Shiksha Mandal's
Bajaj College of Science, Wardha
(An Autonomous Institution)

Department of Chemistry

Proposed Syllabus for Two Year M.Sc. Chemistry

Department Specific Course (DSC)

Semester III courses

Syllabus under Autonomy

(Discussed in BOS Meeting of 10-October-2023 and approved in BOS Meeting of 28-March-2024 to be implemented from Academic Session 2024-25)

Shiksha Mandal's

Bajaj College of Science, Wardha

Syllabus of M.Sc. II Semester III

DSC IX (Theory)

PCH631T: Organic Special I

[60 Hrs] **[4 Credits]**

Course Objectives

1. To learn the theory/principal of photochemistry, types of photochemical reactions and its applications in organic synthesis.
2. To understand the basis of pericyclic reactions, its types and applications in chemistry.
3. To know the chemistry of some famous oxidizing and reducing agents in organic chemistry with major focus on its synthesis and synthetic applications.
4. To study chemistry of some phosphorous, sulphur, silicon and boron compounds with respect to its preparation, synthetic applications and stereochemistry.

Course Outcomes

By the completion of the above course the students will be able to

1. Recognize concept of photochemistry and will demonstrate its applications in organic synthesis.
2. Reproduce pericyclic reactions, its types and will implement its applications in chemistry.
3. Report the synthesis and evaluate the applications of some oxidizing and reducing agents in organic chemistry.
4. Recognize the chemistry of some phosphorous, sulphur, silicon and boron compounds along with its applications.

Contents: -

Unit-I Photochemistry **(15Hrs)**

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 isomerization addition and substitution Photochemical isomerization of cis and trans alkenes, Photochemical cyclization of reaction, Photo-Fries rearrangement, di-π-methane rearrangement, Photo theory reaction of anilides, photochemistry of vision, Applications of photochemical methods in synthesis: Isocomene, Cedrene, Hirsutene

Unit-II **(15Hrs)**

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1, 3, 5-hexatriene, allyl system, classification of pericy clicreaction. FMO approach, Woodward-Hoffman correlation diagram ethod and Perturbation of Molecular Orbital (PMO) approach of pericyclic reaction under thermal and photochemical conditions Electro cyclic 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 effectsin [4+2] cycloaddition. Stereochemical effect sand 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, Enereaction.

Unit-III Oxidation and Reduction: **(15Hrs)**

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. 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

ii) 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)

a) 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: **(15Hrs)**

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

<u>Reference books</u>:

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

DSC X (Theory)

PCH632T: Organic Special II

[60 Hrs] **[4 Credits]**

Course Objectives

1. To learn the terpenoids and porphyrins with major focus on their classification, occurrence, structure determination, stereochemistry and synthesis.
2. To understand the biology, role, classification, structure determination, stereochemistry, synthesis and biosynthesis of some alkaloids and prostaglandins.
3. To learn the steroids and plant pigments with respect to their occurrence, isolation, nomenclature, structure determination and synthesis.
4. To learn the chemistry of some biomolecules like carbohydrates, amino acids, proteins and peptides with respect to their types, structures, derivatives, structure determination.

Course Outcomes

By the completion of the above course, the students will be able to

1. Report the classification, occurrence, structure determination, stereochemistry and synthesis of terpenoids and porphyrins.
2. Illustrate the role, classification, structure determination, stereochemistry, synthesis and biosynthesis of some alkaloids and prostaglandins.
3. Reproduce the chemistry of steroids and plant pigments.
4. Recognise the classification, structure and chemistry of some biomolecules like carbohydrates, amino acids, proteins and peptides.

Contents:-

Unit-I Terpenoids and Porphyrins: (15Hrs)

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 (15Hrs)

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 Alkaloids and Prostaglandins **(15Hrs)**

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 **(15Hrs)**

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 **(15Hrs)**

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.

<u>Reference books</u>:

- Chemistry of Alkloids-S. W. Pelletier
- Chemistry of Steroids-L. F. Fisher and M. Fisher
- The Molecules of Nature-J. B. Hendricsion
- Biogenesis of Natural Compound - Benfield
- Natural Product Chemistry and Biological Significance- J. Mann, R. S Devison, J. B. Hobbs, D. V. Banthripde and J. B. Horborne
- Introduction to Flavonoids-B. A. Bohm, Harwood
- Chemistry of Naturally Occurring Quinines-R. H. Thomson
- The Systematic Identification of Flavonoids- Marby, Markham, and Thomos
- Text Book of Organic Medicinal Chemistry-Wilson, Geswold

- Medicinal Chemistry Vol I and II-Burger
- Synthetic Organic Chemistry -Gurudeep Chatwal.
- Organic Chemistry of Natural Products Vol I and II-O. P. Agrawal Organic Chemistry of Natural Products -Gurudeep Chatwal
- A Textbook of Pharmaceutical Chemistry-Jayshree Ghosh
- Synthetic Dyes Series -Venkatraman
- Chemistry Process Industries-Shreve and Brink
- Principal of Modern Heterocyclic Chemistry-L. A. Paquelte
- Heterocyclic Chemistry-J. Joule and G. Smith
- Heterocyclic Chemistry-Morton
- An Introduction to Chemistry of Heterocyclic Compound-J. B. Acheson
- Introduction to Medicinal Chemistry-A. Gringuadge
- Wilson and Gisvold Text Book of Organic Medicinal and Pharmaceutical Chemistry-Ed. Robert F Dorge
- An Introduction to Drug Design-S. S. Pandey and J. R. Demmock Polymer Science-V. Govarikar
- Principle of Polymer Chemistry-P. J. Flory
- An Outline of Polymer Chemistry-James Q. Allen
- Organic Polymer Chemistry-K. J. Saunders

DSC XI (Theory)

PCH633T: Spectroscopy

[60 Hrs] **[4 Credits]**

Course Description

This course is introduced to impart the knowledge of various spectroscopic techniques such as Microwave, IR, Raman, and Mossbauer spectroscopy along with diffraction techniques and group theory to the students.

Course Objectives

The main objectives of the course are –

1. To relate important concepts related to symmetry elements and symmetry operations with spectroscopy.
2. To provide the basic knowledge about the principles and instrumentation of these spectroscopic techniques - Microwave, IR, Raman, and Mossbauer spectroscopy - along with their application for the structure elucidation of different organic and inorganic compounds.
3. To study the principles behind various diffraction techniques such as X-ray, neutron and electron diffraction.

