*
2. *To know the generation, stability, structure and reactivity of free radicals, carbenes, nitrenes, carbanions, carbocations and arynes.*
3. *To describe the methods of determining reaction mechanism.*
4. *To understand correlation analysis.*
5. *To know concepts of chirality and Configurational nomenclature.*
6. *To understand and define the important terms in stereochemistry.*
7. *To describe the nomenclature and configuration of geometrical isomers.*
8. *To analyze the dynamic stereochemistry.*
9. *To know concepts of Aromaticity of Organic Cyclic compounds.*
10. *To Know the Preparation, Properties & Applications of the various heterocyclic compounds.*

UNIT I

Nomenclature and reaction intermediates

Naming of linear and branched alkenes, polyenes and alkynes without and with functional groups by IUPAC nomenclature. Aromatic and hetero aromatic systems – nomenclature of heterocycles having not more than two hetero atoms such as oxygen, nitrogen and sulphur. Nomenclature of alicyclic, bicyclic and tricyclic compounds.

Free radicals, carbenes, nitrenes, carbanions, carbocations and arynes – generation, stability, structure and reactivity.

Electronic effects: inductive effect, resonance effect, hyperconjugation (Baker-Nathan effect) - hydrogen bonding (inter and intra molecular).

UNIT II

Stereochemistry-I

Optical Isomerism: Concepts of chirality- Newman, Sawhorse and Fisher notations – representations and interconversions of compounds with two asymmetric centres. Configurational nomenclature – D and L notations – R-S notations of acyclic and cyclic compounds.

Asymmetric synthesis – Creation of chiral centre - Cram‘s rule and Prelog‘s rule. Concepts of prochirality, enantiotopic and diastereotopic groups Atropisomerism- Stereochemistry of allenes, spiranes and biphenyls. Catropisomerism–Stereochemistry of ansa compounds, cyclophanes and transcycloalkanes.

UNIT III

Stereochemistry-I

Geometrical isomerism: Cis-trans, E/Z and syn/anti nomenclature for C=C and C=N bonds. Determination of configuration of the geometrical isomers. Cis and trans nomenclature and configuration of mono and disubstituted cyclohexanes. Energy comparison and energy profile diagram of mono and disubstituted cyclohexanes. Geometrical isomerism in decalins. Dynamic stereochemistry - qualitative correlation between conformations and reactivity – Winstein - Eliel equation – Curtain - Hammett principle. Conformation analysis of cyclohexane - saponification of ester, esterification of an alcohol and chromic acid oxidation of cyclohexanols. Neighbouring group participation – deamination of 2-aminocyclohexanol– stereo specific and stereo selective reactions.

UNIT IV

Reaction mechanism and Correlation Analysis

Methods of determining reaction mechanism: Thermodynamic and kinetic aspects of organic reaction- energy profile diagrams – intermediates versus transition states, isotope effects - kinetic and non-kinetic method of determining reaction mechanism, product analysis and its importance – cross over experiments – isotopic labeling studies-stereo chemical studies – substituent effects.

Correlation analysis: linear free energy relationship s- Hammett equation – significance of sigma and Rho applications – Yukawo –Tsuno equation - Taft equation- Grunwald – Winstein equation and their applications.

UNIT V

Aromaticity and Heterocyclic compounds

Aromaticity: Huckel's theory of Aromaticity, concept of homoaromaticity and antiaromaticity Aromatic character in five, six, seven and eight membered rings – other systems with aromatic sextets – Huckel‘s rule – Craig‘s rule – NMR concept of aromaticity and antiaromaticity – systems with 2,4,8 and 10 electrons – systems with more than 10 electron (annulenes) , Mobius Aromaticity– Alternant and non - alternant hydrocarbons. Chemistry of cyclopentadienyl anion – Fullerenes, Azulene, Tropolones, Sydnones and Annulenes. Bonding properties of system with(4n+2) and 4n π electrons.

Heterocyclic compounds: Structure - synthesis and reactions of the following systems - indole - isoindole -quinoline - isoquinoline - oxazoles- carbazole - imidzole- thiozole- chromones - pyridines- pyrimidines, pyridazine,pyrazoles and pyrazines.

Course outcomes:

Student understood the knowledge about:

1. *Identify ,classify and draw structures of organic molecules*
2. *Apply the basic rules of organic nomenclature to interrelate between structures of organic molecules*

References:

1. Advanced Organic Chemistry, Part A & B, F.A.Carey and Sundberg, III Edn. PlenumPress, 1990.
2. Organic Chemistry, S.H.Pine, J.B. Hendrickson, D.J.Cram and G.S.Hammond, IV Edn. McGraw-Hill Company 1980.
3. Mechanism and Theory in Organic Chemistry – T.H. Lowry and K.S. Richardson, Harper and Row, NY 1976.
4. Organic Reactions and Mechanisms, P.S.Kalsi, II Edn. New Age International Publishers,2000.
5. Fundamentals of Organic Reaction Mechanisms- J.M.Harris and C.C. Wamser, JohnWiley & Sons, Inc. 1976.
6. R Panico, W H Powell, L Jean and C Ridcher, Agenda of nomenclature of organic compounds, 1993.
7. R S Cahn and O L Dermer, Introduction to chemical nomenclature, 5th Edition, Butterworth, 1979.
8. Jerry March, Advanced Organic Chemistry, 4th Edition, Wesley, 1999.
9. D.Nasipuri, Stereochemistry or organic compounds.
10. I L Finar, Organic Chemistry, Vol.I and II.
11. P S Kalsi, Stereochemistry conformation and mechanism.
12. P J Carratt, Aromaticity, McGraw Hill, 1971

CC - II: INORGANIC CHEMISTRY – I

SEMESTER: I **SUBJECT CODE: 21PCH2**

CREDITS: 5 **TOTAL HOURS: 6**

Objectives:

1. *Bonding, structure and reactivities of compounds formed by main group elements, and basic knowledge on acid and base concept.*
2. *Basic concepts describing structure of solids and properties of solids.*
3. *Basis of nuclear chemistry and types of nuclear reactions*
4. *Basic concepts of bonding and catalysis in organometallic chemistry*

UNIT-I

Main Group Chemistry - I

VSEPR- dπ-pπ bonding, Bent‘s rule; Theories of acid and base. The HSAB concept. Theoretical basis of hardness and softness. Structure and bonding of boranes - diborane and higher boranes, borazines, S-N compounds, phosphazenes and cyclic phosphazene, silicates and silicones; Interhalogen and Noble gas compounds - Hybridisation, Geometry and properties.

UNIT-III

Inorganic Solids

Lattice, unit cell, crystal systems and Bravais lattices-Miller indices and labelling of planes – symmetry properties –c rystallographic point groups and space groups –fundamentals of X-ray diffraction - Laue equation and Brag‟s law - powder and single crystal X-ray diffraction-Debye - Scherrer formula - systematic absences, electron and neutron diffraction. Ionic bonds - lattice energy of ionic crystals - Born-Haber cycle - Born lande equation - Madelung constant – Structures – cesium chloride – wurtzite – zinc blende – rutile – fluorite..

UNIT-IV

Nuclear Chemistry - I

Nuclear properties: Nuclear spin and moments, origin of nuclear forces, salient features of the liquid drop and the shell models of the nucleus. Models of Radioactive Decay: Orbital electron capture: nuclear isomerism, internal conversion, GM and Scintillation counters. Nuclear Reactions: Types, reactions, cross section, Q-value, nuclear fission and fusion reactions as energy sources; direct reactions; photonuclear and thermo nuclear reactions.

UNIT-IV

Nuclear Chemistry - II

Stellar energy: synthesis of elements, hydrogen burning, carbon burning, Nuclear Reactors: fast breeder reactors, particle accelerators, linear accelerators, cyclotron and synchrotron.

Radio analytical Methods: Isotope dilution analysis, Radiometric Titrations, Radio immune assay, Neutron activation analysis. Applications of nuclear science in agriculture and biology. Radiation risks and medical benefits – natural and manmade isotopes.

UNIT-V

Organometallic Chemistry & Catalysis

Carbon donors - Alkyls and Aryls-preparation and properties; Carbonyls -18 electron rule, isolobal concept - application to structure of carbonyls (simple and polynuclear); Nitrosyls - bridging and terminal nitrosyls, bent and linear nitrosyls; dinitrogen complexes; Chain Carbon donors - Olefins, acetylene and allyl complexes - synthesis, structure and bonding; Cyclic Carbon donors - Metallocene - synthesis, structure and bonding (Ferrocene only).

Hydrogenation of olefins (Wilkinsons catalyst); hydroformylation of olefins using Cobalt or Rhodium catalysts (oxo process); Oxidation of olefins to aldehydes and ketones (Wacker process); polymerization (Zeigler-Natta catalyst); Cyclooligomerization of acetylene using Nickel catalyst (Reppe‘s catalyst); polymer bound catalysts.

Course outcomes:

Student understood the knowledge about:

1. The concepts of acids and bases, structure and bonding
2. The systematic structures of solids
3. The awareness of nuclear properties and atomic energy resources
4 The applications of nuclear science in agriculture and biology
5. The hydrogenation, hydroformylation and oxidation process

Reference Books

Unit-I

1. Inorganic Chemistry - Principles of structure and reactivity, Fourth Edition, J. E. Huheey, E. A. Keiter and R. L. Keiter - Addition Wesley Publishing Co, NY, 1993.

Unit-II

2.West, A. R. Solid State Chemistry and its Applications, John Wiley & Sons: New York, 1989

3. L.V.Azaroff – Introduction to solids, John Wiley.

4. W.E.Addision – structural principles of Inorganic Chemistry, Longman, 1961.

Unit – III &IV

5.S.Glasstone – Source book on atomic energy, Von Nostrand Co., 1969.

6. G.Friedlander, J.W.Kennedy, - Nuclear and Radiochemistry, John Wiley and sons, 1981.

7. H.J.Arnikar – Essentials of Nuclear chemistry, Wiley Easter Co., 4thedition, 1995

Unit-V

8. Cotton and Wilkinsin, Advanced Inorganic Chemistry, 5th Edition, John Wiley & Sons, New York.

EC - I: CHOICE – I

PHOTOCHEMISTRY AND PERICYCLIC REACTION

SEMESTER: I **SUBJECT CODE: 21PCHE1**

CREDITS: 5 **TOTAL HOURS: 6**

Objectives:

1. *To study the photo-physical processes and experimental techniques in photochemistry*
2. *To learn the various types of photochemical reactions of alkenes and aromatic system*
3. *To know the photochemistry of singlet molecular oxygen and polymers*
4. *To study the molecular orbital symmetry, molecular orbital approaches*
5. *To learn the cyclo-addition and various photochemical rearrangements*

UNIT – I

Chemistry of Photophysical Processes

Photo physical processes in electronically excited molecules – Radiation less transitions –Jablonski diagram - Internal conversion and intersystem crossing. Fluorescence emission – Fluorescence and structure. Triplet states and phosphorescene emission – Photo physical kinetics unimolecular processes – Stern-Volmer equation. Photochemical techniques-Experimental techniques in photo chemistry –Chemical actinometry – Ferrioxalate, uranyl oxalate, photochromic, Reinecke‘s salt actinometeres – Lasers and their applications.

UNIT – II

Photochemical Reaction I

Photochemistry of carbonyl compounds: Norrish type I and type II reactions, Photoreduction. Photochemistry of α, β and β,γ – unsaturated carbonyl compounds, Photodimerization, Barton reaction and Paterno-buchi reaction.

Photochemistry of aromatic compounds: Photochemical isomerization, addition (1,2 additon 1,3 addition 1,4 addition) and substitution (Electrophilic and nucleophilic).

Photochemistry of Alkenes: Cis -Trans Isomerization - Sensitised cis - trans isomerization - Photochemistry of Conjugated Dienes. Rearrangement of 1,4 - and 1,5- dienes

UNIT – III

Photochemical Reaction II

Photo oxidation and Photo oxygenation, Singlet molecular reaction, Photo oxidation of alkenes. Photochemical Cyclization, Di - π-methane rearrangement, Aza di – π methane rearrangement, Photo - Fries Rearrangement, Hoffmann-Loefller-Freytag reaction.

Photochemistry of polymers: Photopolymerization, photochemical cross linking of polymers, photodegradation of polymers (vinyl, polyethylene and polypropylene), photostabilisers.

Photobiology, Chemiluminescence, Bioluminescence, dyes and pigments

UNIT – IV

Pericyclic Reactions I

Construction of molecular orbitals, symmetry in π Molecular Orbitals, filling of electrons in molecular orbitals, Frontier Molecular Orbitals, conrotatory and disrotatory motions in ring opening reactions, conrotatory and disrotatory motions in ring closing reactions, Open chain conjugated system having 4nπ, (4n+2)π conjugated electrons, Frontier Molecular Orbital (FMO) Method, electrocyclic ring - closure and electrocyclic ring opening reactions. Correlation diagram for 4nπ and (4n+2)π system. Woodward - Hoffmann rule for thermal electrocyclic reaction. Huckel - Mobius Method or Perturbation Molecular Orbital (PMO) Method.

