Bajaj College of Science, Wardha (Autonomous College)
SUBJECT: CHEMISTRY
BOARD OF STUDIES MEETING (13th April, 2022)

Syllabus of M.Sc. II/Semester III (WEF 2022-23)

Course Code: PG–CHEM(02)-S3-T1-SP1

Paper–IX : Special I-Organic Chemistry [L-T-P = 4-0-0]

60 h (4 h per week): 15 h per unit **80 Marks**

Unit-I

Photochemistry: 15L

Interaction of radiation with matter, types of excitation, rate of excited molecules, quenching, Quantum efficiency, quantum yield, transfer of excitation energy, singlet and triplet states, experimental methods in photochemistry of carbonyl compounds, and transition, Norrish type I and Norrish type II reactions Paterno–Buchi reaction, Photoreduction, Photochemistry of enones, Hydrogen abstraction rearrangement of unsaturated ketones and cyclohexadienones, Photochemistry of parabenzoquinones, photochemistry of Aromatic compounds with reference to isomerisation additon and substitution Photochemical isomerization of cis and trans alkenes, Photochemical cyclization of reaction, Photo-Fries rearrangement, di-pi methane rearrangement, Photo theory reaction of anilides, photochemistry of vision, Applications of photochemical methods in synthesis: Isocomene, Cedrene, Hirsutene

Unit-II

Pericyclic Reactions: 15L

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1, 3, 5-hexatriene, allyl system, classification of pericyclic reaction. FMO approach, Woodward-Hoffman correlation diagram method and Perturbation of Molecular Orbital (PMO) approach of pericyclic reaction under thermal and photochemical conditions Electrocyclic reactions, conrotatary and disrotatary motion 4n and (4n+2) systems, Cycloaddition reaction with more emphasis on [2+2] and [4+2], Cycloaddition of ketones Secondary effects in [4+2] cycloaddition. Stereochemical effects and effect of substituents on rate of cycloaddition reaction, Diels-Alder reaction, 1,3-dipolar cycloaddition and chelotropic reaction. Sigmotropic rearrangement, suprafacial, and antarafacial shift involving carbon moieties, retention and inversion of configuration, [3,3] and [3,5] sigmotropic rearrangements, Claisen, Cope, Sommelet-Hauser rearrangements, Ene reaction.

Unit-III

Oxidation and Reduction: 15L

a) Oxidation:

i) Oxidation of alkanes, aromatic hydrocarbons and alkenes, Dehydrogenation with S, Se, Fremy's salt, DDQ, chloranil and $PhI(OAc)_2$, Oxidation with SeO_2, Epoxidation of olefins, Sharpless asymmetric epoxidation, Dihydroxylation of olefins using $KMnO_4$, OsO_4, Woodward and Prevost dihydroxylation, Oxidative cleavage of olefins, Ozonolysis.

ii) Oxidation of alcohols: Chromium reagents, pyridinium chlorochromate (PCC), pyridinium dichromate (PDC), Collin and Jones reagent, Combination of DMSO with DCC, $(COCl)_2$, NCS and $(CH_3CO)_2O$ for oxidation of alcohols, Oxidation with MnO_2, Oppenauer oxidation

iii) Oxidation of aldehydes and ketones, Conversion of ketones to α, β-unsaturated ketones and α-hydroxy ketones, Baeyer-Villiger oxidation , Chemistry and synthetic applications of $Pb(OAc)_4$, Dess-Martin periiodinane, IBX.

(Advantages and limitations of reagents should be covered during teaching)

b) Reduction:

i) Catalytic heterogeneous and homogeneous hydrogenation, Hydrogenation of alkenes, alkynes and arenes, Selectivity of reduction, Mechanism and stereochemistry of reduction of Raney Ni-catalyst, Adam catalyst, Lindlar catalyst, Wilkinson catalyst.

ii) Reduction by dissolving metals, Reduction of carbonyl compounds, conjugated systems, aromatic compounds and alkynes. Birch reduction, Hydrogenolysis

iii) Reduction by hydride transfer reagents: Meerwein-Pondorff-Verley reduction, Reduction with $LiAlH_4$ and $NaBH_4$, stereochemical aspects of hydride addition, Derivatives of $LiAlH_4$ and $NaBH_4$, Selectivity issues, Diisobutylaluminium hydride (DIBAL-H), Sodium cyanoborohydride, Reduction with boranes and derivatives, Reduction with Bu_3SnH, Reduction of carbonyl group to methylene, Reduction with diimide and trialkylsilanes

(Advantages and limitations of reagents should be covered during teaching)