Course Outcomes

On completion of theory course, students will be able to:

1. Recognize symmetry elements and symmetry operations and describe the multiplication table of C_{2V}, C_{3V} and character tables of H_2O and NH_3 using great orthogonality theorem.
2. Interpret spectra and identify compounds using Microwave and Mossbauer spectroscopy.
3. Determine the functional group and structure of compounds using IR, and Raman spectroscopy.
4. Analyse the nature and structure of samples using diffraction techniques viz. X-ray, electron, and neutron diffraction.

Contents:-

Unit-I Symmetry properties of molecules and group theory: **(15Hrs)**

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: **(15Hrs)**

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: **(15Hrs)**

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), Rule of mutual exclusion, Numericals.

Unit-IV Diffraction techniques: **(15Hrs)**

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:

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

DSC XII (Practical)

PCH634P: Special Organic Chemistry Practical

[60 Hrs] **[2 Credits]**

Course Objectives

The main objective of this course is to

- Study the quantitative estimation organic compound, isolation of organic compound from natural source & qualitative analysis of mixture of three organic compound.
- Provide basic knowledge of principle and techniques of separation, purification and identification of ternary mixture of organic compounds.
- Perform qualitative analysis for a separation and identification of the components of a mixture of three organic compounds.

Course Outcomes:

The students will be able to

1. Demonstrate quantitative estimation of vitamin "C", formaldehyde, phenol, amine, glucose & carbonyl compounds.
2. Isolate an organic compound (caffeine, casein, dipricrate, β-carotene etc.) from natural source (tea leaves, milk, tobacco, carrot etc.)
3. Analyse qualitatively a separation and identification of the components of a mixture of three organic compounds.

Contents: -

[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 byacetylation 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 Rfvalue 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 andseparation 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

Reference books:

- Synthesis and Characterization of Inorganic Compounds, W. L. Jolly, Prentice Hall.
- Inorganic Experiments, J. Derck Woollins, VCH.
- Practical Inorganic Chemistry, G. Marrand, B. W. Rockett, Van Nostrand.
- A Text Book of Quantitative Inorganic Analysis, A. I. Vogel, IIIrd Edition
- EDTA Titrations. F. Laschka
- Instrumental Methods of Analysis, Willard, Merit and Dean (CBS, Delhi).
- Inorganic Synthesis, Jolly
- Instrumental Methods of Chemical Analysis, Yelri Lalikov
- Fundamental of Analytical Chemistry, Skoog D.A. &West D.M Holt Rinehart &Winston Inc.
- Experimental Inorganic Chemistry, W.G. Palmer, Cambridge.
- Quantitative Analysis: Day and Underwood
- Physical Methods In Inorganic Chemistry: R. S. Drago
- General and Inorganic Chemistry: N. Akjmetov

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Proposed Syllabus for Two Year M.Sc. Chemistry

ELECTIVE

Semester III courses

Syllabus under Autonomy

(Discussed in BOS Meeting of 10-October-2023 and approved in BOS Meeting of 28-March-2024 to be implemented from Academic Session 2024-25)

Shiksha Mandal's

Bajaj College of Science, Wardha

Syllabus of M.Sc. II Semester III

ELECTIVE - I

PCH635T: Modern Separation Techniques and Instrumental Analysis

Course Description

This course aims to provide students with a comprehensive understanding of instrumental methods of analysis, enabling them to apply these techniques effectively in research, industry, and various scientific disciplines.

Course Objectives

The Course is aimed at-

1. **Instrumentation Familiarity:** To introduce students to a range of modern analytical instruments and techniques used in chemical analysis, such as spectroscopy, chromatography, and electrochemical methods.
2. **Instrumental Operation:** To teach students the principles of operation, components, and maintenance of various analytical instruments, ensuring they can use them effectively and safely.
3. **Calibration and Standardization:** To instruct students on how to calibrate instruments, create calibration curves, and use standards for accurate and precise measurements.
4. **Quantitative Analysis:** To develop students' ability to quantitatively determine the concentration of specific analytes in a sample using various instrumental methods.
5. **Data Analysis and Interpretation:** To equip students with the skills needed to analyze, interpret, and present data obtained from instrumental methods, including statistical analysis and error propagation.

Course Outcomes

Course outcomes for a course on Instrumental Methods of Analysis are designed to specify the knowledge, skills, and abilities that students should gain upon completing the course. Here are some typical course outcomes for such a course:

1. **Understanding of Instrumentation:** Students should demonstrate a solid understanding of the principles and operation of various analytical instruments commonly used in chemical analysis, such as spectroscopy, chromatography, and electrochemical methods.

2. **Instrument Selection:** Students should be able to select the most appropriate analytical instrument or technique for a given analytical problem based on its strengths, limitations, and suitability for specific sample types.
3. **Instrument Calibration:** Students should have the ability to calibrate analytical instruments accurately, including setting up calibration curves, determining instrument sensitivity, and ensuring proper instrument performance.
4. **Data Analysis:** Students should be capable of performing data analysis, including peak integration, spectral interpretation, and statistical analysis, to extract meaningful information from instrument-generated data.

Course Contents

Theory

[30 Hrs] **[2 Credits]**

Unit-I

Modern separation techniques:

a) Gas Chromatography: Principle including concept of theoretical plates and van-Demeter equation. Instrumental set up- carrier gas, sampling system, column and detector. Types of columns, their advantages and limitations. Detectors in GC analysis. Temperature programmed GC. Factors affecting retention, peak resolution, and peak broadening.

b) Liquid chromatography: Principle, Instrumentation, Advantages and applications of HPLC. Types of columns and detectors. Principle and applications of size exclusion, gel permeation, ion retardation, normal phase and reverse phase chromatography.

c) Supercritical fluid chromatography: Introduction and applications.

Unit-II

Optical methods of analysis

Flame photometry: Principle. Instrumentation and types of burners. Factors affecting flame photometric determination. Limitations of flame photometry. Interferences in flame photometry. Applications.

Atomic absorption spectroscopy: Principle. Atomic energy levels. Grotrian diagrams. Population of energy levels. Instrumentation. Sources: Hollow cathode lamp and electrodeless discharge lamp, factors affecting spectral width. Atomizers: Flame atomizers, graphite rod and graphite furnace. Cold vapour and hydride generation techniques. Factors affecting atomization efficiency, flame profile. Monochromators and detectors. Beam modulation. Detection limit and sensitivity. Interferences and their removal. Comparison of AAS and flame emission spectrometry. Applications of AAS.