UNIT-V

Pericyclic Reactions II

Cycloaddition reaction: [2+2] and [4+2] Cycloaddition reactions with FMO approach, Correlation diagram for cycloaddition reactions, The Woodward - Hoffmann rule for cycloaddition reactions, Huckel - Mobius method for cycloaddition reaction. Antarafacial and Suprafacial addition. Chelotropic Reactions: Chelotropic Cycloaddition reaction.

Sigmatropic rearrangement: Mechanism of sigmatropic rearrangement, Frontier Molecular Orbital method, Sigmatropic shift of alkyl groups, Selection Rules for sigmatropic rearrangement. The Woodward - Hoffmann rule for sigmatropic rearrangement (where migrating group is hydrogen and not hydrogen). Huckel - Mobius method for sigmatropic rearrangement, [1, 3], [1, 5] and [3, 3] sigmatropic rearrangement, Cope rearrangement and Aza cope rearrangement. Fluxional Tautomerism.

Course outcomes:

Student understood the knowledge about:

1. *The photo-physical processes and experimental techniques in photochemistry*
2. *The various types of photochemical reactions*
3. *The photochemistry of alkenes and carbonyl compounds*
4. *The photochemistry of polymers*
5. *The molecular orbital symmetry, molecular orbital approaches*
6. *The cyclo-addition and various photochemical rearrangements*

References

Unit-I, II&III

1. K K.Rohatgi Mukherjee, Fundamentals of photo chemistry. Wiley Eastern Ltd. 1988.
2. N J Turro, Molecular photochemistry, New York, W A Benjamin, 1966.
3. S. Arunachalam, Inorganic photochemistry, Kala Publications.

Unit-IV&V

4. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, 1st Ed., Oxford University Press, 2001.
5. M.B. Smith & J. March, March's Advanced Organic Chemistry, 5th Ed., John Wiley & Sons, New York, 2001.
6. F.A. Carey and R.A. Sundberg, Advanced Organic Chemistry, Part A and Part B, 5th Ed., Kluwer Academic/Plenum Publishers, New York, 2004
7. P. G. M. Wuts, Greene's Protective Groups in Organic Synthesis, 5th Ed., Wiley, 2014.

EC - I: CHOICE – II

CHEMISTRY OF MACROMOLECULES

SEMESTER: I **SUBJECT CODE: 21PCHE1**

CREDITS: 5 **TOTAL HOURS: 6**

Objectives:

1. *To know about the processes involved in the polymerisation*
2. *To learn the synthesis and importance of various types of polymers.*
3. *To understand the properties of different types of polymers.*

UNIT -I

Concept of Macromolecules

Principle of duality and molecular design - tetrahedral model of product development.Polymers-Nomenclature and classification. Raw material for the synthesis of polymers. Synthetic schemes. Petroleum and petrochemicals - Naphtha as a source of petrochemicals.

UNIT -II

Polymerization Process

Free radical addition polymerization - kinetics and mechanism. Chain transfer. Molecular weight distribution and molecular weight control. Cationic and anionic polymerization: Kinetics and mechanism. Living polymers. Step growth polymerization - Linear Vs cyclic polymerization. Other methods of polymerization - bulk, solution, melt, suspension, emulsion and dispersion techniques.

UNIT -III

Polymer Stereochemistry

Configuration and conformation. Tacticity. Chiral polymers. Polymer characterization. Molecular weights - Methods for determining molecular weights - static, dynamic, viscometry, light scattering and GPC. Crystalline and amorphous states. glassy and rubbery States. Glass transition temperature and crystalline melting of polymers.Degree of crystallinity - X-ray diffraction. Thermal stability of polymers.

UNIT -IV

Polymer Solutions

Flory-Huggins theory. Chain dimension - chain stiffness. End – to - end chain distance of polymers. Conformation - random coil, solvation and swelling. Determination of degree of cross linking and molecular weight between cross links. Industrial polymers - synthesis, structure and applications of polyethylene, PVC, Teflon, poly styrene, polymethylmethacrylate, poly urethane, phenol formaldehyde resins, ureaformaldehyde resins and epoxy polymers.

UNIT -V

Specialty Polymers

Polymer degradation: Types of degradation- thermal, mechanical, photo, hydrolytic and oxidative degradations.Additives for polymers: Fillers, plasticizers, thermal stabilizers, photo stabilizers, anti oxidants and colourants.

Polymers as aids in organic synthesis. Polymeric reagents, catalysts, substrates. Liquid crystalline polymers - Main chain and side chain liquid crystalline polymers. Phase morphology. Conducting polymers - Polymers in optical lithography - Drug delivery - Drug carriers.

Course outcomes:

Student understood the knowledge about:

1. *Sort the process of different polymerization methods.*
2. ***Appreciate the physical properties of different polymers and its application.***

TEXT BOOKS

1. F.W. Billmayer. Textbook of Polymer Science. 3rd Edn, Wiley. N.Y. 1991.
2. J.M.G Cowie. Polymers: Physics and Chemistry of Modern Materials. Blackie. London, 1992.
3. R.J.Young, Principles of Polymer Science, 3rd Edn. , Chapman and Hall. N.Y. 1991.
4. P.J. Flory. A Text Book of Polymer Science. Cornell University Press. Ithacka, 1953.
5. F. Ullrich, Industrial Polymers, Kluwer, N.Y. 1993.
6. H.G.Elias, Macromolecules, Vol. I & II, Academic, N.Y. 1991.

EC - I: CHOICE – III

ADVANCED PHARMACEUTICAL CHEMISTRY

SEMESTER: I **SUBJECT CODE: 21PCHE1**

CREDITS: 5 **TOTAL HOURS: 6**

Objectives

1. *To learn about the inorganic molecules used for the treatment of wide range of diseases*
2. *To study the herbal drug action*
3. *To study the drug formulation and mechanism of synthetic drug molecules*

UNIT - I

Inorganic pharmaceuticals I

Antioxidants : Introduction, criteria for action as anti oxidants, mechanism of action.

Preparation, properties and assay of hypophosphorus acid and sodium meta bisulphate.

Gastrointestinal agents: Acidifiers, antacids. Acidifiers - dil. HCl; Antacids - evaluation of antacid activity, drug interactions. Aluminium compounds- aluminium hydroxide gel, dry tablets, dried aluminium phosphate gel; calcium compounds- calcium phosphate, calcium carbonate; magnesium compounds- milk of magnesia, magnesium oxide; sodium compounds - sodium bicarbonate; combination of antacids.

Antidiarrhoeals: Bismuth compounds - bismuth sub carbonate

Laxatives: Magnesium sulfate, milk of magnesia

UNIT - II

Inorganic pharmaceuticals I

Dental products. Introduction, anticaries agents-sodium flouride, dentifriers - dibasic calcium phosphate.

Inhalants: Introduction, role of oxygen, carbon dioxide and ammonia, nitrous oxide as inhalant.

Expectorants - Ammonium chloride and Potassium iodide.

Respiratory stimulants: Dil. ammonia solution, aromatic spirit of ammonia.

Emetics: Ammonium chloride, potassium iodide.

Intra cellular and extra cellular electrolytes- body fluid compartments, role of major physiological cations and anions, sodium chloride.

UNIT - III

Herbal Drugs

Classification of herbal drugs - Taxonomical, Morphological, Pharmacological and Chemical Classification - Adulteration and evaluation of drugs - Different chemical groups of Herbal Drugs - Alkaloids, Terpenoids, Glycosides, Volatile oils, Isolation of volatile oils, Tannins and carbohydrates.

Herbal drugs and their therapeutic efficacy - Laxative- Barbarian, Aloe emodin from Aloes. Ricinolic acid from castor oil.

Nervous system drugsDepressants - Reserpine from Rawolfia, Hallucinogens- LSD (ergot), Stimulants - Caffeine (coffee), Cocaine (coca), Analeptics - Strychnine (St.Nuxvomica), Camphor (Cinnamonam camphora) - Analgesics- Morphine and Codeine (Phapaver somniferum) - Depressants- Tropane alkaloids (belladonna), Cannabinol (cannabis) - Anti-hypertensive- Reserpine (rawolfia) - Anti-rheumatics - Guggulosterol (Guggul), Colchicin (colchicum) – Anti – tumor - Colchicin (colchicum), Vinblastin (vincarosea), Taxol (taxus bacetta) - Anti-diabetics - Neem oil (Neem). Anti – malarial - Quinine (cinchona).

UNIT - IV

Synthetic pharmaceuticals I

Synthesis and pharmacological activity of Diclofenac (anti - inflammatory), Tinidazole (anti - amebic), Pheniramine (anti - histamine), Ciprofloxacin (anti - bacterial), Cloxacillin, Cephalexin (anti - biotics), Miconazole (anti - fungal), Cisplatin (anti-neoplastic), Ethambutal (antitubercular) and Enalapril (anti - hypertensive).

UNIT - V

Synthetic pharmaceuticals II

Benzocaine (localanesthetic), Phenobarbitone, Nitrazepam (Hypnotic), Isoprenalin (sympathomimetic), Celecoxib (antiinflammotory), Procainamide (cardiovascular), Omeprazole (antiulcer), 5-Floro uracil (anticancer), Ciprofloxacin, norfloxacin (antibacterials), Lamivudine (anti AIDs) and Clofazimine (anti leprosy and anti T.B).

Course outcomes:

1. *Drug action of inorganic molecules*
2. *Therapeutic efficacy of herbal drugs*
3. *Pharmacological activity of synthetic drugs*

References

1. Practical pharmaceutical chemistry. By A.H.Backette, J.B.Stenlake.
2. British Pharmacopoeia vol I,II
3. Indian Pharmacopoeia vol I,II
4. Pharmaceutical analysis. By Takeru,Higuchi
5. Pharmaceutical analysis By. David G.Watson
6. Bently's Text book of pharmaceutics by Rowlins
7. The science and practice of pharmacy by Remington
8. Natural products. By P.S.Kalsi
9. Medicinal chemistry. By Chatwal.
10. Medicinal chemistry. By Ashtoshkar.
11. Chemistry of Drugs. By V.N.Ivers.
12. May's chemistry of synthetic drugs. Hand Book of Reagents for organic synthesis By Reich,Rigby
13. The organic chemistry of Drug synthesis.vol 1-6 By Ledneicer etal.
14. Top Drugs: The synthetic routes. J.Saunders

CP - III: INORGANIC CHEMISTRY PRACTICAL – I

SEMESTER: I **SUBJECT CODE: 21PCH3P**

CREDITS: 5 **TOTAL HOURS: 6**

Objectives:

1. *To learn the qualitative analysis by semimicro method*
2. *To know the usage of photoelectric colorimeter for quantitative estimation*
3. *To study the volumetric analysis by iodimetric titration method*
4. *To learn the gravimetric estimations by using sintered crucibles*
5. *To know about the complex preparations*

1. **Semi micro qualitative anlaysis of a mixture containing two common and two Rare cations.**
2. **Colorimetric estimation of Copper, Ferric, Nickel, Chromium and Manganese using photoelectric colorimeter.**
3. **Titrimetry and Gravimetry**

   (i) Cu(V), Ni(G); (ii)Cu(V), Zn(G); (iii)Fe(V), Zn(G); (iv)Fe(V), Ni(G); (v)Zn(G), Cu(V)
4. **Preparation of the following complexes**
   1. Tetramminecopper(II) sulphate
   2. Potassiumtrioxalatochromate(III)
   3. Hexathiourealead(II)nitrate
   4. Potassium trioxalaoaluminate(III)
   5. Tristhioureacopper(II) sulphate
   6. Tristhioureacopper(II) chloride

Course outcomes:

Student understood the knowledge about:

1. *The qualitative analysis by semi micro method*
2. *The usage of photoelectric colorimeter for quantitative estimation*
3. *The volumetric analysis by iodimetric titration method*
4. *The gravimetric estimations by using sintered crucibles*
5. *The complex preparations*

CP - IV: ORGANIC CHEMISTRY PRACTICAL – I

SEMESTER: I **SUBJECT CODE: 21PCH4P**

CREDITS: 5 **TOTAL HOURS: 6**

Objectives:

1. *To study the separation of organic compounds and qualitative analysis*
2. *To know the synthesis of organic compounds by single stage*
3. *To learn the estimation of organic compounds by quantitative analysis*
4. *To study the synthesis of organic compounds by two stage*

1. Qualitative analysis of organic mixture

Pilot separation, bulk separation, Analysis, Derivative, determination of m.p/ b.p of the derivative.