Unit-IV

Chemistry of P, S, Si, and Boron compounds: 15L

a) Phosphours and sulphur ylide: Preperation and their synthetic application along with stereochemistry.

b) Umpolung concept: Dipole inversion, generation of acyl anion, use of 1,3-dithiane, ethylmethylthiomethylsulphoxide, bis-phenylthiomethane, metallated enol ethers, alkylidene dithiane, ketone thioacetals, 2-propenethiobismethyl thioallyl anion, thiamine hydrochloride based generation of acyl anion.

c) Organoboranes: preparation and properties of organoborane reagents e.g. RBH_2, R_2BH, R_3B, 9-BBN, catechol borane, Thexyl borane, cyclohexyl borane, $ICPBH_2$, IPC_2BH, Hydrboration- mechanism, stereo and regeoselectivity, uses in synthesis of primary, secondary tertiary alcohols, aldehydes, ketones, alkenes, Synthesis of EE, EZ, ZZ dienes and alkyenes. Mechanism of addition of IPC_2BH. Allyl boranes- synthesis, mechanism and uses.

d) Organo silicon compounds in organic synthesis: Me_3SiCl, Me_3SiH and Paterson synthesis

Reference books:

1] Books as suggested in Semester I for organic chemistry
2] Organic Synthesis, The disconnection approach-S. Warren
3] Designing Organic Synthesis-S. Warren
4] Some Modern Methods of Organic Synthesis-W. Carruthers
5] Advance Organic Chemistry Part-B-F. A. Caray and R. J. Sundberg Plenum Press
6] Protective Group in Organic Synthesis-T. W. Greene and PGM
7] The Chemistry of Organo Phosphorous-A. J. Kirbi and S.G. Warren
8] Organo Silicon Compound-C. Eabon
9] Organic Synthesis via Boranes-H. C. Brown
10] Organo Borane Chemistry-T. P. Onak
11] Organic Chemistry of Boron-W. Gerrard
12] Fundamentals of Photochemistry-K. K. Rohatgi-Mukharji, Wiley Eastern Limited
13] Photochemistry-Cundau and Gilbert
14] Aspects of Organic Photochemistry-W. M. Horspoot
15] Photochemistry-J. D. Calvert
16] Photochemistry-R. P. Wayne

Course Code: PG–CHEM(02)-S3-T2-SP2

Paper–X Special II-Organic Chemistry [L-T-P = 4-0-0]

60 h (4 h per week): 15 h per unit **80 Marks**

Unit-I

Terpenoids and Porphyrins: 15L

A] Terpenoids: Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Structure determination, stereochemistry, and synthesis of the following representative molecules: Citral, Geraniol, α-terpeneol, Menthol, Farnesol, Zingiberene, Santonin, Phytol, Abietic acid and β-carotene, Vitamin A Genesis of biological isoprene unit, Biosynthesis (ONLY) of the following terpenoids: α & β-myrecene, linalool, geraniol, α-terpeneol, limonene, camphor, α-pinene, β-pinene, farnesol, β-bisabolene and squalene.

B] Porphyrins: Structure and synthesis of Haemoglobin and Chlorophyll.

Unit-II

Alkaloids and Prostaglandins: 15L

A] Alkaloids: Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, role of alkaloids in plants Structure, stereochemistry, and synthesis of the following: Ephedrine, (+)-Coniine, Nicotine, Atropine, Quinine, Reserpine and Morphine. Biosynthesis (ONLY) of the followings: Hygrine, Tropinone, Nicotine, Pelletierine, Conine.

B] Prostaglandins: Occurrence, nomenclature, classification, biogenesis and physiological effects. Synthesis of PGE_2 and $PGF_{2\alpha}$.

Unit-III

Steroids and Plant Pigments: 15L

A] Steroids: Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of Cholesterol, Bile acids, Androsterone, Testosterone, Estrone, Progesterone and Aldosterone.

Biosynthesis of steroids (lanosterol)

B] Plant Pigments: Occurrence, nomenclature and general methods of structure determination, isolation and synthesis of Apigenin, Luteolin, Quercetin, Myrcetin, Quercetin-3-glucoside, Vitexin, Diadzein, Butein, Cyanidin-7-arabinoside, Cyanidin, Hirsutidin.

Biosynthesis of flavonoids: Acetate pathway and Shikimic acid pathway

Unit-IV

Carbohydrates, amino acids, proteins and peptides: 15L

A] Carbohydrate: Types of naturally occurring sugars, deoxy sugars, amino sugars, branched chain sugars, methyl ethers and acid derivatives of sugars, general methods of structure and ring size determination with reference to maltose, lactose, sucrose.

Chemistry of starch and cellulose.