Unit-III

Electrochemical methods of analysis

a) Polarography: Principle of DC polarography. Instrumentation in polarography. Advantages and limitations of DME. Types of currents- residual current, migration current, diffusion current, limiting current, adsorption current, kinetic current and catalytic current. Ilkovic equation-diffusion current constant and capillary characteristics. Derivation of equation of polarographic wave and half wave potential. Experimental

determination of half wave potential. Reversible, quasi reversible and irreversible electrode reactions. Polarographic maxima and maximum suppressor. Oxygen interference and deaeration. Introduction to pulse, a.c. and oscillographic techniques and their advantages. Applications of polarography in determination of dissolved oxygen, metal ion quantification and speciation, simultaneous determination of metal ions, analysis of organic compounds. Limitations of polarography.

b) Amperometric titrations: Principle, types and applications in analytical chemistry.

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

PCH635P: Instrumental techniques Practical

Practicals

[60 Hrs] **[2 Credits]**

Instrumental techniques

Section (A) : Electroanalytical techniques

1) Analysis of commercial vinegar by conductometric titration.
2) Estimation of phenol by conductometric titration with NaOH.
3) Determination of strength of HCl and CH_3COOH in a mixture conductometrically.
4) Determination of strength of HCl and oxalic acid in a mixture conductometrically.
5) Determination of strength of oxalic acid and CH_3COOH in a mixture conductometrically.
6) Determination of degree of dissociation and dissociation constant of acetic acid conductometrically.
7) Estimation of phenol in dilute solution by conductometric titration with NaOH.
8) Determination of strength of HCl and CH_3COOH individually and in a mixture potentiometrically.
9) Determination of Fe(II) by potentiometric titration with $K_2Cr_2O_7$.

10) Determination of three dissociation constants of H_3PO_4 by pH-metric/potentiometric titration

Section (B) : Optical methods

1) Determination of pK of indicator by colorimetry.
2) To estimate the amount of NH_4Cl colorimetrically using Nesseler's Reagent.
3) To study the complex formation between Fe(III) and salicylic acid and find the formula and stability constant of the complex colorimetrically (Job's method).
4) To determine the dissociation constant of phenolphthalein colorimetrically.
5) Estimation of iron in wastewater sample using 1,10-phenanthroline.

(Note: One experiment from each section should be performed in the examination.)

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

ELECTIVE - II

PCH635T: Environmental Chemistry I

Course Description

The course is designed to make students aware of the chemistry behind environmental aspects like atmosphere, pollution of water and air. Students will learn sampling of polluted water, air, soil and investigate them chemically.

Course Objectives

The course is designed with following course objectives -

- To learn about atmosphere, relation of air pollution with climate change and analysis of air pollution.
- To learn about water resources, water pollution and important water analysis methods.
- To understand soil chemistry, soil management and effect of pesticides.

Course Outcomes

The expected course outcomes are given below:

1. Students will correlate air pollution with climate change and analyse the quality of air.
2. Students will explain water management methods and apply analytical skills to test the water samples.
3. Students will determine the type of soil, demonstrate correct techniques of soil management and investigate the effect of pesticides.

Course Contents

Theory

[30 Hrs] **[2 Credits]**

Unit –I: Atmosphere, Climate Change, Air Pollution and Analysis 10 hrs

Major regions of the atmosphere, composition of the atmosphere, Natural versus polluted air, temperature inversion and air pollution episodes, photochemistry of the atmosphere, depletion of the stratospheric ozone, greenhouse effect, greenhouse gases, remedial measures for reversion of greenhouse effect, acid rain, photochemical smog, particulate matter. air quality standards, air sampling, analysis and control of Particulates, Chemistry and analysis of Sox, NOx, CO, ozone, hydrocarbons, CFCs. Chemistry of gaseous, liquid and solid fuels- gasoline and additives, antiknock agents.

Unit-II: Water Pollution and Analysis 10 hrs

Origin, physico-chemical properties of water, sources of water, hydrological cycle, criteria of water quality, Water management- water shed management, rain water harvesting, water pollution- sources, consequences and harmful effects of water pollution, strategies for water pollution control. physico –chemical, organoleptic and chemical analysis of water, electro-analytical, optical (UC-visible spectrophotometry, AAS, flame photometry, XRF, ICPAES) & chromatographic (GC and HPLC) techniques.

Unit-III: Soil Pollution and Analysis **10 hrs**

Soil: Chemical and mineralogical composition of soil, classification of soil, types of soil-saline and alkaline, physical properties – texture, bulk density, permeability, chemical properties—Ion exchange capacity, soil pH and micro and macro nutrient availability. Soil management— Management of saline and alkaline soil, soil indicator plants.

Pesticides: Chemistry of chlorinated organic compounds, Polychlorinated biphenyls(PCB), Insectiside, Second generation of Pesticides, Long term effects of organochloro compounds, current position of pesticides in India.

Practical

PCH635P –Environmental Chemistry Practical

[60 Hrs] **[2 Credits]**

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

1. Analysis of nitrite in water sample by Spectrophotometry
2. Analysis of chromium in water sample 15 Analysis of chloride in water sample 16 Analysis of sulphate in water sample
3. Determination of turbidity of a given water sample
4. Estimation of Na, K, by flame photometry in given water

AIR ANALYSIS

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:

- Water analysis : J. Rodier
- A Text book of Inorganic Analysis : A.I.Vogel
- Colorimetric Determination of metals : E.B.Sandell
- Environmental Chemistry : Moore J W and Moore E A. Academic Press, New York, 1976.
- Environment and Man Vol VII: The Chemical Environment Edited by J Lenihar and W Fleecher Vlackie Publication, 1977.
- The Chemistry of Environment: R A Horne, Wiley Interscience Publication 1978.
- Fundamentals of Air Pollution: A C Stern
- Instrumental Methods of Analysis: Willard,Merrit and Dean
- Analytical Chemistry: Meites and Thomas
- Standard Methods for Examination of water and waste water: A E Greenberg, A D Eaton, APHA, AWWA,WEF
- Chemistry for Environmental Engineering and Science: C N Sawyer, P L McCarty and G FParkin
- Laboratory Manual for the Examination of Water, waste water and soil: H H Rupa

ELECTIVE - III

PCH635T: Medicinal Chemistry I

Course Objectives

This course is aimed at keeping the students abreast with important developments in medicinal chemistry. The students will be introduced with important methods and procedure followed in drug design and some drug types. Students will practically analyse and synthesize some common drugs.