2. Preparation of oraganic compounds (single stage)

1. methyl-m-nitrobenzene from methylbenzoate (nitration)
2. Glucose pentaacetate from glucose (Acetylation)
3. Resacetophenone from resorcinol (Acetylation)
4. o-Chlorobenzoic acid from anthranilic acid (Chlorination &Diazotisation)
5. Phenyl azo-2-naphthol from aniline (diazotization)

3. Quantitative analysis of organic compounds

Estimation of phenol, aniline, ketone, glucose, saponification value and iodine value of oil.

4. Preparation of organic compounds (double stage)

1. p-Bromoacetanilide from aniline (Acetylation + Bromination)
2. Acetyl salicylic acid from methyl salicylate (Hydrolysis + Acetylation)
3. 1, 3, 5 – tribromobenzene from aniline (Bromination + Diazotisation + Hydrolysis)
4. p-Nitroaniline from acetanilide (Nitration + Hydrolysis)
5. Benzilic acid from benzoin (Rearrangement)
6. Benzanilide from benzophenone
7. p-Aminobenzoic acid from paranitrotoluene (Oxidation + Reduction)
8. p-Bromo aniline from acetanilide (Bromination + Hydrolysis)
9. m-Nitroaniline from nitrobenzene (Nitration + Reduction)

Course outcomes:

Student understood the knowledge about:

1. *The separation of organic compounds and qualitative analysis*
2. *The synthesis of organic compounds by single stage*
3. *The estimation of organic compounds by quantitative analysis*
4. *The synthesis of organic compounds by two stage*

SEMESTER – II

CC - V: PHYSICAL CHEMISTRY – I

SEMESTER: II **SUBJECT CODE: 21PCH5**

CREDITS: 5 **TOTAL HOURS: 6**

Objectives:

1. *To understand the theories of chemical kinetics in reaction mechanisms.*
2. *To know the applications of classical thermodynamics in the evaluation of macroscopic properties.*
3. *To learn the concepts of statistical thermodynamics for the study of equilibrium reactions and reaction rates.*
4. *To differentiate electrode kinetics from other types of kinetic studies*

UNIT- I

Chemical Kinetics – I

Theories of reaction rates and factors influencing the reaction rate: ARRT (Eyring's theory), Thermodynamic derivation of ARRT- comparison of ARRT with collision theory (A , $\Delta S^{\#}$, E_a and $\Delta H^{\#}$) – kinetic isotope effects, Marcus electron transfer theory - inner and outer electron transfer. Theory of unimolecular reactions - Lindemann's theory – Steady State approximation-chain reactions - photochemical reaction between hydrogen and halogens (Cl_2 and Br_2) – gas phase auto - oxidations, explosions-hydrogen-oxygen reaction.

UNIT- II

Chemical Kinetics – II

Application of ARRT to solution kinetics-effects of solvents, double sphere model, effect of ionic strength on ionic reactions – influence of pressure on reaction rates in solution significance of volume of activation-substituent effects – Hammett and Taft equations.

Homogeneous catalysis, acid-base catalysis – types and mechanism, derivation of rate law for protolytic acid catalysis and explanation for Arrhenius and van't Hoff intermediates, Bronsted relations - Hammett-Deyrup acidity function – enzyme catalysis-mechanism of single substrate reaction – Michaelis - Menton equation - Influence of pH, concentration and temperature, Line Waver plot and Eddi – Hofstee plot. Fast reactions - study of kinetics by stopped flow technique, relaxation methods, T and P - jump methods, flash photolysis and magnetic resonance method.

UNIT –III

CLASSICAL THERMODYNAMICS

Partial molar properties – chemical potential, relationship between partial molar quantities and thermodynamic functions – Gibbs - Duhem equation - calculation of partial molar quantities from experimental data,

Thermodynamic properties of real gases - activity - fugacity concept - calculation of fugacity of real gas and activity coefficient – definition and experimental determination of activity coefficients of non - electrolytes.

UNIT –IV

STATISTICAL THERMODYNAMICS – I

Probability – types of events-theories of probability- multiplicative nature of probability permutations and combinations – Stirling‘s Approximation. Statistical mechanics – calculation of thermodynamic probability of system – Assembly , ensembles, phase space-definition of micro and macro states - different methods of counting macro and micro states – distinguishable and indistinguishable particles - classical statistics - derivation of Maxwell Boltzmann distribution law - Its application to gaseous system – energy, velocity distribution - concept of negative Kelvin temperature. Quantum statistics - Bose Einstein and Fermi Dirac statistics-comparison with Maxwell- Boltzmann statistics – application of BE statistics to photon gas - Application of FD statistics to electron gas and to thermionic emission – derivation of thermionic energy.

UNIT- V

STATISTICAL THERMODYNAMICS – II

Partition function – characteristics - translational, rotational, vibrational, electronic partition function - expression for enthalpy, internal energy, Gibb‘s energy, entropy (Sackur – Tetrode equation), work function and equilibrium constant in terms of partition functions – partition function of mono atomic and diatomic molecules.

Heat capacity of solids – Derivation of Einstein‘s equation and its limitations, Debye T - cubed law and its significance. Non - equilibrium thermodynamics, Steady – State - phenomenological laws and Onsager‘s reciprocal relations.

Course outcomes:

Student understood the knowledge about:

1. *At the end of this course, the students will be able*
2. *Calculate the thermodynamic and kinetic properties*
3. *Relate microscopic properties of molecules with macroscopic thermodynamic observables*

4. *To analyse the fundamental concepts of atoms and molecules and their arrangements in different energy levels by statistical approach.*
5. *To apply the mathematical concepts in chemical systems at molecular level.*

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3. M.C.Gupta, ―Statistical Thermodynamics‖, Wiley Eastern Ltd., New Age International,
    a. New Delhi, 1998.
4. R.P. Rastogi and R.R. Mishra, ―An introduction to Chemical Thermodynamics‖, Vikas
    a. Publishing House, New Delhi, 2000.
5. B.R. Puri, L.R.Sharma and M.S. Pathania, ―Principles of Physical Chemistry‖, Vishal Publishing Co., Jalandar, 2017.
6. Peter Atkins and Julio de Paula, ―Physical Chemistry‖ Oxford University Press, 2018.
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8. A.A. Frost and R.G. Pearson, ―Kinetics and Mechanisms‖, John Wiley & Sons, New York, 1961.
9. I. Amdur and G.G. Hammes, ―Chemical Kinetics – Principles and Selected Topics‖, McGraw Hill, New York, 1966.
10. J.I. Steinfeld, J.S. Francisco and W.L.Hase, ―Chemical Kinetics and Dynamics‖, Prentice Hall, New Jersey, 1999.
11. Horia Metiu, ―Physical Chemistry-Kinetics‖, Taylor and Francis, New York, 2006.
12. R.K.Dave, ―Chemical Kinetics‖, Campus Books, 2000.
13. R. Stephen Berry, Stuart A.Rice and John Ross, ―Physical Chemistry‖, Oxford University Press, New York, 2000.
14. D.A. Mcquarrie, J.D. Simon, ―Molecular Thermodynamics‖, University Science books, California, 1999.
15. F.W.Sears, Thermodynamics, ―Kinetic theory of Gases and statistical mechanics‖, 2nd Edition, Wesley, 1972.
16. Horia Metiu, ―Physical chemistry- Thermodynamics‖, Taylor and Francis, 2006.
17. Peter Atkins and Julio de Paula Atkins ―Physical Chemistry‖, Oxford University Press, Oxfored, 2018.
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19. Robert J. Silbey, Robert A. Alberty, ―Physical Chemistry‖, John Wiley and Sons, New York, 2006.

CC - VI: INORGANIC CHEMISTRY – II

SEMESTER: II **SUBJECT CODE: 21PCH6**

CREDITS: 5 **TOTAL HOURS: 6**

Objectives:

1. *Basis of the principles of coordination chemistry*
2. *Fundamental theories describe bonding in coordination complexes and structure, stability and reactivity of coordination complexes.*
3. *Electron transfer reactions in inorganic compounds*
4. *Electronic transitions in metal complexes and photochemical reactions*
5. *Understand the chemistry of carbonyls, nitriles and metal clusters*

UNIT – I

Coordination Chemistry: Principles

Studies of coordination compounds in solution – detection of complex formation in solution – Stability constants – stepwise and over-all formation constants – simplemethods (Potentiometric, pH metric and photometric methods) of determining theformation constants - Factors affecting stability – statistical and chelate effects – Forced configurations.

UNIT – II

Theories of Metal-Ligand Bond

Crystal field theory – shapes of d orbitals – splitting of d orbitals in octahedral symmetry - CFSE-strong field and weak field splitting-calculation of CFSE for dn system- splitting in tetrahedral symmetry- only weak field splitting-reasons- tetragonal symmetry - differences between tetrahedral and tetragonal symmetry - John Teller distortion- splitting pattern in trigonal, squreplanar, trigonalbipyramidal, square pyramidal, cubic symmetries. Factors affecting the magnitude of splitting (10Dq) -oxidation state of the metal ion, nature of the metal ion, number and geometry of the ligands, nature of the ligands – Spectrochemical studies, Jorgenson relation, evidences for CFT. Magnetic properties, computation of lattice energies, enthalpies of hydration, stability of particular oxidation states.

M.O. theory - octahedral, tetrahedral and square planar complexes. Pi bonding and M.O theory - ligands having filled and empty pi bonds-effect on 10 Dq.- evidences for Pi bonding

UNIT – III

Kinetics and Reaction Mechanism of Coordination Compounds

Kinetics and mechanism of reactions in solution – labile and inert complexes – Ligand displacement reactions in octahedral and square planar complexes – acid hydrolysis, base hydrolysis and anation reactions – trans effect – theory and applications. Electron transfer reactions – electron exchange reactions – complementary and non-complementary types – inner sphere and outer sphere processes – Application of Electron transfer reactions in inorganic - isomerisation andracemisation reactions of complexes – Molecular rearrangement – Reactions of fourand six-coordinate complexes – Interconversion between stereoisomers. Reactions ofcoordinated ligands – Template effect and its application for the synthesis of Macrocyclic ligands – Unique properties.

UNIT - IV

Inorganic Photochemistry

Electronic transitions in metal complexes, metal-centered and charge-transfer transitions – Various photophysical and photochemical processes of coordination compounds – Unimolecular charge-transfer photochemistry of cobalt(III) complexes. Mechanism of CTTM photoreduction. Ligand-field photochemistry of chromium(III)complexes, Adamson‘s rules, photoactive excited states, V-C model – photophysics and photochemistry of ruthenium-polypyridine complexes, emission and redox properties–photochemistry of organometallic compounds, metal carbonyl compounds, compounds with metal-metal bonding Reinecke‘s salt chemical actinometer.

UNIT – V

Chemistry of Metal carbonyls and clusters

Metal carbonyls, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls, preparation, bonding, structure and important reactions of transition metal nitrosyl, dinitrogen and dioxygen complexes, tertiary phosphine as ligand. Polyhedral model of metal clusters, effect of electronic configuration and coordination number, Structures of metal carbonyl clusters of three atoms M3(CO)12 (M=Fe, Ru &Os), Four metal atoms (tetrahedra) [M4(CO)12 {M= Co, Rh &Ir}] and octahedron of type M6(CO)16 [M= Co & Rh]

Course outcomes:

Student understood the knowledge about:

1. Principles of coordination chemistry, Crystal field splitting energy and molecular orbital theory

2. The kinetics and reaction mechanism of organic compounds

3. Electron transfer reactions, complementary and non-complementary reactions

4. Photochemical reactions of coordination and organometallic compounds

5. Application of IR to identify the terminal and bridging carbonyls

6. Vibrational spectra of metal carbonyls for bonding and structural elucidation

References

Unit – I, II &III
1. Keith F Purchell and John C Koltz, Inorganic Chemistry, Saunders Golden Sunburst Series
2. F A Cotton and Wilkinson, Advance Inorganic Chemistry, V Edition, John Wiley and Sons
3. A B P Lever, Inorganic Electronic Spectroscopy, Elsevier
4.. M. C. Day and J. Selbin, Theoretical Inorganic Chemistry, Affiliated East West Press Pvt. Ltd.
2nd ed.,1985.
5. J.E. Huheey, Inorganic Chemistry 3rd. ed., Harper & Row publisher, Singapore
6. F.Basolo and R.G.Pearson, Mechanism of Inorganic Reactions, John Wiley, New York.
Unit – III, IV & V
7. . A.W.Adamson, Inorganic Photochemistry, John Wiley & Sons, New York.
8. . W. Adamson and P. D. Fleischauer, Concepts of Inorganic Photochemistry, Wiley, New York, 1975.
9. J. Ferraudi, Elements of Inorganic Photochemistry, Wiley, New York, 1988.
10. H.J. Emeleus and A.G.Sharpe , Modern aspects of inorganic chemistry.