B] Amino acids, protein and peptides: Amino acids, structural characteristics, acid-base property, stereochemistry of amino acids, optical resolution, Strecker synthesis, peptide and proteins structure of peptide and protein, primary, secondary, tertiary and quaternary

structure. Reaction of polypeptide, structure determination of polypeptide, Solid phase peptide synthesis, end group analysis.

Reference books:

1] Chemistry of Alkloids-S. W. Pelletier
2] Chemistry of Steroids-L. F. Fisher and M. Fisher
3] The Molecules of Nature-J. B. Hendricsion
4] Biogenesis of Natural Compound - Benfield
5] Natural Product Chemistry and Biological Significance- J. Mann, R. S Devison, J. B. Hobbs, D. V. Banthripde and J. B. Horborne
6] Introduction to Flavonoids-B. A. Bohm, Harwood
7] Chemistry of Naturally Occurring Quinines-R. H. Thomson
8] The Systematic Identification of Flavonoids- Marby, Markham, and Thomos
9] Text Book of Organic Medicinal Chemistry-Wilson, Geswold
10] Medicinal Chemistry Vol I and II-Burger
11] Synthetic Organic Chemistry -Gurudeep Chatwal.
12] Organic Chemistry of Natural Products Vol I and II-O. P. Agrawal
13] Organic Chemistry of Natural Products -Gurudeep Chatwal
14] A Textbook of Pharmaceutical Chemistry-Jayshree Ghosh
15] Synthetic Dyes Series -Venkatraman
16] Chemistry Process Industries-Shreve and Brink
17] Principal of Modern Heterocyclic Chemistry-L. A. Paquelte
18] Heterocyclic Chemistry-J. Joule and G. Smith
19] Heterocyclic Chemistry-Morton
20] An Introduction to Chemistry of Heterocyclic Compound-J. B. Acheson
21] Introduction to Medicinal Chemistry-A. Gringuadge
22] Wilson and Gisvold Text Book of Organic Medicinal and Pharmaceutical Chemistry-Ed. Robert F Dorge
23] An Introduction to Drug Design-S. S. Pandey and J. R. Demmock
24] Polymer Science-V. Govarikar
25] Principle of Polymer Chemistry-P. J. Flory
26] An Outline of Polymer Chemistry-James Q. Allen
27] Organic Polymer Chemistry-K. J. Saunders

Course Code: PG –CHEM(02)-S3-P1
Practical –V Special Organic Chemistry Practical I [L-T-P = 0-0-8]

8 h per week **100 Marks**

[A] Quantitative Analysis

Student is expected to carry out following estimations (minimum 6 estimations)

1. Estimation of Vitamin "C" Iodometry.
2. Estimation of Phenol by $KBrO_3$-KBr.
3. Estimation of Aniline by Bromate/ Bromide solution.
4. Estimation of Formaldyde by Iodometry.
5. Estimation of Glucose by Benedict's solution.
6. Estimation of given carbonyl compound by hydrazone formation.
7. Estimation of Aldehyde by Oxidation method.
8. Determination of percentage of number of hydroxyl group in an organic compound by acetylation method.

[B] Isolation of Organic Compounds from Natural Source (Any Six)

a) Isolation of caffeine from tea leaves.
b) Isolation of casein from milk (the students are required to try some typical colour reactions of proteins)
c) Isolation of lactose from milk (purity of sugar should be checked by TLC and PC and Rf value reported.)
d) Isolation of nicotine dipicrate from tobacco
e) Isolation of cinchonine from cinchona bark
f) Isolation of piperine from black pepper
g) Isolation of lycopene from tomatoes
h) Isolation of β-carotene from carrots
i) Isolation of cysteine from hair
j) Isolation of oleic acid from olive oil (involving the preparation of complex with urea and separation of linoleic acid
k) Isolation of eugenol from cloves
l) Isolation of (+) limonine from citrus rinds

[C] QUALITATIVE ANALYSIS

Separation of the components of a mixture of three organic compounds.

Three solids, two solids and one liquid, two liquids and one solid, all three liquids and identification of any two components using chemical methods or physical techniques. (Minimum 10-12 mixtures to be analyzed)

Course Code: PG –CHEM(02)-S3-T3-EL1

Paper–XI Elective I - Environmental Chemistry I [L-T-P = 4-0-0]

60 h (4 h per week): 15 h per unit **80 Marks**

Unit –I: Concept and scope of Environmental Chemistry: **15 h**

Biosphere, Lithosphere, Hydrosphere and Atmosphere, Ecological principles- aspects of ecology, classification, and types of ecosystems.

