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 I courses

Syllabus under Autonomy

(Draft discussed and approved in BOS Meeting 08-July-2023 to be implemented from Academic Session 2023-24)

Shiksha Mandal's

Bajaj College of Science, Wardha

Programme Objectives M.Sc. Chemistry

- The main aim of the programme M.Sc. Chemistry is to make students abreast with sound knowledge about the fundamentals and applications of chemical and scientific theories.
- The important objectives of this programme are to enable students to
    1) become familiar with the different branches of chemistry like analytical, organic, inorganic, physical, environmental chemistry.
    2) be able to easily assess the properties of different elements.
    3) learn to apply appropriate techniques for the qualitative and quantitative analysis of chemicals in laboratories and in industries.
    4) develop analytical skills and problem solving skills requiring application of chemical principles.
    5) acquire the ability to synthesize, separate and characterize compounds using laboratory and instrumentation techniques.
- The students should be applying the scientific knowledge to design, carry out, record and analyze the results of chemical reactions.
- The students may acquire some of the skills required to work efficiently in laboratory of any academic/research institution or industrial unit.
- They should become capable of solving a problem by thinking methodically, independently to draw a logical conclusion.

Shiksha Mandal's

Bajaj College of Science, Wardha

Programme Outcomes M.Sc. Chemistry

- After successful completion of the programme the students will have sound knowledge about the fundamentals and applications of chemical and scientific theories.
- They will become familiar with the different branches of chemistry like analytical, organic, inorganic, physical, environmental chemistry.
- They will be able to easily assess the properties of different elements.
- Students can apply appropriate techniques for the qualitative and quantitative analysis of chemicals in laboratories and in industries.
- Students will develop analytical skills and problem solving skills requiring application of chemical principles.
- They acquire the ability to synthesize, separate and characterize compounds using laboratory and instrumentation techniques.
- The graduates achieve the skills required to work efficiently in the **chemical industry like cement industries, agro product, paint industries, rubber industries, petrochemical industries, food processing industries, fertilizer industries** etc.
- They acquire the laboratory skills to transfer and interpret knowledge entirely in the working environment.
- They can understand the causes of environmental pollution and can open up new methods for environmental pollution control.
- Students can find out the green route for chemical reaction for sustainable development.
- They will be able to solve the problem and also think methodically, independently and draw a logical conclusion.
- Students will learn to employ critical thinking and the scientific knowledge to design, carry out, record and analyze the results of chemical reactions.

Shiksha Mandal's

Bajaj College of Science, Wardha

Syllabus of M.Sc. I Semester I

DSC I (Theory)

PGCH1T1: Inorganic Chemistry

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

Course Objectives

1. Understand the stereochemistry and bonding of various molecules on the basis of various theories viz. VSEPR theory, Crystal field theory and Molecular orbital theory.
2. Determine the structure of complex using electronic spectra and magnetic susceptibility measurement studies.
3. Understand the structure, bonding and topology of boron hydrides and its application.
4. Determine the classification of metal clusters containing metal-metal bonds and learn about the factors affecting the stability of metal complexes.
5. Learn about the isopolyacids and heteropolyacids and their structures.
6. Describe the role of metal in biological system and their function.
7. Describe the structural and functional relationships, mechanisms and importance of metalloenzymes.

Course Outcomes

This will equip the learners to gain understanding of:

1. Importance of various theories in determining the stereochemistry and bonding of various molecules.
2. Magnetic and electronic properties of complexes for structure elucidation.
3. Structure and reactivity of boranes, stability of metal clusters and structures of iso and heteropolyacids.
4. Validate the role of bioinorganic chemistry in every day action.

Contents:-

Unit-I

a) Stereochemistry and Bonding in Main Group Compound:
VSEPER-Shape of simple inorganic molecules and ions containing lone pairs, various stereochemical rules and resultant geometry of the compounds of non-transitional elements, short coming of VSEPR model, bent rule, and energetic of hybridization.

b) Crystal Field Theory:
Splitting of d-orbital in tetragonal, square planar and trigonal bipyramidal complexes. Jahn teller effect, spectrochemical series, nephelauxetic effect. Limitations of crystal field theory.

c) Molecular Orbital Theory:
Molecular orbital theory for octahedral, tetrahedral, and square planar complexes with and without π-bonding.