EC - II: CHOICE – I

NANO MATERIALS AND GREEN CHEMISTRY

SEMESTER: II **SUBJECT CODE: 21PCHE2**

CREDITS: 5 **TOTAL HOURS: 3**

Objectives:

1. *To know about the Techniques for the synthesis of nanoscale materials*
2. *To learn the synthesis and applications of nanomaterials*
3. *To study the principles and basics of green chemistry*
4. *To understand the various methods of green synthesis*

UNIT – I

Introduction and methods of synthesis of nanomaterials

Nanomaterials – Introduction – Classification - Quantum confinement - synthesis and processing - Methods of synthesis nanostructures –Mechanical grinding, spray pyrolysis, Gas Condensation Process, Sputtered Plasma Processing, Microwave Processing, Sonochemical method, Laser ablation, Hydrodynamic cavitation, Sol-gel process, Precipitation method, Reverse Micelle method, Solvothermal method, Hydrothermal method, Combustion method.

Properties of nanomaterials : Electrical properties, Mechanical properties, Magnetic properties and optical properties - Application of nanomaterials - Disadvantages of Nanomaterials.

UNIT – II

Carbon nanomaterials

Nature of carbon bond, new carbon structures, carbon clusters: discovery of C60, alkali doped C60, superconductivity in C60, larger and smaller fullerenes, carbon nanotubes: synthesis, single walled carbon nanotubes, structure and characterization, mechanism of formation, chemically modified carbon nanotubes, doping, functionalizing nanotubes, application of carbon nanotubes, nanowires, synthetic strategies, gas phase and solution phase growth, growth control, properties.

UNIT – III

Characterization Techniques for Nanomaterials

Techniques for characterization of nanoscale materials: atomic force microscope (AFM), transmission electron microscope (TEM), resolution and scanning electron microscope (SEM), scanning tunneling microscope (STM), scanning near field optical microscope (SNOM).

UNIT – IV

Principle of Green Chemistry

Green chemistry definition, Twelve principles of Green Chemistry with their explanations and examples; Designing a Green Synthesis using these principles; Prevention of Waste/byproducts; maximum incorporation of the materials used in the process into the final products (Atom Economy); prevention/minimization of hazardous/toxic products; designing safer chemicals different basic approaches to do so; selection of appropriate auxiliary substances (solvents, separation agents), green solvents, solvent less processes, immobilized solvents and ionic liquids; energy requirements for reactions – use of microwaves, ultrasonic energy.

Green Synthesis of the following compounds: adipic acid, catechol, BHT, methyl methacrylate, urethane, aromatic amines (4- aminodiphenylamine), benzyl bromide, acetaldehyde, ibuprofen, paracetamol, turtural.

UNIT V

Methods of Green Synthesis

Microwave assisted reactions in water: Hofmann Elimination, Hydrolysis (of benzyl chloride, benzamide, n-phenyl benzamide, methylbenzoate to benzole acid), and Microwave assisted reactions in organic solvents: Esterification, Diels Alder Reaction, and Decarboxylation. Ultrasound assisted reactions: Esterification, saponification, Alkylations, Cannizaro reaction, Strecker synthesis, Reformatsky reaction.

Ionic liquids: Properties and application, Organic reaction in water, lewis acid catalysis.

Green catalysis: Role of catalysis, catalysis in water, Process integration.

Zeolite catalysts, description and denomination of Zeolites, commercially used zeolites, shape selectivity, application of zeolites in chemical synthesis.

Green chemistry in everyday life

Course outcomes:

Student understood the knowledge about:

1. *various types of Electron Microscopes*
2. *some important recent discoveries in nanoscience and nanotechnology*
3. *Chemical methods in preparation of nanomaterials*
4. *Structure, characterization, mechanism and formation of carbon nanotubes*
5. *Twelve principles of Green Chemistry with their explanations*
6. *Synthesis of different compounds by green method*
7. *Uses of Microwaves and Ultra sounds in green synthesis*

References

Unit – I, II & III

1. http:/www.inflibnet.ac.in
2. http:/www.springerlink.com
3. http:/www.rsc.org
4. http:/www.pubs.acs.org
5. Kenneth . Klabunde, Nanoscale Materials in Chemistry, John Wiley & Sons,
6. Nanotechnology: basic science and emerging technologies – Mick Wilson KamaliKannangara, Geoff Smith, Michelle Simmons, BurkhardRaguseas Overseas Press (2005).

Unit – IV & V

7. Paul T. Anastas Green Chemistry
8. Sanghi A Shrivastav Green Chemistry
9. M.Kidwai&Ahlavalia V.K. Green Chemistry
10. V. Kumar, An Introduction to Green Chemistry, Vishal Publishing CO. Jalandhar, 2007

EC - II: CHOICE – II

DRUG DESIGN AND DISCOVERY

SEMESTER: II **SUBJECT CODE: 21PCHE2**

CREDITS: 5 **TOTAL HOURS: 3**

Objectives:

1. *To enable students identify Lead compounds*
2. *To understand the various drug – Receptor interactions*
3. *To outline the steps to synthesize a drug molecule.*

UNIT- I

Introduction to Drug Design

Historical background- -drug targets: lipids, carbohydrates, proteins , enzymes, and nucleic acids as drug targets and receptors. Receptor Pharmocology –Agonists and Antagonists (partial and full) - Allosteric Modulators – Pharmacokinetics and pharmacodynamics: administration, absorption, distribution, metabolism, elimination of drugs - bioavailability of drugs - side effects - Case study : serotonin and dopamine receptors and transferring drugs.

UNIT -II

Drug Identification and Validation

Steps in drug discovery – Lead identification – Hits - Drug validation-Natural products as drugs – molecular recognition in drug design – thermodynamic considerations – physical basis and inter molecular interactions between drugs and targets like electrostatic interactions – ionic bonds-hydrogen bonds – Inductive interactions – dispersive forces. Stereochemistry in drug designing – stereospecificity of drug targets – Eudesmic ratio – Examples of Eutomers and Distomers

UNIT - III

Reterosynthetic Strategies for Drug Synthesis

Introduction to retrosynthetic analysis and disconnection approach – synthons acceptor and donor – synthetic equivalents - umpolungs – planning a synthesis – relay and convergent routes - Guidelines for disconnection – one group C-X and C-C disconnections – Chemoselectivity. Two group C-C disconnections in dicarbonyls – Case Study : Synthesis of Amelfolide.

UNIT- IV

Computer Aided Drug Design

Molecular modeling in drug design – Energy Minimization methods – both Molecular Mechanics and Quantum mechanical Methods – Energy minimization – Conformational analysis – Structure based and Ligand based Drug design – QSAR – parameters – Quantitative models of QSAR – Hansch methods – free Wilson model -3D pharmacophore modeling – Docking – Introduction - Preparation of protein and ligands - Types of docking- rigid and flexible methods of docking - Online docking tools - Post docking analysis.

UNIT -V

Cheminformatics

Introduction- Molecular representation and Topological indices -2D & 3D, SMILES-ROSDAL-MDL number, Z-Matrix and Cartesian coordinates-Types of database-Online Cheminformatics database - Chemspider - MOLBASE-ADMET property calculator, DruLiTo, Episuite and molinspiration.

Course outcomes:

Student understood the knowledge about:

1. *Identify the lead compounds and its influences*
2. *Assess the drug receptor interactions and mode of action of different drugs*
3. *Synthesize a drug molecule using retro synthetic strategy*
4. *Employ the principle involved in analyzing drug molecules*
5. *Design a new drug molecule based on the principles of SAR and QSAR*

REFERENCES

1. Andrew R. Leach, Valerie J Gillet, An Introduction to Cheminformatics, Revised Edition, Springer, Netherland, 2007. **(Unit I, II & IV)**

2.Stuart Warren **"**Organic Synthesis The Disconnection Approach‖ Wiley; 2nd Edition, 2008 **(Unit III)**

1. Larsen et al,Text book of Drug Design and Discovery,4th Edition, London and Newyork , Taylor and Francis, 2004. **(Unit I, II)**

2. Graham L. Patrick, An Introduction to Medicinal Chemistry, 4th Edition, Oxford University Press, 2009. **(Unit I, II)**

3. Johann Gasteiger, Thomas Engel, Cheminformatics : A Textbook,Wiley VCH, Weinheim, 2003. **(Unit V)**

EC - II: CHOICE – III

SENSORS AND TRANSDUCERS

SEMESTER: II **SUBJECT CODE: 21PCHE2**

CREDITS: 5 **TOTAL HOURS: 3**

Objectives:

1. To learn the working principles of various transducers.
2. To measure the non - electrical quantities
3. To acquire knowledge of measurement techniques of thermal conductivity
4. To enhance the knowledge on integrated sensors.
5. To know the usage of electrolytic sensors
6. To learn about biosensors and MEMS based sensors
7. To learn the signal conditioning circuits used in bio- instrumentation
8. To analyze the operations of various sensors used in industries

UNIT - I

Transducers

Introduction to measurement - Direct and indirect measuring methods - Accuracy - Errors - Transducers - Resistive transducers - Potentiometers - Non-linear potentiometers function generators - Strain gauges - Types of strain gauges - Resistance thermometers – Variable inductance transducers - Linear variable differential transformer - Capacitive transducers – Piezo electric transducers - Hall Effect transducers - Magneto resistors

UNIT - II

Measurement of non-electrical quantity

Measurement of vibrations - Seismic transducers - Measurement of flow rate - Measurement of thickness - Measurement of humidity – Measurement of sound using microphones - Measurement of pH value - Measurement of thermal conductivity - Measurement of pressure.

UNIT - III

Integrated Sensors

LM 35 temperature sensor - DS18s20 1-wire digital thermometer - TSOP 17 photo modules for PCM remote control system - MOC3041 zero cross optoisolators - TL173L linear hall effect sensor - KMZ51 magnetic field sensor - MPXV5004G pressure sensor - A1425 analog speed sensor - LM1830 water level sensor - HC610 humidity sensor - ICM105A VGA CMOS sensor

UNIT - IV

Biosensors and MEMS based Sensors

Introduction - FET & MOSFET chemical sensor - Bio sensors - Ion exchange membrane electrodes - Oxygen electrodes - CO_2 electrodes enzyme electrode - Construction - ISFET for glucose, urea - Electrolytic sensors - Opticalsensor - Fiber optic sensors - ADXL 335 accelerometer - MPU 6050 IMU Sensor.

UNIT - V

Signal Conditioning Circuits

Signal conditioning basics – type of signal conditioning: analog and digital – analog signal conditioning amplification - attenuation – level shifting - Clippers – clampers - data sampling and optimization - Filters: RC filter - active filter - Wheatstone bridge - AC bridges- noise reduction techniques. Comparators – Schmitt trigger for noise removal – Current amplification – isolation.

Course outcomes:

Student understood the knowledge about:

1. *Function of transducer*
2. *Measurement of non-electrical quantity*
3. *Integrated, MEMS and bio sensors*
4. *Types of signal conditioning*

References

1. A.K. Sawhney, ‒A course in Electrical and Electronic Measurements and Instrumentation‖, Dhanpat Rai & Co. publishers,2011.
2. N.Mathivanan, ‒PC Based Instrumentation: Concepts and Practice‖, PHI, 2007.
3. H. S. Kalsi, ‒Electronic Instrumentation‖, Tata McGraw-Hill publishers
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6. Gabor Harsanyi, Sensors in Biomedical Applications - Fundamentals, Technology and Applications, CRC Press, 2000.
7. Raluca-Ioana Stefan, Electrochemical Sensors in Bioanalysis, CRC Press, 2001.

EDC - I: SUPRAMOLECULAR CHEMISTRY

SEMESTER: II **SUBJECT CODE: 21PCHED1**

CREDITS: 5 **TOTAL HOURS: 3**

Objectives:

1. *To understand the Basic concepts of supramolecular chemistry*
2. *To know the synthesis and different structures*
3. *To study the crystal engineering*
4. *To learn the designs and various interactions*
5. *To study molecular electronic devices*

UNIT-I

Basic Concepts of Supra Molecular Chemistry

Basic concepts Terminology and nomenclature in supramolecular chemistry, definition of supramolecular chemistry,

Selectivity, Complementarity, Co-operativity and the chelate effect, Preorganisation, Binding constants, Kinetic and thermodynamic selectivity, Supramolecular interactions

Chemical interactions leading to supramolecular assemblies, nature of binding interactions in supramolecular structures: ion-ion, ion-dipole, dipole-dipole, H-bonding, cation-π, anion-π, π-π, Van der Waals interactions and Hydrophobic effects.