Course Objectives

The main objectives of this course are

- To study basic concepts related to drug design and to understand important aspects of pharmacokinetics and pharmacodynamics.
- To realize mode of action and synthesis of some common diuretics, analgesics and antipyretics.
- To learn about synthesis and uses of important cardiovascular drugs and antineoplastic agent.

Course Outcomes

At the end of this course -

1. Students will illustrate a clear comprehension of fundamental concepts in drug design, including the principles of molecular interactions, target identification, and drug discovery strategies.
2. Students will apply key principles of pharmacokinetics and pharmacodynamics to analyze drug absorption, distribution, metabolism, and excretion, as well as the drug's effects on the body.
3. Students will apply their knowledge of cardiovascular drug synthesis and usage, as well as antineoplastic agent synthesis and application in the context of clinical scenarios.

Course Contents

Theory

[30 Hrs] **[2 Credits]**

UNIT-I Drug Design **10 hrs**

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: **10 hrs**

A] Pharmacokinetics and pharmacodynamics: Introduction, 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: 10 hrs

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.

PCH635T - Medicinal Chemistry Practical

[60 Hrs] [2 Credits]

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 andaniline
15. 1-phenyl-1,2-pentadine-3-one frombenzaldehyde
16. 1,5 diphenyl-1,3-pentadiene-2-onefrom benzaldehyde
17. 1,3-diphenyl-prop-2-ene-1-one
18. 3-methy pyrazol-5-one fromethylacetoacetate
19. 6-methyl uracil from ethylacetoacetate
20. Sulphanilamide from acetanilide
21. Barbituric acid (4-hudroxyuracil) fromdiethylmalonate.
22. 2,3-dimethyl-1-Phenylpyrazol-5- one(Antipyrin)from ethylacetoacetate
23. Fenbufen
24. 2-Phenylbenzo-4-pyrone (falvone)fromo-hydroxyacetophenone
25. Chlorobutanol from acetone
26. 2,4-dioxypiperazine from glycine

Reference books:

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

Shiksha Mandal's

Bajaj College of Science, Wardha

(An Autonomous Institution)

Department of Chemistry

Proposed Syllabus for Two Year M.Sc. Chemistry

Department Specific Course (DSC)

Semester IV courses

Syllabus under Autonomy

(Discussed in BOS Meeting 10-October-2023 and approved in BOS Meeting 28-March-2024 to be implemented from Academic Session 2024-25)

Shiksha Mandal's

Bajaj College of Science, Wardha

Syllabus of M.Sc. II Semester IV

DSC XIII (Theory)

PCH641T: Organic Chemistry Special III

[60 Hrs] **[4 Credits]**

Course Objectives

The main objective of this course is to

1. Learn the carbanion chemistry and its applications in various organic name reactions.
2. Study the properties, synthesis and applications of various organometallic reagents of Li, Mg, Zn, Cu, Hg etc. and some transition metals in organic chemistry.
3. Understand the applications of advanced stereochemistry and protection/deprotection of functional groups in organic chemistry.
4. Design the organic synthesis based on retrosynthetic analysis.

Course Outcomes

By the completion of the above course the students will be able to

1. Recognise the carbanion chemistry and will analyze its applications in various organic name reactions.
2. Describe the properties, synthesis and applications of various organometallic reagents of Li, Mg, Zn, Cu, Hg etc. and some transition metals in organic chemistry.
3. Demonstrate the applications of advanced stereochemistry and protection/deprotection of functional groups in organic chemistry.
4. Develop a synthetic route for organic synthesis based on retrosynthetic analysis.

Contents:-

Unit-I **15 Hrs**

A] Carbanions in organic Chemistry

Ionization of carbon hydrogen bond and prototopy, Base and acid catalysed halogenation of ketones, keto-enol equilibria, structure and rate in enolisation, concerted and carbanion mechanism for tautomerism, geometry of carbanions, kinetic and thermodynamic control in the generation of enolates, LDA, hydrolysis of haloforms, use of malonic and acetoacetic esters, Aldol, Mannich, Cannizzaro, Darzens, Dieckmann, Claisen Baylis-Hillman reactions, Knoevenagel, benzoin condensation, Julia olefination, alkylation of enolates and stereochemistry thereof, Conjugate additions, enamines in organic synthesis

B] Organometallic reagents -I

Synthesis and applications of organo Li and Mg reagents, nucleophilic addition to aldehyde, ketones, ester, epoxide, CO_2, CS_2, isocyanates, ketenes, imines, amides, lactones, Stereochemistry of Grignard addition to carbonyl compounds, *o*-metallation of arenes using organolithium compounds.

Unit-II **15 Hrs**

A) Organometallic reagents-II

Organozinc reagents: Preparation and applications, Reformatsky reaction, Simon-Smith reaction. Organocopper reagents: Preparation and applications in C-C bond forming reaction, mixed oragnocuprates, Gilman's reagent. Organo Hg and Cd reagents in organic synthesis.

B) Transition metals in organic synthesis:

Transition metal complexes in organic synthesis- Introduction-oxidation states of transition metals, 16-18 rule, dissociation, association, insertion, oxidative addition, reductive elimination of transition metal.

Organopalladium in organic synthesis - Heck reaction, carbonylation, Wacker oxidation, coupling reactions: Kumada Reaction, Stille coupling, Sonogashira, Negishi and Suzuki coupling reactions and their importance

Applications of $Co_2(CO)_8$**,** $Ni(CO)_4$, $Fe(CO)_5$ in organic synthesis. Wilkinson catalyst of Ruthenium and Rhodium – synthesis and uses its use in hydrogenation reactions-deallylation, C-C, C-O, C-N bond cleavages. Olefin metathesis by I^{st} and II^{nd} generation catalyst, reaction mechanism and application in the synthesis of homo and heterocyclic compounds.