Unit-II

a) Electronic spectra:

Spin-orbit (L-S) coupling scheme, calculation of spectral term symbols for ground state and excited states, selection rules, vibronic coupling, electronic spectra of transition metal complexes, charge transfer spectra, band intensities, band energies, band width & shapes, construction and application of Orgel diagrams, Tanabe-Sugano diagrams, spectra of octahedral, tetrahedral and square planar complexes with examples, Jahn teller effect, calculation of crystal field parameters (10Dq, B and β) for octahedral Ni(II) and Co(II) complexes from electronic spectra. Spectrochemical series, nephelauxetic effect and nephelauxetic series of ligands. Magnetic moment, electronic spectra, and structure of complexes.

b) Magnetochemistry:

Concept of magnetic susceptibility, types of magnetic bodies, magnetic properties of free ions and transition metal complexes of different geometries, factors affecting the magnetic properties, orbital splitting and magnetic properties, quenching of orbital angular momentum, and effect of ligand field on spin-orbit coupling. Temperature dependence of paramagnetism, high spin-low spin crossover, spin crossover in coordination compounds, spin equilibria, magnetic interactions, ferromagnetism and antiferromagnetism. Anomalous magnetic moments and magnetic exchange coupling.

Unit-III

a) Boron hydride:

Classification, nomenclature, structure, bonding and topology of boranes, 4 digit coding (STYX) number for higher borane and their utilities, study of metalloborane, carborane, and metallocarborane with reference to preparation and structure.

b) Metal ligand equilibria in solution:

Stepwise and overall formation constants, trends in stepwise formation constant, factors affecting stability of metal complexes with reference to nature of metal ion, ligand, chelate effect, and thermodynamic origin, determination of formation constant by:

(1) spectrophotometric method (Job's and Mole ratio method)

(2) Potentiometric method (Irving-Rossotti Method)

Unit-IV BIOINORGANIC CHEMISTRY:

a) Role of metals in bioinorganic chemistry

i) Classification as enzymatic and non-enzymatic metals, enzymatic redox metals such as Cu (SOD) and enzymatic non redox metals such as Zn (Hydrolase).

ii) Role of metal ions in non-enzymatic process, Na, K, Ca, Mg (one example of each and brief discussion).

iii) Role of metals in enzymatic processes, transition metals, catalase, peroxidase and nitrogenase (Redox active).

b) Metalloproteins: Iron proteins, introduction of Fe-S proteins, electron transfer proteins (Fe-S, Fe_2S_2, Fe_3S_4, Fe_4S_4). Transport protein (transferrin) and storage protein (ferritin).

c) Bioinorganic Chemistry of Fe: Hemoglobin and myoglobin, its structure and functions.

d) Bioinorganic Chemistry of Co: Vitamin-B_{12}, its structure and function.

References -

- S. F. A. Kettle, J. N. Murral & S. T. Teddler: Valency Theory
- C. A. Coulson: Valency
- J. E. Huheey: Inorganic Chemistry

- F .A. Cotton & G. Wilkinson: Advanced Inorganic Chemistry 3rd, 5th& 6th Editions.
    - F. Willims: Theoretical Approach in inorganic chemistry.
- Mannas Chanda: Atomic Structure and chemical Bonding
- L. E. Orgel: An introduction to transition metal chemistry, Ligand field theory, 2nd Edition.
- J. J. Logowski: Modern Inorganic Chemistry
- Durrant and P. J. Durrant: Advanced Inorganic Chemistry
- J. C. Bailar: Chemistry of co-ordination compounds.
- W. L. Jolly: Modern Inorganic Chemistry
- R. S. Drago: Physical methods in inorganic chemistry.
- K. Barnard: Theoretical Inorganic Chemistry
- F. A. Cotton: Chemical Applications of Group theory.
- N. Figgis: Introduction to Ligand field.
- S. F. A. Kettle: Co-ordination chemistry.
- M. C. Day and J. Selbin: Theoretical Inorganic Chemistry.
- J. Lewin and Wilkins: Modern Co-ordination chemistry.
- Gowarikar, Vishwanathan and Sheedar: Polymer science.
- R. L. Dutta and A. Symal: Elements of magneto chemistry
- P. Atkins: Inorganic Chemistry 4th Edition, Oxford University Press.
- Bertini, et al: Bioinorganic Chemistry (Viva)
- Fenton, David E.: Bio coordination chemistry, Oxford
- Selected Topics in Inorganic Chemistry by Wahid U Malik, Tuli, Madan.
- A Logical Approach to Modern Inorganic Chemistry by Jagdamba Singh
- Essentials of Bio Inorganic Chemistry by Monal Singh Neerja Gupta
- Concise Coordination Chemistry by R. Gopalan , V. Ramalingam
- Advanced inorganic chemistry Volume I by Madan malik Tuli Prakash S.Chand publication
- Advanced inorganic chemistry Volume II Madan malik Tuli Prakash S.Chand publication

DSC II (Theory)

PGCH1T2: Physical Chemistry

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

Course Objectives

1. To recapitulate fundamentals of chemical thermodynamics and extending the study to Maxwell's relations and third law of thermodynamics.
2. To learn advanced concepts and theories of chemical kinetics.
3. To understand fundamentals of quantum mechanics and its applications.
4. To study theories of electrolytes and fundamentals of conductometry, potentiometry and their applications.