UNIT-II

Synthesis and Different Structures

Host-Guest chemistry: Macrocyclic versus acyclic hosts, High-dilution synthesis and Template synthesis. Synthesis and structure of crown ethers, lariat ethers, podands, cryptands, spherands, hemispherands, crypytaspherands and hetcrowns. calixarenes, cyclodextrins, cyclophanes, cryptophanes, carcerands, and hemicarcerands.

Biological ligands: ion channels and siderphores. Anion binding, charged receptors, neutral receptors, metal containing receptors, lewis acid receptors, ditopic receptors and zwitterion receptors.

UNIT-III

Crystal engineering

Crystal engineering: Concepts in crystal engineering, Crystal engineering with hydrogen bonds, π interaction and other common synthon, solid state reactivity and engineering crystals. Coordination

polymers, cocrystals, polymorphs and their physic - chemical properties, coordination polymers, Interpenetrating networks, metal organic frameworks and their properties.

UNIT-IV

Designs and Various Interactions

Self - Assembly Self - assembly of molecules: Definitions and basic concepts of self-assembly, Self-assembly with modification, Design, synthesis and properties of the molecules. Biological self-assembly. Ladders, polygons and helices, Racks, ladders and grids, helicates and molecular polygons. metallomacrocycles, catenanes, rotaxanes, rotaxanes and catenanes as molecular devices.

UNIT-V

Molecular devices

Molecular devices: Molecular Electronic Devices – Controlling Electricity Using Supermolecules, Reading Signals from Molecular Device, Molecular Photonic Devices – Controlling Light with Supermolecules, Molecular Computers, Molecular Machines, Molecular Devices with Directional Functionality, molecular wires, molecular rectifiers, molecular switches, molecular logic.

Course outcomes:

Student understood the knowledge about:

1. *Binding interactions in supramolecuar structure*
2. *Synthesis and structure of crown ethers*
3. *H-bonding, halogen bonding and other interactions*
4. *Metal organic frame works and their properties*
5. *Design, synthesis and properties of the molecules*
6. *Metal – ligand and other weak interactions*
7. *Molecular electronic devices*

References:

Unit-I, II & III

1. J.M. Lehn, Supramolecular Chemistry-Concepts and Perspectives, Wiley-VCH, 1995.
2. P. D. Beer, P. A. Gale and D. K. Smith, Supramolecular Chemistry, Oxford University Press, 1999.
3. J. W. Steed and J. L. Atwood, Supramolecular Chemistry, 1st Ed., Wiley, 2000.
4. J.W. Steed, Core Concepts in Supramolecular Chemistry and Nanochemistry,1st Ed., John Wiley & Sons, 2007.

Unit- IV & V

5. J.D. Seader, I. W. Hamley, Introduction to soft mater Synthetic and Biological selfassembly materials, Separation process principles, 2nd Ed., Wiley, 2010.
6. G. R. Desiraju, J. J. Vittal and A. Ramanan, Crystal Engineering: A Textbook, World Scientific, 2011.

SEMESTER – III

CC - VII: ORGANIC CHEMISTRY – II

SEMESTER: III **SUBJECT CODE: 21PCH7**

CREDITS: 5 **TOTAL HOURS: 6**

Objectives

1. *To learn the preparation, properties of amino acids and proteins.*
2. *To study the activity of enzymes and cofactors.*
3. *To know basics of lipids and nucleic acids.*
4. *To learn the concept of bioenergetics.*
5. *To learn the principles of lead and analogue synthesis.*

UNIT - I

Structure and Bonding

Nomenclature of alicyclic, bicyclic and tricyclic compounds (Basic skeletal structures only with or without ene substituent). Localized chemical bonding: electronic structure of molecules: VB, MO, HOMO - LUMO theory. Electro negativity, dipole moment, inductive and field effect, bond distances, bond angles and bond energies. Delocalized chemical bonding and bond distance in compound containing delocalized bond, cross conjugation, Resonance, steric inhibition of resonance, hyper conjugation, and keto -enol tautomerism.

UNIT – II

Alkaloids and Steroids

General methods of determining structure. Classification of alkaloids – structural elucidation of (-) quinine, morphine, conine, atropine, reserpine, ephedrine. Biosynthesis of alkaloids.

Steroids – Occurrence, nomenclature, basic skeleton, diel‘s hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of cholesterol, bile acids, androsterone, testosterone, estrone, progesterone, aldosterone, bio synthesis of steroids.

UNIT - III

Biomolecules

Carbohydrates: Structure of mono saccharides and disaccharides - Polysaccharides–structure of starch and cellulose- photosynthesis.

Peptides and proteins: Synthesis of peptides – primary, secondary, tertiary and quaternary structure of proteins-protection of N-terminal and C-terminal groups of proteins-Biosynthesis of proteins.

Nucleic acids: Chemistry of nucleic acids – structure of DNA – properties, biological implications of DNA-replication of DNA. Structure of RNA – types of RNA and their functions.

Antibiotics: Synthesis and applications of penicillin, streptomycin and cephalosporin.

UNIT – IV

Reagents in Organic Synthesis

Oxidation: Baeyer-Villiger, Jacobsen epoxidation, Shi epoxidation, Jones reagent.PCC, PDC, IBX, DMP, CAN, TPAP, NOCl, $Mn(OAc)_3$, Cu(OAC)2, Bi_2O_3. Swern oxidation, Sommelet reaction, Elbs reaction, Oxidative coupling of phenols, Prevost reaction and Woodward modification.

Reduction: palladium /platinum /rhodium /nickel based heterogeneous catalysts for hydrogenation, Wilkinson‘s catalyst, Noyori asymmetric hydrogenation. Reductions using Li/Na/Ca in liquid ammonia.

UNIT – V

Retrosynthesis

Concepts in organic synthesis: retrosynthesis, disconnection, synthons, linear and convergentsynthesis, umpolung of reactivity, protecting functional groups, protection of NH and OH groups, acetals as protecting groups for diols, protection of carbonyl groups in aldehydes and etones, protection of the carboxyl group, protection of double and triple bonds.

Course outcomes:

At the completion of this course the student will be able to

1. *Identify ,classify and draw structures of organic molecules*
2. *Apply the basic rules of organic nomenclature to interrelate between structures of organic molecules*
3. *Learning about Organic Photochemistry, Pericyclic reaction & Retrosynsynthesis.*

References:

1. P.S.Kalsi, Organic reactins and mechanisms, II Edition, New Age International Publishers (2000).
2. Jerry March, Advanced Organic Chemistry, IV Edition, Wiley-Interscience Publication (1992).
3. I.L.Finar, Organic Chemistry, Vol. II, V Edition, First Indian reprint, Pearson Education Asia Pvt. Ltd. (2000).
4. O.P.Agarwal, Chemistry of Natural Products, Vol. I, Green Publishing House (1997).

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7. S.M. Mukherji and S. P. Singh, Reaction Mechanism in Organic Chemistry, 1st Edition, Macmillan (1976).
8. Organic chemistry VII edition, Morrison and Boyd.(Retro synthesis)
   Strateges and tactics in organic synthesis, M. Harmata.
   Organic synthesis – Disconnection approach, Stuart Warren

CC - VIII: PHYSICAL CHEMISTRY – II

SEMESTER: III **SUBJECT CODE: 21PCH8**

CREDITS: 5 **TOTAL HOURS: 6**

Objectives:

1. *To understand about the classical mechanics and wave mechanics*
2. *To study the approximation methods*
3. *To learn the fundamentals of Group theory*
4. *To know the application of Group theory to Spectroscopy*
5. *To study the Rotational, Vibrational, Raman and Electronic spectrum*

UNIT – I

Basic concepts of Quantum mechanics

Classical mechanics – #General principles, basic assumptions, postulates of classical mechanics, conservation laws, Lagrange's and Hamilton's equations of Motion (no derivation)#.

Wave particle dualism – uncertainty principles – functions-orthogonality and Normalisation - operator - operator algebra. Linear and Hermitian - eigen function and eigen values. Angular momentum operator--commutation relations.

Postulates of quantum mechanics – Solving the Schrodinger wave equation (SWE) to simple systems viz., particle in a box – one and three dimensional, (1D and 3D box).

UNIT – II

Applications of Quantum Mehanics

Setting and solving Schrodinger wave equation for harmonic oscillator, rigid-rotator, hydrogen and hydrogen like atoms (He^+ and Li^{2+}). Shapes of atomic orbitals - radial and angular probability distribution functions.

Approximation methods – linear variation principle, application to hydrogen and helium atoms, perturbation method for non-degenerate systems, application of perturbation theory to helium atom. Pauli's principle and Slater determinants – variation method – application of perturbation theory to helium atom. Hertree – Forkself consistent field method. L – S and J – J coupling.

Born – Openheimer approximation: Hydrogen molecule ion. LCAO method. MO and VB treatments of the hydrogen molecule. Hybridization and molecular orbitals of H_2O, NH_3 and

CH_4.Huckel pi-electron method for butadiene and benzene.

UNIT – III

Concepts of Group Theory

Elements of group theory – definition – group multiplication tables for C_2V and C_3V point groups – conjugate classes, conjugate and normal subgroups – symmetry elements and operations – point groups – assignment of point groups to molecules, - Matrix representation of geometric transformation and point groups – reducible and irreducible representations– Great Orthogonality Theorm -properties of irreducible representation – construction of character tables – C_2V, C_3V, C_2h.

UNIT – IV

Application of Group Theory to Spectroscopy

Symmetry of Normal modes of vibrations, application of Group theory to normal modes of vibrations and normal mode analysis – symmetry properties of integrals – application for spectral selection rules-Vibration spectra – IR and Raman active fundamentals symmetry of molecular orbitals and symmetry selection rule for electronic transitions in simple molecules like H_2O, NH_3 and CO_2 - Construction of hybrid orbitals and predicting hybridization for the molecules CH_4 and. BF_3.

UNIT - V

Fundamentals of molecular spectroscopy

Rotational spectrum: Diatomic molecules. Energy levels of a rigid rotor selection rules. Poly atomic molecules - Isotope effect. Vibrational spectrum: Infrared spectrum: vibrating diatomic molecules, diatomic vibrating rotator-. Raman spectrum: Rayleigh and Raman scattering stokes and antistokes lines, concept of polarizarity, pure rotational Raman spectra - vibrational Raman spectra Electronic spectrum : Electronic spectra of diatomic molecules – Born-Oppenheimer approximation – Franck -Condon principle – Dissociation energy – Rotational fine structure - Fortrat diagram

Course outcomes:

Student understood the knowledge about:

1. *Classical mechanics and applications of wave mechanics*
2. *The Variation and Perturbation method*
3. *LCAO, MO and VB treatments of the Hydrogen molecule*
4. *Symmetry elements, operations and point groups*

References

Unit – I &II

1. R.K. Prasad, Quantum Chemistry, third Reprint new age International limited.
2. Quantum Chemistry, Ira N. Levine Prentice Hall.
3. Introduction to Quantum Chemistry, A.K. Chandra Tata Megraw Hill.

Unit – III & IV

4. P.W. Atkins, Physical chemistry, ELBS.
5. Chemical Applications of group theory, F.A. Cotton.

Unit – V

6. C.N. Banwell, Fundamentals of molecular spectroscopy

CC - IX: INORGANIC CHEMISTRY – III - BIOINORGANIC CHEMISTRY

SEMESTER: III **SUBJECT CODE: 21PCH9**

CREDITS: 5 **TOTAL HOURS: 6**

Objectives:

1. *To study about the metal ions in biological system*
2. *To learn about the metalloproteins and metalloenzymes*
3. *To study the characterization techniques for the biological process*
4. *To study the Nitrogen fixation and photo systems*
5. *To know the medicinal bioinorganic chemistry*

UNIT – I

Metal ions in biological systems

Classification of metallobiomolecules - Occurrence and availability of metal ions - Role of metal ion in biological system – Biomineralization, Function of biominerals, calcium, silica and iron biominerals – Role of nonmetals in biological systems.

Transport across the membrane: Gibbs - Donnen equilibrium, Macrocyclic crown ethers, cryptands and spherands – Ionophores - Na^+/K^+ pump – Calcium pump. Bioenergetics: Oxidation of glucose and role of phosphate – Glycolysis – Citric acid cycle.

UNIT – II

Metalloproteins and Metalloenzymes

Copper: Blue copper proteins, ceruloplasmin – Calcium binding proteins – Important iron proteins.

Heme proteins and oxygen uptake, structure and function of haemoglobin, myoglobin, hemocyanins, and hemerythrin – Synthetic oxygen carriers.

Electron transfer proteins: Iron-Sulphur proteins, Ferridoxins, Rubrdoxins.