Atmospheric chemistry: Composition of atmosphere; photochemical reactions in atmosphere; smog formation, types of smog (sulphur smog and photochemical smog), aerosols; chemistry of acid rain, reactions of NO_X and SO_X; free radicals and ozone layer depletion, role of CFCs in ozone depletion.

Toxic elements & their hazards: Essential & non-essential elements, Impact of toxic chemicals on enzymes, Biochemical effects of As, Cd, Pb and Hg, their metabolism, toxicity and treatment.

Unit-II: Water **15 h**

Origin, physico-chemical properties of water, sources of water, hydrological cycle, criteria of water quality. Types and sources of water pollution. Impact on humans, plants and animals. Measurement of water quality parameters: sampling and analysis for pH, EC, turbidity, TDS, hardness, chlorides, salinity, DO, BOD, COD, nitrates, phosphates, sulphates, heavy metals and organic contaminants. Microbiological analysis MPN. Indian standards for drinking water (IS:10500, 2012).

Unit-III: **Soil** **15 h**

Chemical and mineralogical composition of soil, classification of soil, types of soil- saline and alkaline, Types and sources of soil pollution, classification of soil pollutants, impact of soil pollution on air quality, Specifications for disposal of sewage and effluent on land for irrigation and ground water recharge.

Soil Pollution control: Methodology of waste water disposal on land in India. Management of saline and alkaline soil, soil indicator plants.

Unit IV: Air **15 h**

Major regions of the atmosphere, composition of the atmosphere, temperature inversion and air pollution episodes, photochemistry of the atmosphere, depletion of the stratospheric ozone, green house effect, green house gases, remedial measures for reversion of green house effect, acid rain, photochemical smog, particulate matter. Natural versus polluted air, air quality standards.

Air pollution control: Control of automobile emission and control measures in thermal power stations.

Course Code: PG –CHEM(02)-S3-P2

Practical –VI : Elective-Environmental Chemistry Practical [L-T-P = 0-0-8]

8h per week **Marks-100**

WATER ANALYSIS

1. Sampling of water-tap water, overhead storage tank water, pond water and lake water
2. Physico –chemical and organoleptic characteristics of the above water sample
3. Statistical evolution of the data obtained for optimization of result
4. Determination of total solids, total dissolved solids and total suspended solids and its significance
5. Determination and comparison of chlorine content in tap water, storage tank and swimming pool

6 Determination of acidity and alkalinity in water samples
7 Determination of total, permanent and temporary hardness of water sample
8 Determination of DO, COD, and BOD of water sample
9 Analysis of chemicals used in water and waste water treatment-alum, bleaching powder, activated carbon
10 Analysis of iron and manganese in water sample by visual titrimetry
11 Analysis of copper and nickel in water sample by Spectrophotometry
12 Analysis of phenol in water sample by Spectrophotometry
13 Analysis of nitrite in water sample by Spectrophotometry
14 Analysis of chromium in water sample
15 Analysis of chloride in water sample
16 Analysis of sulphate in water sample
17 Determination of turbidity of a given water sample
18 Estimation of Na, K, by flame photometry in given water

AIR ANALYSIS

1 Determination of SOx and NOx and TSPM (total suspended particulate matter) and RSPM in ambient air

SOIL ANALYSIS

1 Analysis of different parameters of soil like pH, conductivity, alkalinity etc.
2 Determination of N,K, P of soil by flame photometry
3 Analysis of nutrients-nitrogen (total, ammonia, nitrite & nitrate), phosphate total
4 Determination of macro &micro nutrients in soil

Reference books:

1. Water analysis : J. Rodier
2. A Text book of Inorganic Analysis : A.I.Vogel
3. Colorimetric Determination of metals : E.B.Sandell
4. Environmental Chemistry : Moore J W and Moore E A. Academic Press, New York, 1976.
5. Environment and Man Vol VII: The Chemical Environment Edited by J Lenihar and W Fleecher Vlackie Publication, 1977.
6. The Chemistry of Environment: R A Horne, Wiley Interscience Publication 1978.
7. Fundamentals of Air Pollution: A C Stern
8. Instrumental Methods of Analysis: Willard,Merrit and Dean
9. Analytical Chemistry: Meites and Thomas
10. Standard Methods for Examination of water and waste water: A E Greenberg, A D Eaton, APHA, AWWA,WEF
11. Chemistry for Environmental Engineering and Science: C N Sawyer, P L McCarty and G F Parkin
12. Laboratory Manual for the Examination of Water, waste water and soil: H H Rupa and H Krist, V C H Publication
13. Manual on Water and Waste water analysis: D S Ramteke and C A Moghe, NEERI
14. Environmental Chemistry: B K Sharma and H Kaur
15. Environmental Chemistry: A K De
16. Environmental Pollution- Management and control for sustainable Development: R K Khatoliya
17. Environmental Chemistry: A K Bhagi and G R Chatwal
18. Environmental Chemistry : P.S. Sindhu