Course Outcomes

On successful completion of this Course the students should be able to-

1. Derive the Maxwell's relations and understand third law of thermodynamics and related concepts.
2. Learn modern concepts and theories of reaction dynamics.
3. Understand and execute quantum mechanical problems and their applications
4. Understand the theories of electrolytes, apply conductometric and potentiometric titrations for analysis

Contents:-

Unit-I CLASSICAL THERMODYNAMICS:

a) Recapitulation of Laws of thermodynamics, Exact and inexact differentials, condition of exactness, Ptaff differential expression and equations, Applications of Ptaff differential equations to first and second law of thermodynamics, homogeneous function of degree 0 and 1, extensive and intensive properties, derivation of thermodynamic equations of state, Maxwell's relations, Applications of Maxwell's Relations

b) Third law of thermodynamics, Nernst Heat Theorem, Evaluation of Absolute Entropy, Entropy of reaction, Concept of residual entropy, Numericals based on absolute entropy.

Unit-II CHEMICAL KINETICS

a) Recapitulation, Activation energy, Arrhenius Equation and Numericals. Collision Theory and Transition state theory of bimolecular reactions, Thermodynamic formulation of Transition state theory (Eyring equation), Comparison of Transition state theory with Collision Theory.

b) Bodenstein steady state approximation, Rice-Herzfeld mechanism of chain reaction, Kinetics of photochemical chain reaction between H_2 & Cl_2 and H_2 & Br_2, Kinetics of Enzyme catalyzed reaction (Michaelis-Menten equation), salt effect.

Unit-III FORMULATION OF QUANTUM MECHANICS

a) Introduction of Quantum Mechanics, Wave Function, Acceptability of Wave Functions, Normalized and Orthogonal Wave Functions, Operators, Operator Algebra, Eigen

Functions and Eigen Values of Quantum Mechanical Properties e.g. Linear, Angular momentum, etc. Hermitian Operators, Orbital and generalized Angular Momentum, Postulates of Quantum Mechanics, Numericals on Operator algebra, Eigen Values and Average Values of quantities.

b) Application of Schrödinger Wave Equation to Simple Systems: Particle in a 3-Dimensional Box, Concept of degeneracy and breakdown in degeneracy, Rigid Rotor, Potential Well of Finite Depth, Tunneling Effect, Simple Harmonic Oscillator, The Hydrogen Atom.

Unit-IV ELECTROCHEMISTRY

a) Electrolytic conductance (Specific, Equivalent and molar), Variation of Eq./molar conductance with dilution, Transport number and its determination using Hittorf's method and Moving boundary method, Kohlrausch's law, calculation of molar ionic conductance, conductometric titrations, High frequency titrations, Ostwald dilution law, Determination of ionic mobility, numerical.

b) Principle of potentiometry, Indicator electrodes: hydrogen electrode, quinhydrone electrode, antimony electrode and glass electrode. Reference electrodes: Calomel electrode and Ag/AgCl electrode. potentiometric titrations, Basic Electrochemical Thermodynamics, Nernst equation, standard electrode potential, Determination of cell potential.

List of books

- R. P. Rastogi and R. R. Mishra, An Introduction to Chemical Thermodynamics, Vikas Publication,
- Gorakhpur, 2010.
- P. W. Atkins and D .Paula, Physical Chemistry, 8th Edition, Oxford University Press, 2010.
- E. N. Yenemin, Fundamentals of Chemical Thermodynamics, MIR, Publications.
- S. M. Blinder, Advanced Physical Chemistry,
- D. Mcquarie and J .Simon, Physical Chemistry –A Molecular Approach, University Press, 2000
- G. M. Barrow, Physical Chemistry, Tata Mc-Graw Hill, V edition 2003.
- H. K. Moudgil, Text Book of Physical Chemistry, Pretice Hall of India, New Delhi, 2010.
- G. M. Panchenkov and V. P. Labadev, "Chemical Kinetics and catalysis", MIR Publishing
- E. A. Moelwyn - Hughes, "Chemical Kinetics and Kinetics of Solutions", Academic
- K. J. Laidler, Chemical Kinetics, Third Edition) 1987(Harper and Row, New York.
- J. Raja Ram and J. C. Kuriacose, Kinetics and Mechanism of Chemical Transformations MacMilllan IndianLtd., New Delhi, 1993
- C. H. Bamford and C. F. H. Tipper, Comprehensive Chemical Kinetics, Vol 1., Elsevier Publications, New York, 1969.
- C. H. Bamford and C. F. H. Tipper, Comprehensive Chemical Kinetics, Vol 2., Elsevier Publications, New York, 1969.