Metalloenzymes: Catalase, peroxidase (Fe) – Superoxide dismutase, Cytochrome C oxidase (Cu) – Carboxy peptidase and Carbonic anhydrase (Zn) – Urease (Ni)

UNIT – III

Physical Methods in Bioinorganic Chemistry

Important methods used to analyze bioinorganic species: X-ray Diffraction, X-ray Absorption Spectroscopy (XAS), Electron Paramagnetic Resonance (EPR) Spectroscopy, Nuclear Magnetic Resonance (NMR) Spectroscopy, Mossbauer Spectroscopy, Electronic and Vibrational Spectroscopy, Circular Dichroism and Magnetic Circular Dichroism, Mass Spectrometry

UNIT – IV

Nitrogen Fixation and Photosystem

Biological Nitrogen fixation: Definition – Kinetic and thermodynamic aspects – Nitrogenase: Occurrence, composition, structural aspects, Nitrogenase-substrate reactions and different functions in nitrogenase – Reaction pathway for the reduction of N_2 – Binding of N_2 at Mo center – Abiological nitrogen fixation by complexation – Vanadium nitrogenase – Model systems for nitrogenase.

Chlorophylls, photo system I, photo system- II in the cleavage of water, model systems.

UNIT – V

Medicinal Bioinorganic Chemistry

Metal ion toxicity-Sources –general mechanism of metal ion toxicity – chemical speciation of metals in environment – Toxic effects of metals: Cadmium, Mercury, Aluminium, Iron and Copper. Detoxification – Basic requirements of chelating drug - Detoxification by metal chelates (representative chelating drugs). Chemotherapy – Cisplatin in chemotherapy – Drug action and mechanism – Gold containing drugs as Anti-Rheumatic agents – Lithium in Psychopharmacological drugs.

Course outcomes:

Student understood the knowledge about:

1. *Significance of metal ions*
2. *Composition and function of the biominerals*
3. *Role of macrocyclic ligands in the transport of ions*
4. *Metallo proteins and its role in the biological process*
5. *Structure and function of metalloenzymes*
6. *Characterization tools for the biological process*
7. *Mechanism of biological nitrogen fixation and photosynthesis*

8. *Toxic effects of metals*
9. *Detoxification of metal ions*
10. *Metal containing drugs for the treatment of variety of diseases*

References

Unit – I, II, III, IV &V

1. Principles of Bioinorganic chemistry, S.J.Lippard and J.M.Berg. University Science Book.
2. Bioorganic chemistry, I.Bertini, H.B.Gray, S.J.Lippard and J.S.Valentine, University Science Books.
3. Inorganic Biochemistry Vol.I&Vol.II L. Ed. G. Eichhorn, Elsevier.
4. Hussain Reddy, Bioinorganic chemistry.

EC – III – CHOICE - I

PHYSICAL METHODS IN CHEMISTRY

SEMESTER: III **SUBJECT CODE: 21PCHE3**

CREDITS: 5 **TOTAL HOURS: 6**

Objectives

1. To understand the electronic transitions in inorganic compounds
2. To identify the vibrational characteristics of inorganic molecules.
3. To learn the magnetic environment of magnetically active atoms present in the molecules
4. To know the structure of inorganic compound using NMR technique.
5. To understand the concept of Mossbauer spectroscopy and its applications.
6. To interpret the structure of crystals by X-ray analysis

UNIT I

Electronic Spectra of Transition metal complexes

Spectroscopic ground states, spectral terms, R-S coupling and J-J couplings- term symbol – selection rules—microstates—Pigeon hole diagram for p^2 and d^2 configuration. Orgel and Tanabe – sugano diagrams for transition metal completes (d^1-d^9 states) electronic spectra of transition metal complexes—calculation of Dq values -- Racah parameters and Beta parameters, Nephelexatic effect, charge transfer spectra.

Magnetic properties—Types of magnetism, quenching of orbital angular momentum (A,E and T term).determination of magnetic susceptibility by Guoy method. Magnetic properties of lanthanides and actinides.

UNIT – II

IR and Raman Spectroscopy

Combined uses of IR and Raman spectroscopy in the structural elucidation of simple molecules likeH_2O, ClF_3, NO_3 ion, ClO_3 ion, - effect of coordination on ligand vibrations - uses of group vibrations in in the structural elcidation of metal complexes of urea, thiourea, cyanide, thiocyanate, nitrate, sulphate, and dimethyl sulphoxid e - effect of isotopic substitution on the vibrational spectra of molecules - vibrational Spectra of metal carbonyls with reference to the

nature of bonding, geometry, nd number of C-O stretching vibrations- group theoretical treatment.-

UNIT – III

NMR spectroscopy

Nuclear spin, Nuclear resonance, saturation, Shielding of magnetic nuclei - chemical shift and its measurement, factors influencing chemical shift --deshielding, spin-spin interaction. Factors influencing coupling constant, spin decoupling.^{13}C NMR, ^{31}P NMR, P-NMR, FT-NMR. Spectrum of paramagnetic molecules – Isotropic shift—lanthanide shift reagents – fluxional behaviour of molecules.

ESR- Zeeman effect, hyperflinesplittings (isotropic systems) – coupling constants –Zero field splitting and Kramers degeneracy – esr of transition metal complexes. McConnell equation - g-value - factors affecting g-value.

UNIT – IV

Mossbauer spectroscopy

Experimental considerations-the sample- temperature measurement-spectrometer - Fundamentals-Doppler effect –spectrum and its parameters-simple spin states - higher spinstates-magnetic splitting - Isomer shift - Quadrupole splitting-the additive model – Interpretation - Iron, antimony, Tin and gold compounds -unusual intensities - recoil free fraction- non zero asymmetry parameter - magnetic ordering and magnetic relaxation.

UNIT –V

Crystallographic Analysis

Lattices and symmetries Reciprocal lattice Crystal symmetry Point groups Plane groups and space group - Difference between crystal symmetry and molecular symmetry Diffraction of light – principles of X-ray diffraction: geometry -X-ray diffraction: intensity- Electron diffraction - Neutron diffraction - crystal structures and diffraction patterns - Practical aspects of X-ray diffraction Practical aspects of electron diffraction

Photo electron spectroscopy (PES) – principle and applications.

Course outcomes:

Student understood the knowledge about:

1. The concept of electronic transitions in transition metals are learnt

2. Vibrational frequencies of ligand and their complexes are understood.
3. The difference between IR and Raman spectroscopy and their applications are learnt.
4. The applications of NMR spectroscopy to know the chemical environment in inorganic complexes are learnt.
5. Concept of Mossbauer spectroscopy and their applications are understood
6. Interpretation of crystal structure.

References

1. Modern spectroscopy, J.M.Hollas, John Wiley.
2. Physical methods in chemistry, R.S.Drago, SaundersCollege
3. Introduction to Molecular Spectroscopy, G.M.Barrow, Mc.Graw Hill.
4. Introduction to Magnetic Resonance, A.Carrington and A.D.Maclachalan.
5. Group theory and Application to Chemistry, K.V.Raman, New Delhi, Tata. Mc Graw Hill.

EC – III – CHOICE - II

FOOD CHEMISTRY AND ADULTERATION

SEMESTER: III **SUBJECT CODE: 21PCHE3**

CREDITS: 5 **TOTAL HOURS: 6**

Objectives:

1. *On completion of this course student will have knowledge of*
2. *Basics of food groups and water purification process*
3. *Constituents of food*
4. *Food Additives*
5. *Food and Pesticides*
6. *Food Adultration*

UNIT I

Introduction

Food: source, functions of food – food groups – food guide – basic five food groups, usage of the food guide – food in relation to health – objectives of cooking. Water: Purification processes – Ion exchangers, reverse osmosis, activated charcoal treatment - Use of chlorination, ozone, and UV light disinfection. Specification of drinking water.

UNIT II

Constituents of Foods

Carbohydrates: Classification, Principles involved in the analysis of carbohydrates – estimation of carbohydrates. Proteins: amino acids – peptides - Analysis of proteins – Separation of amino acids by paper chromatography. Minerals and vitamins: Sources, functions, deficiency of the following minerals (calcium, iron, iodine, fluorine, sodium and potassium (elementary treatment). Vitamins - classification, sources, Vitamins – A, D, E and K, C, B Complex, - B6 & B12.

UNIT III

Food Additives

Artificial sweeteners – saccharin, cyclomate, asparatame – food flavours – esters, aldehydes and heterocyclic compounds. Antioxidants. Food colours – changes in cooking..Restricted use. Spurious colours. Emulsifying agents, preservatives – leavening agents. Baking powder –Yeast. Taste enhancers – MSG-vinegar.

UNIT IV

Pesticides Control

Spoilage of foods by insects and pests. Loss in food quantity and quality. Various pesticides used in agriculture and post-harvest storage, uses of pesticides for food grain application.

UNIT V

Food Adulteration

Common adulterants in different foods – milk and milk products, vegetable oils, and fats, spices and condiments, cereals, pulses, sweetening agents and beverages. Contamination with toxic chemicals – pesticides and insecticides. .

Course outcomes:

1. *To know about the basic criteria of food and water standards for consumption*
2. *To get a basic idea about the chemical constituents of food*
3. *To learn about the various food additives, their chemical composition and their permissible level of usage in foods.*
4. *To know about the various organisms which spoil the crops pre and post harvest and their control using pesticides*
5. *To know about the various food adulterants for different types of food and methods to detect those adulteration.*

Reference

1. Owen R Fennema, ‒Food Chemistry‖, Marcel Decker Inc., New York. 1996.
2. M. Swaminathan ‒Text Book on Food chemistry‖, Printing and Publishing CO., Ltd. 1993.
3. B. Siva Sankar, ‒Food Processing and Preservatio‖, Prentice – Hall of India Pvt. Ltd., New Delhi. 2002.
4. S. Ramakrishnan, K. G. Prasannam, R. Rajan, ‖Principles - Text book of medical biochemistry‖, Orient Longman Ltd. Third Edition

EC – III – CHOICE - III

CATALYSIS AND CATALYTIC PROCESSES

SEMESTER: III **SUBJECT CODE: 21PCHE3**

CREDITS: 5 **TOTAL HOURS: 6**

Objectives:

1. *To learn about acid base and asymmetric catalysis*
2. *To study the surface phenomena and micellar catalysis*
3. *To study the reaction mechanism of heterogeneous catalysis*
4. *To know the importance of PTC*
5. *To study the characterization techniques for catalysts*

UNIT - I

Introduction to catalysis

Types of catalysis, characteristics of catalyst, catalyst supports, promoters, general mechanism of catalysis, equilibrium treatment and steady state treatment. Activation energies of catalyzed reactions.

Acid - base catalysis, specific acid - base catalysis, general acid base catalysis, mechanism of acid – base catalysis, catalytic activity and acid - base strength - Bronsted relationships.

Acidity functions: Types of acidity functions. Hammett acidity function. Measurement of Hammett acidity function (Ho), usefulness of Hammett acidity function in understanding the mechanism of an acid catalyzed reactions. Zucker - Hammett hypothesis and its applications. Bunnett – Olson‘s criteria of acid-base catalyzed reactions with examples. Catalysis by transition metal ions and their complexes. Use of Ziegler – Natta and metallocene catalysts as homogeneous catalysts for polymerization of olefins. Application of metal ion catalysis to the hydrogenation of alkenes, hydroformylation, oxidation and isomerization reactions.

Asymmetric Catalysis–Introduction, Catalysts, Commercial Applications, Asymmetric Hydrogenation, Enantioselective Isomerization: L-Menthol, Asymmetric Epoxidation.

UNIT - II

Micellar catalysis

Surface tension, Curved interfaces, The Laplace equation and Capillary action. Thermodynamics

of surface layers – Adsorption: Types of adsorption, factors effecting adsorption, Chemistry and thermodynamics of adsorption. Determination of heats and entropies of adsorption. Surface versus bulk structures. Adsorbate - induced restructuring of surfaces.

Micelles: Classification of surface active agents. Micellization and micellar interactions. Structure of micelles – spherical and laminar. Critical micellar concentration (CMC). Factors affecting the CMC of surfactants. Counter ion binding to micelles. Thermodynamics of micellization. Phase separation and mass action models, solubilization, micro emulsion, reverse micelles. Reactions assisted by micelle formation. Examples of micelle - catalyzed reactions and their mechanisms.

UNIT - III

Heterogeneous catalysis

Heterogeneous catalysis. Broad categories of catalysts – metals, bimetals, semiconductors, insulators, zeolites, oxides, nanomaterials. Preparation of metal catalysts, supported metal catalysts and non- metallic catalysts. Coprecipitation, Impregnation, sol-gel method, deposition-precipitation, hydrothermal synthesis, pulsed laser methods, plasma chemical methods, chemical vapor deposition methods

Steps in heterogeneous catalyzed reactions. Diffusion and adsorption. Mechanism of surfacecatalyzed reactions. Adsorption isotherms - Langmiur Hinshelwood model, Rideal - Eley mechanism, Kinetics and thermodynamics of catalysed reactions. Catalytic activity – the determining factors. Structure sensitive and structure insensitive catalysts.