Unit-III **15 Hrs**

A] Advanced Stereochemistry: Conformation of sugars, monosaccharides, disaccharides, mutorotation, Recapitulation of Stereochemical concepts-enantiomers, diastereomers, homotopic and heterotopic ligands, Chemo-, regio-, diastereo- and enantio-controlled approaches; Chirality transfer, Stereoselective addition of nucleophiles to carbonyl group: Re- Si face concepts, Cram's rule, Felkin Anh rule, Houk model, Cram's chelate model. Asymmetric synthesis use of chiral auxiliaries, asymmetric hydrogenation, asymmetric epoxidation and asymmetric dihydroxylation.

B] Protection and Deprotection of functional groups: Protection and deprotection of functional groups like, hydroxyl, amino, carbonyl and carboxylic acids groups, Solid phase peptide synthesis.

Unit-IV Designing the synthesis based on retrosynthetic analysis **15Hrs**

A) Disconnection Approach: An introduction to synthons and synthetic equivalents, disconnection approach, functional group inter-conversions, the importance of the order of events in organic synthesis, one group C-X and two group C-X

disconnections, chemoselectivity, reversal of polarity, cyclisation reactions, amine synthesis.

B) **One Group C-C Disconnections:** Alcohols and carbonyl compounds, regioselectivity, alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis.

Two Group C-C Disconnections: Diels-Alder reaction, 1,3-difunctionalised compounds, α,β- unsaturated carbonyl compounds, control in carbonyl condensations, 1,5-difunctionalised compounds, Michael addition and Robinson annulation, Methods of ring synthesis, Linear and convergent synthesis.

Reference books:

1] Principle of Organic Synthesis R. O. C. Norman and J. M. Coxon
2] Modern Synthetic Reaction. H. O. House and W. A. Benjamin
3] Organic Synthesis: The Disconnection Approach-S. Warren
4] Designing Organic Synthesis-S. Warren
5] Some Modern Methods of Organic Synthesis-W. Carruthers
6] Advance Organic Reaction. Mechanism and Structure-Jerry March
7] Advance Organic Chemistry Part-B-F. A. Caray and R. J. Sundberg
Plenum Press
8] Organic Reaction and their Mechanism-P. S. Kalsi
9] Protective Groups in Organic Synthesis-T. W. Greene
10] The Chemistry of Organo Phosphorous-A. J. Kirbi and S. G. Warren
11] Organo Silicon Compound-C. Eabon
12] Organic Synthesis via Boranes-H. C. Brown
13] Organo Borane Chemistry-T. P. Onak
14] Organic Chemistry of Boron-W. Gerrard

DSC XIV (Theory)

PCH642T: Organic Chemistry Special IV

[60 Hrs] **[4 Credits]**

Course Objectives

The main objective of this course is to provide

1. Fundamental knowledge of enzymes and its catalysis in biological systems.
2. Knowledge of chemistry of some heterocyclic compounds with major focus on their synthesis and reaction.
3. Information of the chemistry of bioactive compounds and biomolecules like nucleic acids, lipids and vitamins.
4. Knowledge of chemistry of some dyes, drugs and polymers with respect to its classification, structure and applications.

Course Outcomes

By the completion of the above course the students will be able to

1. Recognise chemistry of enzymes and its catalysis in biological systems with mechanistic details.
2. Demonstrate the chemistry of some heterocyclic compounds (like azoles, diazenes, benzofused heterocycles) with major focus on their synthesis and reactions.
3. Reproduce the chemistry of bioactive compounds and biomolecules like nucleic acids, lipids and vitamins.
4. Recall the chemistry of some dyes, drugs and polymers with respect to its classification, structure and applications.

Content

Unit-I: Enzyme chemistry (15 Hrs)

A] Enzymes: Introduction, chemical and biological catalysis, remarkable properties of enzymes like catalytic power, specificity and regulation. Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes. Nomenclature and classification, Fischer's lock and key and Koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site-directed mutagenesis. Baker's yeast catalyzed reactions

B] Mechanism of Enzyme Action: Transition-state theory, orientation and steric effect, acid- base catalysis, covalent catalysis, strain or distortion. Enzyme mechanisms for chymotrypsin, ribonuclease, lysozyme and carboxypeptidase A.

C] Co-Enzyme Chemistry: Structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD^+, $NADP^+$, FMN, FAD, lipoic acid, biotin as CO_2 carrier. Mechanisms of reactions catalyzed by the above cofactors.

Unit-II: Heterocycles (15 Hrs)

A] Azoles: Structural and chemical properties; Synthesis of pyrazole, isothiazole

and isoxazole; Synthesis of imidazoles, thiazoles and oxazoles; Nucleophilic and electrophilic substitutions; Ring cleavages, Carbonyldiimidazole as coupling agent

B] Benzofused heterocycles: Synthesis of indole, benzofuran and benzo-thiophene, quinoline and isoquinoline Nucleophilic, electrophilic and radical substitutions; Addition reactions; Indole rings in biology.

C] Diazines: Structural and chemical properties; Synthesis of pyridazines, pyrimidines, pyrazines; Nucleophilic and electrophilic substitutions.

D] Synthesis of following bioactive compounds: Vitamin B6, Ondansetron, Serotonin, Indometacin, Cyanamid, fentiazac, trimethoprim, papaverine

Unit-III (15 Hrs)

A] Nucleic Acids: Primary, secondary and tertiary structure of DNA; DNA replication and heredity; Structure and function of m-RNA, t-RNA and r-RNA. Purines and pyrimidine bases ofnucleic acids and their preparation.

B] Lipids: Fatty acids, essential fatty acids, structures and functions of triglycerols, glycerophospho lipids, spingolipids, lipoproteins, composition and function, role in atherosclerosis.

Properties of lipid aggregates, micells, bilayers, liposomes and their biological functions, biological membranes, fluid mosaic model of membrane structure, Lipid metabolism, β- Oxidation of fatty acids

C] Vitamins: Structure determination, and synthesis of vitamin A, E and H.

Unit-IV (15 Hrs)

A] Dyes: General Introduction, classification on the basis of structure and methods of application dying mechanism, methods of dying, such as direct dying, vat dying, dispersive dying, formation of dye in fibre, dying with reactive dyes, study of quinoline yellow, cyamine dye, ethyl red, methylene blue, Alizarin, cyamine-green, fluorescein, cosin, erythrosine, Rhodomines and Indigo.