Course Code: PG –CHEM(02)-S3-T3-EL1

Paper–XI Elective I - Polymer Chemistry I [L-T-P = 4-0-0]

60 h (4 h per week): 15 h per unit **80 Marks**

Unit-I: Introduction to polymers **15h**

Basic Concept, raw materials for polymers. Nomenclature and classification of polymers, Polymerization: condensation, addition, radical chain- ionic and co-ordination and co-polymerization and their mechanisms, Types of polymers- linear, branched, crosslinked, ladder, thermoplastic, thermosetting, fibres, elastomers, natural polymers, addition and condensation polymers. Stereoregular polymers- atactic, syndiotactic and isotactic.

Unit-II: Molar mass and its determination **15h**

Molecular mass and molar distribution. Number average, mass average, viscosity, average molecular mass and relation between them. Molecular mass distribution. Determination of molecular mass- Osmometry (membrane and vapour phase), light scattering, gel permeation chromatography, sedimentation and ultracentrifuge, viscosity method and end-group analysis.

Unit III: Physical characteristics of polymers **15h**

Morphology and order in crystalline polymers. Configuration of polymer chains, crystal structure of polymers. Morphology of crystalline polymers, strain-induced morphology, crystallization and melting. The glass transition temperature (Tg), relationship between T_g and T_T, Effect of molecular weight, dilments, chemical structure, chain topology, branching and cross linking. Methods of determination of glass transition and crystallinity of polymers.

Unit IV: Commercial polymers **15h**

A) Organic polymers: Commercial polymers, synthesis and and application of polyethylene, Cellulose Acetate, PMMA, polyaimdes, polyesters, Urea resins and eposy resins.

B) Functional Polymers: Conducting polymers, polymeric reagents, polymer supports and catalysts, Photoresponsive Polymers, polymers in lithography Immobilization of Enzymes.

Course Code: PG –CHEM(02)-S3-P2

Practical –VI: Elective- Polymer Chemistry Practical [L-T-P = 0-0-8]

8h per week **Marks-100**

1. Synthesis of polymers:
   a) Synthesis of Thiokol rubber (condensation)
   b) Urea-formaldehyde (condensation)
   c) Glyptal resin: glycerine phthalic acid (crosslinked Polymer Chemistry)
   d) Polyacryonitril (bulk polymerization)
   e) Polyacryonitril (emulsion polymerization)
   f) Polymethylomethacrylate (emulsion of suspension Polymer Chemistry)
   g) Nylon-66 (interfacial polycondensation)
   h) Coordination polymers
   i) Conducting polymer (electro- or peroxodisulphate oxidation)
2. Characterization of polymers:
   a) End-group analysis
   b) Viscosity and molecular mass

c) Density of polymer by flotation methods
d) IR spectra.

3. Purification and fractionation of polymer, polystyrene, Nylon 66, PMMA.
4. Magnetic and electrical properties of polymers, magnetic susceptibility and electrical conductivity of coordination and conducting polymers.
5. Thermal analysis and degradation of polymers:
   i. TGA: Isothermal and non-isothermal;
   ii. DTA: Glass transition temperature and melting point
6. Crystallinity of polymers by density measurement.
7. Swelling and solubility parameters of polymers.
8. Synthesis of Graft-Polymers and its characterization by density and IR spectra.
9. Dielectric behavior of polymers.
10. Kinetics of polymerization:
    a) Polycondensation
    b) Peroxide initiation polymerization.

Reference books:

1. Textbook of polymer science: F.W. Billmayer Jr. Wiley.
2. Polymer science: V.R. Gowarikar, N. V. Viswanathan and J. Sreedhar, Wiley-Eastern.
3. Fractional monomers and polymers: K Takemoto, Y. Inaki, and R.M. Ottam Brite.
4. Contemporaty polymer chemistry: H.R. Alcock and F. W. Lambe, Prentice Hall.
5. Principles of polymer Chemistry: Flory, Cornell Univ. press.
6. Introduction to polymer chemistry: R. B. Seymour, McGraw Hill.
7. Principles of polymerization: Odian.
8. A first course in polymer chemistry: A. Strepikheyew, V. Derevistkay and G. Slonimasky, Mir Publishers, Moscow.
9. Laboratory preparation of macro chemistry: EMM effery, McGraw Hill Co.
10. A practical course in polymer chemistry: S. J. Punea , Pergamon Press.