UNIT - IV

Phase transfer and Photo catalysis

Phase-transfer catalysis (PTC): Principles of phase - transfer catalysis. PTC classification. Role of water in phase - transfer catalyzed reactions. Factors influencing the rate of PTC reactions. Inverse phase transfer catalysis. Mechanism of nucleophilic displacement reactions. Crown ethers: Crown ethers as phase transfer catalysts (PTC) in the reaction of alkyl halides with super oxide. Permanganate oxidation of alkenes and phenols in presence of PTC‘s viz., quarternary ammonium salts and crown ethers.

Photo catalysis: Photocatalytic effect, metal semiconductor systems as photo catalysts, nature of the metal loaded, extent of metal loading, nature of semiconductor, doped semiconductors,

coupled Semiconductors. Application of photocatalysis for splitting of water by semiconductor particles, removal of organic and inorganic pollutants, for oxidation and reduction of organic compounds.

UNIT - V

Characterization of catalysts

Surface area by BET method. Determination of pore volume and pore size distribution by BJH method. Pore size and specificity of catalysts. Surface acidity of catalysts - Determination of surface acidity by indicator method, IR spectroscopic method and TPD methods. Surface characterization by XRD, LEED, TEM & AFM, XPS, AES, techniques. Auto exhaust emissions - catalytic converters. Catalytic hydrogenation and oxidation reactions. Cracking and reforming. Fischer-Tropsch synthesis of methanol.

Course outcomes:

1. *Mechanism of acid base catalysis*
2. *Theory of adsorption and micellar interactions*
3. *Steps in heterogeneous catalyzed reactions*
4. *Application of photocatalysis*
5. *Surface characterization by different techniques*

References

1. Principles of Heterogeneous Catalysis in practice, G. C. Bond, Oxford Publishing
2. Heterogeneous Catalysis, C. Satterfield, McGraw Hill
3. Catalysis, Principles and applications, edited by B. Vishwanathan, S. Sivasanker & A. V.Rama Swamy, Narosa Publishing House
4. Catalysis, J. C. Kuriacose, Macmillan
5. Colloidal and surface chemistry , M. Satake, Y. Hayashi, Y.Mido, S.A.Iqbal and M.S.sethi
6. " Physical Organic Chemistry" by L.P.Hammett, chapter 9 , McGraw Hill .
7. Chemical Review, 57, 1935(1957), M.A. Paul and F.A. Long
8. Phase Transfer Catalysis, Fundamentals, Applications and Industrial perspective, C. M. Stark,
C. Liotta & M. Halpern, Academic Press
9. Phase Transfer Catalysis, E. V. Dehmlow & S. S. Dehmlow, Verlag Chemie, Weinheim

10. Phase Transfer Catalysis in Organic synthesis, W. P. Weber & G. W. Gokel, Springer
11. Hand book of phase transfer catalysisEdited by Y. Sasson and R. Neumann
12. Catalysis in Micellar and Macromolecular systems, J. H. Feudler & E. J. Feudler, Acad. Press
13. Reaction Kinetics in Micelles, E. H. Codes (ed), Plenum
14. Micelles – Theoretical and Applied aspets, V.Moroi, plenum
15. Physical Chemistry of surfaces, A.W.Adamson and A.P.gast, Wiley
16. Polymer supported Catalysts, C. U. Pittman Jr, vol 8, Comprensive Organometallic Chemistry
17. Principles and Practice of Heterogeneous Catalysis, J. M.Thomas andW.J.Thomas, VCH1997.
18. Spectroscopy in catalysis – An introduction by J. W. Niemantsverdriet.

CP - VIII: PHYSICAL CHEMISTRY PRACTICAL – I

SEMESTER: III & IV **SUBJECT CODE: 21PCH13P**

CREDITS: 5 **TOTAL HOURS: 6**

Objectives:

1. *To know about the molecular weight determination methods*
2. *To study the determination of distribution coefficient and equilibrium constant*
3. *To learn comparison of acids by kinetic studies*
4. *To understand about Conductometric titrations*
5. *To study the Potentiometric titrations*

Non Electrical

1. Determination of molecular weight of given unknown substance by Rast Method (Determination of K_f value of given solvent)
2. Determination of molecular weight by transition temperature method. (Determination of K_f value of given substance)
3. CST of phenol – water system – Effect of impurities on CST.
4. Determination of eutectic temperature and eutectic composition of a primary mixture of compound A & B (phase diagram of compound formation)
5. i. Determination of partition or distribution coefficient of iodine between CCl_4 and water.
   ii. Determination of equilibrium constant of the reaction between Kl and I_2 and to find out the concentration of the given KI solution.
6. Comparison of strength of acid by kinetics of hydrolysis of ester.
7. Determination of energy of activation (E_a) and Arrhenius factor (A) for the acid catalysed hydrolysis of ester.
8. Effect of ionic strength on kinetics of reaction – primary salt effect (Determination of concentration of the given KNO_3 solution)
9. Determination of concentration of the given oxalic acid by studying the adsorption of oxalic acid on charcoal (Adsorption Isotherm)
10. Determination of solubility and heat of solution of the given oxalic acid.

PHYSICAL CHEMISTRY PRACTICAL (Electrical)

Conductometric titrations

1. Determination of strength of strong and weak acid present in the given mixture of acids using 0.1N NaOH and crystalline NH_4Cl.
2. Determination of strength of NaOH and NaOAc present in the given mixture using 0.1N HCl and crystalline NaOAc.
3. Determination of strength of HCl and NH_4Cl in the given mixture using 0.1N NaOH and crystalling NH_4Cl.
4. Determination of strength of Cl^- and I^- present in the given mixture of halides using 0.1N $AgNO_3$ and crystalline Kcl (conductometric precipitation titration)
5. Determination of ionization constant of a weak acid (determination of cell constant of a conductivity cell)
6. Determination of strength of K_2SO_4 (conductometric precipitation titration) determination of solubility and solubility product of $BaCl_2$.

Potentiometric Titrations

1. Determination of strength of strong and weak acid potentiometrically using 0.1N NaOH and a standard solution of HCl.
2. Determination of strength of given ferrous sulphate solution potentiometrically using ferrous sulphate (standard solution) and 0.1N $K_2Cr_2O_7$ (link solution)
3. Determination of strength of given KI solution using KI (standard solution) and $KMnO_4$ (link solution) (potentiometric redox titration)
4. Determination of strength of Cl^- and I^- ions present in the given solutions using 0.04N $AgNO_3$ solution and 0.02 N KCl (standard solution).

Course outcomes:

Student understood the knowledge about:

1. *The molecular weight determination methods*
2. *Determination of partition coefficients*
3. *Eutectic temperature and eutectic composition of a primary mixture*
4. *Determination of energy of activation and Arrhenius factor*

5. *The adsorption method*
6. *Determination of acid – base strength by conductometric titrations*
7. *Determination of strength of halides by conductometric precipitation titration*
8. *Determination of strength of KI solution by potentiometric redox titration*

SEMESTER – IV

CC - X: ORGANIC CHEMISTRY - III

SEMESTER: IV **SUBJECT CODE: 21PCH10**

CREDITS: 5 **TOTAL HOURS: 6**

Objectives

1. *To develop the knowledge aromatic and Aliphatic Nucleophilic & Electrophilic Substitutions reactions.*
2. *To study the organic applications of different types of spectroscopic techniques.*
3. *To learn the applications of various reaction in organic synthesis.*

UNIT – I

Aliphatic nucleophilic substitution: SN1, SN2, and SNi mechanisms - effect of substrate structure, leaving group, attacking nucleophile and solvent - neighboring group participation - substitution in allylic carbons and reactivity - ambident nucleophiles.

Aliphatic electrophilic substitution : SE1,SE2, and SEi mechanism - effect of substrate structure, leaving groups, attacking electrophiles and solvent-Stark - Enamine reaction - decarboxilation of aliphatic acids- halogenation of aldehydes and ketones.

UNIT – II

Aromatic electrophilic substitution: Aromatic ion mechanism-orientation and reactivity - nitration, halogenation, friedel Craft reaction - Gattermann, Kolbe-Schmidt , Reimer -Tiemann, Hauben - Hoesch reactions.

Aromatic Nucleophilic substitution: SNAr, SN1, benzyne, SRN1 mechanisms – effect of sustrate structure, leaving groups, attacking nucleophiles and solvents – selected reactions – Zeigler alkylation, Chichibabin reaction - reactions involving diazonium group as leaving group – cine substitution – von Richter reaction.

UNIT – III

Elimination reactions: E1, E2, E1cb and Ei mechanisms- stereo chemistry of eliminations – Hoffman and Saytzeff rules - competition between elimination and substitution reactions - Chugaev reaction-dehydration of alcohols - dehydrohalogenation-Hoffman degradation-cope elimination - Bredt‘s rule

Addition reactions : Addition to carbon – carbon multiple bonds-electrophilic addition - nucleophilic free radical additions, orientation and reactivity - Birch reduction, hydroxylation, hydroboration, epoxidation, Diels - Alder reaction, Michael addition, ozonolysis, carbenes and their addition to double bonds.

Addition to carbonyl groups : Mannich , crossed cannizzaro , Stobbe , Benzoin , formation of ketenes , openauer oxidation , MPV reduction , Darzen's glycidic ester condensation, wittig reactions.

UNIT – IV

Molecular rearrangements: Mechanism of the following - wagner Meerwin-Dienone phenol – Wolf – Lozson – Schmidt - Bayer Villiger – Stevens – Wittig - Favoraski rearrangements.

Reagents in Organic Syntheses: Complex metl hydrides – $LiAlH_4$, $NaBH_4$, tri tert-butoxyaluminium hydride, Gilman's reagents, Lithium dimethylcuprate, lithium di - isopropyl amide, dicyclohexylcarbodiimides, 1,3-dithianestrimethyl silyl odide, DDZ, SeO_3 – phase transfer catalyst, Crown ethers and Merrifield resins.

UNIT - V

Natural products: Isolation and detection of natural products – a brief outline to carotenoids, flavonoids and anthocynins with one example each (structural elucidation not needed)

Terpenes: structural elucidation , Medicinal values and synthesis of α-pinene, camphor and zingiberene – biosyntheses of terpenes.

Alkaloids: Structural elucidation, medicinal values and synthesis of quinine, reserpine, morphine, cinchonine and papavarine – biosyntheses of alkaloids.

Vitamins: Physiological importance – structural elucidation of vitamins –B1, B2, B6, E and K.

Course outcomes:

Student understood the knowledge about:

1. *Recall reagents and predict products for a defined set of organic reactions.*
2. *To understand the naming reaction and molecular rearrangement*
3. *To have and importance of natural products, Terpenes Alkaloids and Vitamins*

References:

1. J. March, –Advanced Organic Chemistry : Reactions, Mechanisms and Structure‖,4th ed., Wiley, 1992.
2. R.K. Bansal, –Organic Reaction Mechanisms‖, Tata McGraw Hill, 1975.
3. P. S. Kalsi, –Organic Reactions and their Mechanisms‖, New Age International Publishers.
4. I.L. Finar, –Organic Chemistry‖, Vol.II, 5 th ed., ELBS 1975.
5. O.P. Agarwal, Chemistry of Organic Natural Products, Vol. I & II, Goel Publications, 1997.
6. F.A. Carey and R.J. Sunberg, –Advanced Organic Chemistry, Parts A & B, Plenum, 1984.
7. T.H. Lowry and K.S.Richardson, –Mechanism and Theory in Organic Chemistry‖,Harper and Row, 1976.

CC - XI: PHYSICAL CHEMISTRY - III

SEMESTER: IV **SUBJECT CODE: 21PCH11**

CREDITS: 5 **TOTAL HOURS: 6**

Objectives

1. *To study about the activity of ions*
2. *To know about the electro-kinetic phenomena*
3. *To study about the electro-analytical methods*
4. *To study about thermal methods of analysis*
5. *To learn the computer applications in chemistry*

UNIT – I

Electrochemistry I

Electrode- Electrolyte equilibrium- Thermodynamic quantities from EMF data. Nernst equation- and its limitations- equilibrium electrode potentials- classification of electrodes - concentration cells- liquid junction potentials.

Electrolytic conductance Debye-Huckel-Onsager theory – Debye Falkenhagen and Wien effect. -Electrode – electrolyte equilibrium, electrode potential – concentration cells. Processes at Electrodes- The rate of charge transfer - current density – Electokinetic phenomena: - electro osmosis-electrophopreseis- sedimentation potential - Theories of electrical double layer-Electrical double layer potential -zeta potential- theory of multiple layers at electrode electrolyte interface-double layer capacity- Butler – Volmer Equation – Tafel equation –, Applications: Fuel cells and power storage.