B] Pharmaceutical chemistry:

History, medical terms in pharmaceutical chemistry, classification of drugs, antibacterial and antifungal drugs, specific clinical applications, Synthesis and applications of: Benzocaine, Methyl dopa, dilantin, ciprofloxacin, acyclovir, terfenadine, salbutamol

C] Polymer chemistry: Importance of polymers, Basic concepts: monomers, repeat units, degree of polymerization. Linear, branched and network polymers. Classification of polymers. Polymerization: condensation, addition, radical chain-ionic and co-ordination and co- polymerization and their mechanisms, Polymerization in homogeneous and heterogeneous systems. Ziegler-Natta polymerization with mechanism, Stereo regulated polymers, syndiotactic, isotactic and atactic polymers

Reference books:

1] Textbook of Polymer Science, F. W. Billmeyer Jr, Wiley
2] Polymer Science, V. R. Gowarikar, N. V. Viswanathan and J. Sreedhar, Wiley-Eastern
3] Functional Monomers and Polymers, K. Takemoto, Y. Inaki and R. M. Ottanbrite
4] Bioorganic Chemistry: A Chemical Approach to Enzyme Action, Hermann Dugas and C.Penny, Springer-Verlag

5] Understanding Enzymes, Trevor Palmer, Prentice Hall
6] Enzyme Chemistry: Impact and Applications, Ed. Collin J. Suckling, Chapman and Hall
7] Enzyme Structure and Mechanism, A. Fersht, W. H. Freeman
8] Introduction to Medicinal Chemistry, A. Gringuage, Wiley-VCH
9] Wilson and Gisvold's Text Book of Organic Medical and Pharmaceutical Chemistry, EdRobert F. Dorge
10] Burger's Medicinal Chemistry and Drug Discovery, Vol-1, Ed. M. E. Wolff, John Wiley
11] Strategies for Organic Drug Synthesis and Design, D. Lednicer, John Wiley
12] The Organic Chemistry of Drug Design and Drug Action, R. B. Silverman, Academic Press

DSC XV (Theory)

PCH643T: Spectroscopy

[60 Hrs] **[4 Credits]**

Course Objectives

1. To understand fundamental principles, important techniques and applications of ultraviolet -visible spectroscopy and Photoelectron spectroscopy.
2. To study important concepts related to ESR spectroscopy and mass spectrometry and to understand the interpretation of the spectral data.
3. To know fundamental principles, important techniques and applications of nuclear magnetic resonance spectroscopy and to learn the structure determination of organic molecules by applying 2D-NMR spectroscopy, COSY, HETCOR, NOSEY, DEPT-45, DEPT-90, DEPT-135 etc.
4. To learn to solve the numerical based on the combined spectral data.

Course Outcomes

On completion of theory Course, students will:

1. Describe basic principles and applications of UV visible and photoelectric spectroscopy.
2. Apply principles of ESR spectroscopy and mass spectrometry for structure determination of organic molecules.
3. Explain important concepts of NMR spectroscopy and illustrate FT- NMR, COSY, HECTOR, NOSEY, DEPT, INEPT, APT, INADEQUATE techniques.
4. Elucidate the structure of organic molecules by using combined spectral data of UV, IR, NMR, and mass spectroscopy.

Contents:-

Unit I: (15 hrs)

A] Ultraviolet and visible spectroscopy: Natural line width, line broadening, transitionprobability, Born-Oppenheimer approximation, rotational, vibrational and electronic energy levels. General nature of band spectra. Beer- Lambert Law, limitations, Frank-Condon principle, various electronic transitions, effect of solvent and conjugation on electronic transitions, Fiesher Wooodward rules for dienes, aldehydes and ketones. Structure differentiation of organic molecules by UV Spectroscopy

B] Photoelectron spectroscopy: Basic principles, photoelectric effect, ionization process, Koopman theorem, PES and XPES, PES of simple molecules, ESCA, chemical information from ESCA, Auger electron spectroscopy.

Unit II: (15 hrs)

A] ESR spectroscopy: Introduction, principle of ESR, ESR spectrometer, hyperfine coupling, zero field splitting, factors affecting g values, Kramer's degeneracy, application of ESR spectra to study free radicals like hydrogen, methyl radical, 1,4-semibenzoquinone, naphthalene, transition metal complexes, biological

systems.

B] Mass spectrometry:

Theory, ion production (EI, CI, FD, FAB), ion analysis, ion abundance, isotopic contribution, N- rule, types of fission processes, high resolution mass spectrometry, metastable peak, molecular ion peak, Mclaffferty rearrangement, mass spectral fragmentation of organic compounds alkanes, alkenes, alkynes, alcohols, amines, amides, acids, aldehydes, ketones, halides, Structure determination of organic molecules by mass spectrometry, problem based on mass spectral data.

Unit III: Nuclear magnetic Resonance Spectroscopy (15 hrs)

Magnetic properties of nuclei, resonance condition, NMR instrumentation, chemical shift, spin spin interaction, shielding mechanism, factors affecting chemical shift, PMR spectra for different types of organic molecules, effect of deuteration, complex spin spin interaction (1^{st} order spectra), stereochemistry, variations of coupling constant with dihedral angle, electronegativity, Karplus equation etc., classification of molecules as AX, AX_2, AMX, A_2B_2, Shift reagents. NMR studies of ^{13}C, chemical shift in aliphatic, olefinic, alkyne, aromatic, heteroatomic and carbonyl compounds, ^{19}F, ^{31}P. Structure determination of organic molecules by NMR spectroscopy

Unit IV: (15 hrs)

A] Application of NMR spectroscopy: FT-NMR, advantages of FT-NMR, two dimensional NMR spectroscopy-COSY, HETCOR, NOSEY, DEPT, INEPT, APT, INADEQUATE techniques, Nuclear overhauser effect, use of NMR in medical diagnosis

B] Problems based on structure determination of organic molecules by using NMR (^1H and ^{13}C nuclei) data, Structure elucidation using combined techniques including UV, IR, NMR and mass spectrometry (based on data and copies of the spectra)

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] Practical NMR Spectroscopy-ML Martin, JJ Delpench, and DJ Martyin