Course Code: PG–CHEM(02)-S3-T3-EL1

Paper–XI Elective I - Medicinal Chemistry I [L-T-P = 4-0-0]

60 h (4 h per week): 15 h per unit **80 Marks**

UNIT-I: **15 h**

Drug Design

Development of new drugs, factors affecting development of new drugs, sources of lead compounds, serendipity and drug development. Concept of QSAR, QSAR methods and parameters, procedure followed in drug design, structure activity relationship (SAR) method, Free and Wilson analysis, Hansch analysis, concept of prodrugs and softdrugs, SOFT DRUGS, isosterism, bioisosterism, drug receptors, theories of drug action, types of reversible enzyme inhibitors, some special inhibitors and design of inhibitors.

UNIT-II: **15 h**

A] Pharmacokinetics and pharmacodynamics: Indroduction drugs absorption, distribution and disposition of drugs, excretion and elimination, Pharmacokinetics of elimination and Pharmacokinetics in drug development process.

Pharmacodynamics: Introduction, enzyme stimulation, enzyme inhibition, membrane active drugs, drugs metabolism, biotransformation and significance of drug metabolism

B] Diuretics: Introduction, mode of action, loop diuretics. Synthesis of Bumetanide,

Frusemide, Ethacrynic acid, clorexolone Quinethazone.

C] Analgesics and Antipyretics: Introduction, mode of action, evaluation of analgetic agents. Synthesis of: Aspirin, salsalate, phenacetin, phenylbutazone, Indomethacin, Analgin.

UNIT-III: **15 h**

A] Cardiovascular Drugs: Introduction, cardiovascular diseases, Synthesis and uses of cardiovascular drugs; amyl nitrate, diltiazem, varapamil, methyldopa, atenolol, sorbitrate, quinidine, oxyprenolol.

B] Antineoplastic Agent: Introduction, mechanism of tumor formation, treatment of cancer, types of cancer chemotherapy, role of alkylating agents and antimetabolites in treatment of cancer, carcinolytic antibiotics, mitotic inhibitors, harmones, natural products. Synthesis of melphalan , thiotepa, lomustine.

UNIT-IV: **15 h**

A] Psychoactive drugs: Introduction, neurotransmitters, structure of nerve cell, chemical transmitters, CNS depressants, sedative and hypnotics, Synthesis of Barbiturates, Phenobarbital, thiopental sodium, diazepam, lorazepam, bromazepam, ethosuximide, general anaesthetic: Antianxiety drugs, synthesis of oxazepam, alprazolam, puspirone, antipsychotic drugs and antidepressant drugs, MAO inhibitors, antimanic drugs, synthesis of thiopental sodium, ethiosuxmide, glutethimide, trimethadione, phenytoin.

B] Coagulant and Anticoagulants: Introduction, factors affecting coagulant and anti-coagulant. Mechanism of Blood coagulation and Anticoagulation. Structure of Vitamin K1, Vitamin K2 and heparin. Synthesis of Coumarins and indanediones.

Course Code: PG –CHEM(02)-S3-P2

Practical –VI: Elective- Medicinal Chemistry Practical [L-T-P = 0-0-8]

8 h per week **Marks-100**

1. Volumetric estimation of Ibuprofen.
2. Estimation of aspirin by volumetric and instrumental methods.
3. Analysis of ascorbic acid in biological/tablet sample.
4. Determination of paracetamol by colorimetry.
5. Analysis of ampicillin trihydrate.
6. Determination of vitamin B12 in commercial sample by spectrophotometry.
7. Determination of phenobarbitone in given cough syrup.
8. Determination of tetracycline in given capsule.
9. Determination of iron, calcium and phosphorus from milk or drug sample.
10. To perform I.P. monograph of tablet.
11. Estimation of chloride in serum and Urine.
12. Separation and determination of sulpha drugs in tablets or ointments.

Preparation of Drugs: Synthesis, purification and identification of (8-10) of the following drugs.