UNIT – II

Electrochemisry II

Electrocapillary phenomena: Electrocapillary curves – ECM. Lippmann equation and Lippman potential –Capillary electrometer – contact angle method.

Polarography: Principle, experimental technique – dropping mercury electrode – Residual, migration and diffusion currents – Half-wave potential – Ilkovic equation – Analytical applications of polorography – Differential pulse polorography -cyclic voltametry– principle, experimental setup – application – Amperometric titration – principle and types –Titration between Pb2+and K2Cr2O7. electrogravimetry – theory of electrolysis, experimental set up diagram- applications – ion selective electrodes: principle and applications – DSC: Principle and

applications – TMA: Principle and applications

UNIT – III

Surface Phenomena

Gibbs adsorption isotherm – solid- liquid interfaces – contact angle and wetting – solid-gas interface – physisorption and chemisorption – Langmuir, BET isotherms – surface area determination. Kinetics of surface reactions involving adsorbed species – Langmuir-Hinshelwood mechanism, Langmuir – Rideal mechanism – Rideal –Eley mechanism. Some interfacial aspects on Micelles, Reverse micelles, Micro emulsions and Membranes.

UNIT – IV

Thermal methods of Analysis

Thermal methods of analysis – Principle – instrumentation –methods of obtaining thermogram- TGA curves for $AgNO_3$, $CuSO_4$, CaC_2O_4,H_2O Differential thermal analysis – Principle –instrumentation – DTA curves for the above compounds. Factors influencing DTA - applications of DTA. Study of Organic reactions, Decomposition of complexes, Thermometric titration.Principle and Applications of SEM, TEM and XRD.

UNIT – V

Computer in chemistry

C programming – structure of a C program – Steps for Compiling and executing the Programs – Character set and keywords – Constants – Variables – operator – Loops in C - Data types, variables, constants, keywords, operators, expressions. Statements – if, if-else, nested if-else, while, while-do, for, nested for, go to, continue, break, switch case statements. Arrays– string functions – preprocessors – storage class – structure, union.

Calculation of reduced mass, molecular weight using sub-routine program - Determination of activity coefficient using while loop - Calculation of second order rate constant – solving quadratic equation for the calculation of solubility of a sparingly soluble salt - Determining of Ea and A using call function.

Course outcomes:

Student understood the knowledge about:

1. Transport of ions in solution
2. Nernst electrical equation and its limitations
3. Theories of double layer and theory of multiple layers

4. Primary and secondary batteries and energy storage system
5. Analytical applications of polorography
6. Electro-gravimetric analysis and its applications
7. Applications of Thermo-gravimetric method
8. C programming applications to simple chemistry problems

References

Unit-I & III

1. Bockris J O M and Reddy A K N, Modern electrochemistry Volumes I & II. New York, Plenum Press, 1970.
2. Glasstone S An introduction to electrochemistry, New Delhi, East – West Press Pvt. Ltd., 1956

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3. Noel M and Vasu K I, Cyclic Voltametry and the frontiers of electrochemistry, Oxford & IBH, 1990
4. F.W. Fifield and D. Kealey, ―Principles and practice of Analytical Chemistry‖, Blackwell Publishing,Fifthh Edition, 2000.
5. J.S. Fritz and G.H. Scheink, ―Quantitative Analytical Chemistry‖,Allyn and Bacon, Inc., Boston, Fifth Edition, 1987.

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6. G.D. Christian, Analytical Chemistry‖, John Wiley and Sons, Inc., Fifth Edition, 1994.
7. D.A. Skoog, D.M. West, F.J. Holler and S.R. Crouch, ―Fundamentals of AnalyticalChemistry‖, Thomson-Brooks.Cole, Eigth Edition, 2004.
8. H.H. Willard, L.L Merritt, J.A. Dean and F.A. Settle, Jr., CBS Publishers and Distributors, New Delhi, Sixth Edition, 1986

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9. K.V. Raman, Computers in Chemistry, Tata McGraw Hill, New Delhi, 1993.
10. Kishore Arora ,Computer Applications in Chemistry, Anmol Publications, New Delhi, 2004.

CC - XII: ORGANIC SPECTROSCOPY

SEMESTER: IV **SUBJECT CODE: 21PCH12**

CREDITS: 5 **TOTAL HOURS: 6**

Objectives

1. To understand the electronic transitions in organic compounds
2. To identify the vibrational properties of organic molecules.
3. To learn the magnetic environment of magnetically active atoms present in the molecules
4. To know the structure of organic compound using NMR technique.
5. To understand the concept of mass spectrometry.

UNIT – I

UV – VIS and ORD – CD

UV – VIS: Laws of light absorption – chromophores and auxochromes – types of electronic transitions – bathochromic, hypsochromic, hypochromic and hyperchromic effects; Applications of UV – VIS spectroscopy – use of model compounds and additivity – dienes, polyenes and α, β – unsaturated carbonyl compounds – Woodward – Fieser rules – Calculation of λmax for organic molecules; absorption spectra of polyenes, polyenyenes and aromatic compounds; stereochemical factors in electronic spectroscopy;

ORD – CD: Definition – circular birefringence and circular dichroism; plain dispersion curves and their applications; single and multiple cotton effect curves; structural and stereochemical applications – axial haloketone rule, octant rule for ketones; comparison of ORD and CD.

UNIT – II

IR and Raman

IR **:** Charecteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines - Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance.

Raman **:** Theory, application of Raman spectra to organic, inorganic and biological species, quantitative applications, Resonance Raman spectroscopy.

UNIT – III

^{1}H NMR

General introduction and definition, chemical shift, spin – spin interaction, shielding mechanism. Chemical shift values and chemical exchange, effect of deuteration, complex spin-spin interaction between two, three, four, and five nuclei (first order spectra), virtual coupling, coupling constant. Simplification of complex spectra using - nuclear magnetic double resonance, contact shift reagents - solvent effects. Fourier transform technique - Nuclear Overhauser effect (NOE).

UNIT – IV

^{13}C NMR

^{13}C NMR : Distinction between ^{1}H and ^{13}C NMR – theory and experiment – factors affecting intensity of signals – nuclear Overhauser effect – chemical shift and its dependence on polar and steric effects (gamma gauche effect); additivity relationships - C-C and C-H couplings – off resonance, gated and single frequency decouplings – relationship between coupling constant and _s' character; effect of shift reagents on ^{13}C chemical shifts; applications of ^{13}C NMR to find the different carbon functional groups. COSY, NOESY, ROSY,CIDNP and INDOR.

UNIT – V

Mass spectrometry

Introduction, ion production – EI, CI, FD and FAB, factors affecting fragmentation, Ion analysis, ion abundance. Mass spectral fragmentation of organic compounds. Common functional groups, molecular ion peak, meta stable peak, Mclafferty rearrangement. Nitrogen rule. High resolution mass spectrometry. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

Applicationsof Spectroscopy :UV- Visible, IR, 1H NMR, 13C NMR, MASS-interpretation of common organic compounds.

Course outcomes:

1. The concept of electronic transitions are learnt
2. Assigning vibrational frequencies to different functional groups are understood.
3. The difference between IR and Raman spectroscopy and their applications are learnt.
4. The applications of NMR spectroscopy to know the chemical environment are learnt.

5. Concept of mass spectrometry and their applications are understood
6. Solving spectroscopic problems are learnt.

References

1. William Kemp, Organic Spectroscopy, ELBS II Edition, Spectroscopy of organic compounds.

2. P.S. Kalsi, Organic Spectroscopy, Wiley Eastern Ltd, Madras.

3. R.M. Silverstein, C.G. Bassler and Monsil, Spectrometric identification of organic compounds, John Wiley & Sons, New York.

4. J. Dyer, Application of absorption spectroscopy of organic compounds, Prentice Hall of India Pvt. Ltd., New Delhi.

5. W.Kemp, NMR in Chemistry, MacMillan Ltd, 1986.

6. J.B. Lambert, H.F. Shunnel, L. Verbit, R.G. Cooks and G.H. Stout, Organic structural analysis, MacMillan, 1976.

7. G.C. Levy and G.L. Nelson, Carbon – 13 Nuclear Magnetic Resonance for organic chemists, Wiley – Interscience, 1972.

8. R.A.W. Johnstone, Mass spectrometry for organic chemists, Cambridge, 1972.

9. M.C. Hamming and N.G. Foster, Interpretation of Mass spectra of organic compounds, Academic Press, 1972.

10. C.Djerassi, Optical rotatory dispersion – application to organic chemistry, McGraw Hill, 1960.

11. R.J. Abraham and P. Loftus, Proton and carbon – 13 spectroscopy, Heydon& Sons., 1978.

12. D.H. Williams and I.Fleming, Spectroscopic methods in organic chemistry, Tata McGraw Hill, 4th Edition, 1988.

PW - I: PROJECT WORK

SEMESTER: IV **SUBJECT CODE: 21PCH14**

CREDITS: 5 **TOTAL HOURS: 6**

The student has to submit a comprehensive experimental project report on a selected topic in chemistry.

During the fourth semester the project work may be carried out either in the college laboratory.

General Objectives

1. *To learn about the basic concept of the project work.*
2. *To know about designing new experiments and carry out the experiments.*
3. *To know about the various characterization techniques used to characterize the synthesized compounds.*
4. *To know about the necessities of literature survey and to learn about writing dissertationof project work.*

Course outcomes:

1. To identify the topic with the consideration feasibility.
2. To learn the procedure of literature survey on the concerned topic.
3. To derive a plan for executing the work in the stipulated time with maximum efficiency and success.
4. Understanding and learning various technical and safety aspects of the concerned topic related work.
5. To learn, adapt, and practice the extensive bench work in a research laboratory.
6. To prepare the dissertation report with complete follow up of research methodology.

H.H. THE RAJAH'S COLLEGE (AUTONOMOUS), PUDUKKOTTAI
PG & RESEARCH DEPARTMENT OF CHEMISTRY
QUESTION PAPER PATTERN
M.Sc., CHEMISTRY
(Effective from the academic year 2021 – 2022 onwards)

PG Internal & External Pattern for Theory

	Maximum	Minimum
Internal Marks:	25	13
External Marks:	75	37
Total Marks:	100	50

Part – A Answer All the Questions 10 x 2 = 20 Marks	Part – B Internal Choice Type 5 x 5 = 25 Marks	Part – C Answer any Three Questions 3 x 10 = 30 Marks
Question	Question	Question
1,2 – I Unit	11a (or) 11b – I Unit	16 – I Unit
3,4 – II Unit	12a (or) 12b – II Unit	17 – II Unit
5,6 – III Unit	13a (or) 13b – III Unit	18 – III Unit
7,8 – IV Unit	14a (or) 14b – IV Unit	19 – IV Unit
9,10 – V Unit	15a (or) 15b – V Unit	20 – V Unit

PG Internal & External Pattern for Practical

	Maximum	Minimum
Internal Marks:	40	20
External Marks:	60	30
Total Marks:	100	50

PG INTERNAL PATTERN

PG – THEORY

Internal test	-	50 Marks
Assignment 1&2	-	20 Marks
Seminar	-	05 Marks
Model Exam	-	75 Marks
Total Marks	-	**150 Marks**

PG PRACTICAL

Observation Note	-	20
Program Completion	-	20
Model Exam	-	60
Total Marks	-	100

Internal Assessment reduced to 25 marks for Theory & 40 Marks for Practical

For Practical: Record- 10 Marks, Vivavoce - 05 Marks, Practical - 45 Marks = **60 marks**

For Project

Plan of the Project	- 10 Marks
Execution of the plan/ Collection of data/ Organization of materials/ Fabrication/ Instruments	- 45 Marks
Individual initiative (Internal Assessment)	- 25 Marks
Vivavoce	- 20 Marks
Total	**100 Marks**

மாட்சிமை தங்கிய மன்னர் கல்லூரி (தன்னாட்சி)
புதுக்கோட்டை - 622 001.
வேதியியல் துறை

பாடத் திட்டக் குழுமம் 2021-2023

இத்துடன் இணைக்கபெற்ற இளநிலை, முதுநிலை, ஆய்வியல் நிறைஞர் மற்றும் துணைப் பாடங்களின் பாடத் திட்டங்கள் கீழ்கண்ட குழுவினரால் ஏற்கப் பெற்று அமுல் படுத்த சூன் 2021 முதல் சேர்க்கையாகின்ற மாணவர்களுக்கு பரிந்துரை செய்கிறது.

பாடத் திட்டக் குழுவினர் பெயர்கள்	கையொப்பம்
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