7] Spectroscopic Methods in Organic Chemistry-DH Willson, I Fleming

8] Fundamentals of Molecular Spectroscopy-C.NBanwell

9] Spectroscopy in Organic Chemistry-CNR Rao and JR Ferraro

10] Photoelectron Spectroscopy-Baber and Betteridge

11] Electron Spin Resonance Spectroscopy-J Wertz and JR Bolten

12] NMR –Basic Principle and Application-H Guntur

13] Interpretation of NMR spectra-Roy H Bible

14] Interpretation of IR spectra-NB Coulthop
15] Electron Spin Resonance Theory and Applications-W gordy
16] Mass Spectrometry Organic Chemical Applications, JH Banyon
17] Spectroscopy- H. Kaur

DSC XVI (Practical)

PCH644P: Organic Chemistry Special Practical II

[60 Hrs] **[2 Credits]**

Course Objectives

The main objective of this course is

1. To analyze nitrogen, halogen and sulphur by chemical methods.
2. To estimate some natural products and drugs by spectrophotometric/calorimetric and other instrumental methods.
3. To perform multi-step preparations of some important organic compounds
4. To elucidate structure of organic compounds on the basis of spectral data (UV, IR, ^{1}H and ^{13}CNMR and Mass)

Course Outcomes

By the completion of the above course, students will be able to

1. Estimate nitrogen, halogen and sulphur by chemical methods.
2. Analyse some natural products and drugs by spectrophotometric/calorimetric and other instrumental methods.
3. Demonstrate the multi-step preparations of some important organic compounds
4. Elucidate structure of organic compounds on the basis of spectral data (UV, IR, ^{1}H and ^{13}CNMR and Mass)

Contents

A] Quantitative Analysis based on classical and instrumental technique (any 9-10)

- **Classical methods of estimation**

  1]Estimation of nitrogen.
  2] Estimation of halogen.
  3] Estimation of sulphur.

- **Spectrophotometric/calorimetric and other instrumental methods of estimation**

1] Estimation of streptomycin sulphate.
2] Estimation of vitamin B-12.
3] Estimation of amino acids.
4] Estimation of proteins.
5] Estimation of carbohydrates.
6] Estimation of Ascorbic acid.
7] Estimation of Aspirin.
8] Solvent extraction of oil from oil seeds and determination of saponification value, iodine value of the same oil.

B] Organic multi-step preparations (Two/Three steps): Minimum 10-12 preparations

[1] Aniline → Diaminoazobenzene → p-aminoazobenzene
[2] Benzoin → Benzyl → Dibenzyl
[3] Aniline → acetanilide → *p*-bromoacetanilide → *p*-bromoaniline
[4] Aniline → Acetanilide → *p*-nitroacetanilide → *p*-nitroaniline
[5] Benzaldehyde (thiamine hydrochloride) → benzoin → benzil → benzilic acid
[6] *p*-Nitrotoluene → *p*-nitrobenzoic acid → PABA → *p*-iodobenzoic acid
[7] *p*-Cresol → *p*-cresylacetate → 2-hydroxy-5-methyl acetophenone → 2-hydroxy chalcone
[8] Benzaldehyde → benzilidene acetophenone → 4,5-dihydro-1,3,5-triphenyl-1*H*-pyrazole
[9] Aniline → phenylthiocarbamide → 2-aminobenzthiazole (Microwave in step I)
[10] Chlorobenzene → 2,4- Dinitrochlorobenzene → 2,4- Dinitrophenylhydrazine.
[11] Acetophenone → acetophenone phenyl hydrazone → 2-phenylindole
[12] Benzion → benzoin benzoate → 2,4,5-triphenyl oxazole
[13] Benzophenone → benzpinacol → benzopinacolone (Photochemical preparation)
[14] Benzophenone → Benzophenone oxime → Benzanilide → Benzoic acid + aniline
[15] Aniline → aniline hydrogen sulphate → sulphanilic acid → Orange II
[16] Aniline → N-arylglycine → indoxyl → indigo
[17] Phthalimide → Anthranilic acid → Phenyl glycine-o-carboxylic acid →Indigo
[18] Phalic anhydride → Phthalimide → Anthranilic acid → o-chlorobenzoic acid
[19] Phalic anhydride → Phthalimide → Anthranilic acid →Diphenic acid
[20] Ethyl acetoacetate → 3-methyl-pyrazol-5-one → 4,4-dibromo-3-methyl-pyrazol-5-oneButanoic acid
[21] Biosynthesis of ethanol from sucrose
[22] Enzyme catalyzed reactions

[C] SPECTRAL INTERPRETATION

- Structure Elucidation of organic compounds on the basis of spectral data (UV, IR, ^{1}H and ^{13}CNMR and Mass) (Minimum 12 compounds are to be analysed during regular practicals).

Shiksha Mandal's

Bajaj College of Science, Wardha

(An Autonomous Institution)

Department of Chemistry

Proposed Syllabus for Two Year M.Sc. Chemistry

ELECTIVE

Semester IV courses

Syllabus under Autonomy

(Discussed in BOS Meeting 10-October-2023 and approved in BOS Meeting 28-March-2024 to be implemented from Academic Session 2024-25)

Shiksha Mandal's

Bajaj College of Science, Wardha

Syllabus of M.Sc. II Semester IV

ELECTIVE - I

PCH645T: Statistical Thermodynamics, Macromolecules and Phase

[30 Hrs] **[2 Credits]**

Course Description

The course is designed to cover some important fundamental topics in physical chemistry that will be helpful to students in better understanding of the subject.

Course Objectives

1. To get introduced to fundamentals of Statistical Thermodynamics.
2. To extend the study of Gibbs phase rule to more advanced one, two and three component systems.
3. To understand the concept and methods of determination of molecular mass of macromolecules.

Course Outcomes

The learner will:

1. Correlate the important concepts of statistical ther111111111111modynamics and compare Maxwell Boltzmann, Bose Einestein, Fermi Dirac statistics.
2. Apply Gibbs phase rule to study different one-, two- and three component systems.
3. Explain the concept and methods of determination of molecular mass of macromolecules.

Contents:-

Unit-I Statistical thermodynamics: **10 Hrs**

Lagrange's Method of Undetermined Multipliers (Conditional Maximization), Stirling Approximation, Concept of Distribution, Thermodynamic Probability and most probable distribution, Maxwell Boltzmann, Bose Einestein, Fermi Dirac statistics, comparison between three statistics.