1. Benzocaine from p-nitrobenzoic acid.
2. Dapsone from diphenyl sulphone.
3. Paracetamol from p-nitro phenol.
4. Uracil from sulphanil amide.
5. Diphenyl hydantion from benzoin.
6. Aluminium asprin from salicylic acid.
7. 4,6-diphenyl-thiazine from chalcone.
8. 6/8 nitro coumarin from resorcinol.
9. Copper aspirin from salicylic acid.
10. N-acetyl parabanic acid.
11. Nerolin from 2-naphthol
12. Phenothiazine from diphenylamine
13. Umbelliferon from resorcinol
14. Benzylidene from benzaldehyde and aniline
15. 1-phenyl-1,2-pentadine-3-one from benzaldehyde
16. 1,5 diphenyl-1,3-pentadiene-2-one from benzaldehyde
17. 1,3-diphenyl-prop-2-ene-1-one
18. 3-methy pyrazol-5-one from ethylacetoacetate
19. 6-methyl uracil from ethylacetoacetate
20. Sulphanilamide from acetanilide
21. Barbituric acid (4-hudroxyuracil) from diethylmalonate.
22. 2,3-dimethyl-1-Phenylpyrazol-5-one(Antipyrin)from ethylacetoacetate
23. Fenbufen
24. 2-Phenylbenzo-4-pyrone (falvone)from o-hydroxyacetophenone
25. Chlorobutanol from acetone
26. 2,4-dioxypiperazine from glycine

<u>Reference books</u>:

1. Text book of organic medicinal chemistry-Wilson,Geswold
2. Medicinal chemistry Vil I and II-Burger
3. A textbook of pharmaceitical chemistry-Jayshree Ghosh
4. Introduction to medicinal chemistry-A Gringuadge
5. Wilson andGisvold text book of organic medicinal and pharmaceutical chemistry-Ed.Robert F Dorge
6. An introduction to drug design-S S Pandey,and JR Demmock
7. Goodman and Gilmans pharmacological basis of therapeutics- Stragies for organic drug sythesis and design-D Lednicer
8. Textbook of Medicinal Chemistry- A. Kar
9. Medicinal Chemistry – D Sriram and P. Yogeeswari

Course Code: PG –CHEM(02)-S3-T4

Paper–XII : Spectroscopy – I (Core Subject Centric) [L-T-P = 4-0-0]

60 h (4 h per week): 15 h per unit **80 Marks**

Unit-I

Symmetry properties of molecules and group theory: 15L

Symmetry elements and symmetry operations. Properties of group. Point groups and Schoenflies symbols. Symmetry operations as a group. Matrix representations of groups. Multiplication table for C_{2v} and C_{3v}. Reducible and irreducible representations. Similarity transformation. Classes of symmetry operations. Great Orthogonality Theorem. Derivation of character tables for H_2O and NH_3 using Great Orthogonality Theorem. Application of character tables in selection rules of IR, Raman and Electronic spectroscopy.

Unit-II

Microwave and Mössbauer Spectroscopy: 15L

A] Microwave spectroscopy: Classification of molecules on the basis of M. I., rigid and non rigid rotor, effect of isotopic substitution on transition frequencies, stark effect, microwave spectrometer, application in deriving: molecular structure, dipole moment, atomic mass. Width and intensity of spectral transitions, Fourier transform microwave spectroscopy, rotation spectra of poly atomic molecules. Numericals.

B] Mössbauer spectroscopy:

Basic principle, experimental techniques, recoil emission and absorption, source, absorber, isomer shift, quadrupole interaction, magnetic hyperfine interaction, applications in determining electronic structure, molecular structure, crystal symmetry, magnetic structure, surface studies, biological applications.

Unit-III

Infrared and Raman Spectroscopy: 15L

A] Infrared spectroscopy: Diatomic molecules: Molecules as harmonic oscillator, zero point energy, Anharmonic oscillator, Morse potential energy function, vibrational spectrum, fundamental vibrational frequencies. Force constant, the interactions of rotations and vibrations. P, Q, R branches, vibration of polyatomic molecules, selection rules, normal modes of vibration, IR spectra, regions of IR, Characteristic vibrational frequencies of functional groups, overtone and combination frequencies,. Numericals. Structural information from IR spectroscopy, Structural determination of organic molecules by IR spectroscopy, problems based on IR spectral data.

B] Raman Spectroscopy: Rayleigh scattering. Raman Scattering, classical and quantum theories of Raman effect. Rotational Raman Spectra for linear and symmetric top molecules. Vibrational Raman Spectra, rotational fine structure. Selection rules, coherent anti-Stokes Raman spectroscopy, Structure determination from Raman and Infra-red spectroscopy, Surface enhanced raman spectroscopy(SERS), Numericals.

Unit-IV

Diffraction techniques: 15L

A] X ray diffraction: Braggs condition, Miller indices, Laue method, Bragg method, Debye Scherrer method, identification of unit cells from systematic absences in diffraction pattern, structure of simple lattices and x-ray intensity, structure factor and its relation to intensity and electron density, absolute configuration of molecules.

B] Electron diffraction: scattering intensity vs scattering angle, Wierl equation, measurement techniques, elucidation of structure of simple gas phase molecules, low energy electron diffraction and structure of surfaces.