Unit-II Phase Equilibrium **10 Hrs**

Gibbs Phase rule and its derivation, calculation of degrees of freedom, reduced phase rule, one component systems (Helium, carbon), 1^{st} and 2^{nd} order phase transition, lambda line, two component systems forming solid solutions having congruent and incongruent melting point,

partially miscible solid phase, three component systems, graphical presentation, influence of temperature, systems with 1, 2, 3 pairs of partially miscible liquids, transition points.

Unit-III Macromolecules **10 Hrs**

Definitions, Number and mass average molecular weights, molecular mass determination by Osmometry, Viscometry, Sedimentation, Diffusion, light scattering method, Numericals.

Reference books:

- M. C. Gupta, Statistical Thermodynamics, New Age International.
- K. Huang, Statistical Mechanics, Wiley, New Delhi, 2003.
- Andrew Maczek, *Statistical Thermodynamics*, Oxford University Press Inc., New York (1998).
- G. K. Vemulapalli, Physical Chemistry, Prentice – Hall of India, 1997.
- Findley, The Phase Rule and its Applications, Longmans Green and Co., Mumbai.
- Textbook of polymer science: F.W. Billmayer Jr. Wiley.
- Polymer science: V.R. Gowarikar, N. V. Viswanathan and J. Sreedhar, Wiley-Eastern.
- Fractional monomers and polymers: K Takemoto, Y. Inaki, and R.M. Ottam Brite.

ELECTIVE - II

PCH645T: Environmental Chemistry II

[30 Hrs] **[2 Credits]**

Course Description

The course is designed to make students aware of important types of pollutions – thermal, noise, radioactive and solid waste. Students will learn the sources, harmful effects and preventive measures of these types of pollutions.

Course Objectives

The course is designed with following course objectives -

- To learn about sources, harmful effects and prevention of thermal, noise and radioactive pollution.
- To understand the classification, consequences and management of solid waste pollution.
- To understand synthesis and degradation of plastics.

Course Outcomes

The expected course outcomes are given below:

1. Students will recognize the sources, harmful effects and prevention of thermal, noise and radioactive pollution.
2. Students will classify the solid wastes, assess the impact of toxic chemicals on the metabolism.
3. Students will investigate the photochemical and biological degradation of polymers.

Course Contents

Unit-I **(10 Hrs)**

Thermal pollution—sources, harmful effects and prevention of thermal pollution.
Noise pollution — sources, effects and control of noise pollution.
Radioactive Pollution: Introduction to radiation chemistry, sources of radioactive pollution, effects of radioactive pollution, nuclear disasters in the two decades, protection from radiation, control of radiation.

Unit-II: Solid waste pollution **(10 Hrs)**

Sources, types and consequences, classification of wastes- domestic, industrial, municipal, hospital, nuclear and agricultural and their methods of disposal. Transfer and transport, Recycle, reuse, recovery, conversion of solid wastes -energy / manure. Analysis and monitoring of pesticides. Impact of toxic chemicals on enzymes, Biochemical effects of As, Cd, Pb and Hg, their metabolism, toxicity and treatment.

Unit-III: Polymers & Plastics: **(10 Hrs)**

Polymer synthesis, Polymers degradation, Photochemical degradation, Biodegradation of naturally occurring polymeric substances, Disposable synthetic polymers, polymer recycling, Carry bags- a menace.

Reference books:

1. Environmental Chemistry: B K Sharma and H Kaur
2. Environmental Chemistry: A K De
3. Environmental Pollution- Management and control for sustainable Development: R K Khatoliya
4. Environmental Chemistry: A K Bhagi and G R Chatwal
5. Environmental Chemistry : P.S. Sindhu

ELECTIVE - III

PCH645T: Medicinal Chemistry II

[30 Hrs] **[2 Credits]**

Course Description

The course is aimed at making students aware of legal aspects related to medicinal industry. Students will learn the statistical analysis to interpret the data. Students will be introduced to various drug types and their synthesis methods.

Course Objectives

- To learn the legal aspects related to drugs.
- To understand application of statistical methods in quality control of drugs.
- To study briefly role and few examples of antidiabetic agents, anti-viral agents, anti-malarial agents, local anti-infective drug.

Course Outcomes

On successful completion of this course -

1. Students will analyze the implications of drug regulations, including drug rules and acts, and apply statistical methods to assess the effectiveness of antidiabetic agents in various contexts.
2. Students will synthesize and integrate knowledge about antiviral agents, anti-malarial agents, and local anti-infective drugs, demonstrating a comprehensive understanding of their chemical structures, mechanisms of action, and synthesis methods.
3. Students will synthesize knowledge about histamine and antihistaminic agents, antibiotics, and their synthesis methods, demonstrating a deep understanding of their chemical properties and mechanisms of action.

Course Contents

UNIT-I **10 hrs**

A] Drug rules and drug acts, Overview of Intellectual property right, Indian and International framework for patent protection**.**

B] Statistical method: For sampling and interpretation of results, Statistics in quality control, T-Test, F-Test, Validation of analytical methods as defined proceeding USP Radio immune analysis, Investigational drugs.

C] Antidiabetic Agents- Type-I and Type-II diabetes, Insulin, thiazolidinediones, Synthesis of ciglitazone.

UNIT-II **10 hrs**

A] Anti-Viral agents: Inroduction, viral diseases, viral replication, and transformation of cells, investigation of antiviral agents,. Chemotherapy for HIV. Synhesis of: Idoexuidine, acyclovir, amantadine and cytarabin.

B] Anti-malarial agents: Introduction, malarial parasite, and its life cycle, development of antimalarials, chemotherapy of malaria. Synthesis of: Chloroquin, primaquin, proguanil, and Quinacrine

C] Local Anti-infective drug: Introduction and general mode of action. Synthesis of sulphonamides, ciprofloxacin, norfloxacin, dapsone ,amino salicylic acid, isoniazid, ethionamide, ethambutal, econozole, griseofulvin.

UNIT-III: 10 hrs

A) Histamines and Antihistamic agents: Introduction, histamine H1-receptor antagonists. Inhibitors of histamine release. Synthesis of: alkyl amines, phenothiazines, piperzines derivatives.

B) Antibiotics: Introduction, β-lactam antibiotics, classification, SAR and chemical degradation of penicillin, cephalosporins-classification, tetracycline antibiotics-SAR, miscellaneous antibiotics. Synthesis of ampicillin, cephradine, methacycline, chloramphenicol.

Reference books:

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 FDorge
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