C] Neutron diffraction: Scattering of neutrons by solids and liquids, magnetic scattering, measurement techniques, elucidation of structure of magnetically ordered unit cell.

Reference books:

1] Spectroscopic identification of organic compound-RM Silverstein,GC Bassler and TC Morril, John Wally
2] Introduction to NMR spectroscopy-R. J. Abraham, J. Fisher and P Loftus Wiely
3] Application of Spectroscopy to Organic Compound-J. R. Dyer, Printice Hall
4] Organic Spectroscopy-William Kemp, ELBS with McMillan
5] Spectroscopy of Organic Molecule-PS Kalsi, Wiley, Esterna, New Delhi
6] Organic Spectroscopy-RT Morrison and RN Boyd
7] Practical NMR Spectroscopy-ML Martin, JJ Delpench, and DJ Martyin
8] Spectroscopic Methods in Organic Chemistry-DH Willson, I Fleming
9] Fundamentals of Molecular Spectroscopy-CN Banwell
10] Spectroscopy in Organic Chemistry-CNR Rao and JR Ferraro
11] Photoelectron Spectroscopy-Baber and Betteridge
12] Electron Spin Resonance Spectroscopy-J Wertz and JR Bolten
13] NMR –Basic Principle and Application-H Guntur
14] Interpretation of NMR spectra-Roy H Bible
15] Interpretation of IR spectra-NB Coulthop
16] Electron Spin Resonance Theory and Applications-W gordy
17] Mass Spectrometry Organic Chemical Applications, JH Banyon

OR

Course Code: PG –CHEM(02)-S3-T4

Paper–XII : (Foundation Course-I) Applied Analytical Chemistry–I [L-T-P = 4-0-0]

60 h (4 h per week): 15 h per unit **80 Marks**

Unit-I: Analysis of Pesticides and Fertilizers **15h**

***Pesticides*:** General introduction, analysis of pesticides in general with reference to DDT, Dieldrin, Malathion, Parathion, BHC by different analytical methods such as titrimetric, colorimetric, chromatography and electroanalytical methods.

***Fertilizers*:** Sampling and sample preparation, determination of water, total nitrogen, urea, total phosphates, potassium, acid or base forming quality.

Unit-II: Forensic chemistry **15h**

Introduction: Classification of poisons on the basis of physical states, mode of action and chemical properties with examples of each type. Methods of administration. Action of poisons in body. Factors affecting poisoning. Study of some common poisons used for suicide. Signs and symptoms of As, Pb, Hg and cyanide poisoning. Poisonous effects of kerosene and cooking gas.

Unit-III: Analysis of petroleum and petroleum products **15h**

Introduction, determination of flash and fire point, Pensky Marten's apparatus, cloud and pour point, aniline point, drop point, viscosity and viscosity index, Redwood and Saybolt viscometer, API specific gravity, water and sulphur in petroleum products, carbon residue, corrosion stability, decomposition stability, emulsification, neutralization and saponification number.

Unit-IV: Analysis of alloys **15h**

Definition of alloy. phase diagrams of Fe-C, Pb-Sn, Pb-Ag systems and their applications. Types of steel: hypoeutectic, hypereutectic steels, mild steel, and stainless steel. Uses of steel. Composition and uses of brass, bronze and soldering alloy. Analysis of iron, nickel, chromium and manganese in steel. Analysis of copper and zinc in brass, lead and tin in soldering alloy.

Industrial applications of alloys.

Reference books:

1] Quantitative analysis: Day and Underwood (Prentice-Hall of India)
2] Vogel's Text Book of Quantitative Inorganic Analysis-Bassett, Denney, Jeffery and Mendham (ELBS)
3] Analytical Chemistry: Gary D. Christian (Wiley, India).
4] Instrumental Methods of Analysis: Willard, Merrit, Dean, Settle (CBS Publishers, Delhi, 1986)
5] Instrumental Methods of Chemical Analysis: Braun (Tata McGraw-Hill)
6] Advanced Analytical Chemistry: Meites and Thomas (McGraw-Hill)
7] Instrumental Methods of Analysis: G. Chatwal and S. Anand (Himalaya Publishing House)
8] Analytical Chemistry: Problems and Solution- S. M. Khopkar (New Age International Publication)
9] Basic Concepts in Analytical Chemistry: S. M. Khopkar (New Age International Publication)
10] Advance Analytical Chemistry: Meites and Thomas: (Mc Graw Hill)
11] An Introduction to Separation Science: L. R. Shyder and C. H. Harvath (Wiley Interscience)
12] Fundamentals of Analytical Chemistry: S. A. Skoog and D. W. West
13] Instrumental Methods of Chemical Analysis: G. W. Ewing