- S. Glasstone, K. J. Laidler and H. Eyring, The Theory of Rate Processes, Mc -Graw Hill, New
  York, 1941.
- Santosh Kumar Upadhyay, Chemical Kinetics and Reaction Dynamics, Springer 2006.
- G. K .Agrawal, Basic Chemical Kinetics, Tata-Mc-Graw Hill, 1990.
- Ira .N. Levine, Quantum Chemistry, 5th edition (2000), Pearson educ., Inc.New Delhi
- A.K.Chandra, Introductory Quantum Chemistry, 4th edition (1994), Tata Mcgraw Hill, New Delhi.
- M.W.Hanna, "Quantum Mechanics in Chemistry", Benjamin
- L. Pualing and E. B. Wilson, Introduction to Quantum Mechanics with Applications to Chemistry, McGraw Hill, New York (1935).
- R. K. Prasad, Quantum Chemistry, New Age International, Delhi.
- R. K. Prasad, Quantum Chemistry through problems and solutions, New Age International, New Delhi, 2009.
- B. C. Reed, Quantum Mechanics, Jones and Bartlett, New Delhi, 2010.
- S. Glasstone, An Introduction to Electrochemistry, East-West Press Pvt. Ltd., New Delhi, 2004.
- K. L. Kapoor, Text Book of Physical Chemistry, Vol – I to Vol -VI, 2011.

NPTEL sources weblinks

For Classical Thermodynamics:

- https://archive.nptel.ac.in/courses/104/103/104103112/
- https://digimat.in/nptel/courses/video/104106094/L18.html

For Quantum Chemistry Introduction:

- https://archive.nptel.ac.in/courses/104/108/104108057/
- https://onlinecourses.nptel.ac.in/noc20_cy27/preview
- https://nptel.ac.in/courses/104106083
- https://nptel.ac.in/courses/104108057
- https://www.digimat.in/nptel/courses/video/104108057/L11.html

For Chemical Kinetics

- https://archive.nptel.ac.in/courses/104/101/104101128/
- https://www.youtube.com/watch?v=uep2XeLCGkc

For electrochemistry

- https://onlinecourses.nptel.ac.in/noc23_cy19/preview
- https://www.youtube.com/watch?v=XTt3gXB0a84

DSC III (Practical)

PGCH1P1: Inorganic Chemistry Practical

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

Course Objectives

1. To conduct the experiments for the preparation and characterization of metal complexes.
2. To conduct separation and determination of two metal ions from different alloys using Volumetric, Gravimetric and Spectrophotometric methods.
3. To conduct qualitative analysis of inorganic mixture containing total of five radicals including interfering radicals.

Course Outcomes

1. Students will learn to synthesize various inorganic compounds, purify and characterize them.
2. Students will also be able to perform qualitative and quantitative analysis of different compounds and mixtures.

Contents:-

I. Preparation of Inorganic Complexes and their characterization by:

Elemental analysis and physico-chemical methods (Electronic and IR Spectra, magnetic susceptibility measurements, Thermal analysis and Molar conductance studies).

1. $K_3[Al(C_2O_4)_3](H_2O)$ 2. $[VO(acac)_2]$ 3. $Na[Cr(NH_3)_2(SCN)_4]$
4. $K_3[Cr(SCN)_6]$ 5. $[Mn(acac)_3]$ 6. $K_3[Fe(C_2O_4)_3]$
7. $Hg[Co(SCN)_4]$ 8. $[Co(Py)_2Cl_2]$ 9. $[Cu_2(CH_3COO)_4(H_2O)_2]$
10. $[Ni(DMG)_2]$ 11. $[Ni(NH_3)_6]Cl_2$ 12. $[Cu(NH_3)_4(H_2O)_2]SO_4$

II. Quantitative Analysis:

Separation and determination of two metal ions from the following alloys involving: Volumetric, Gravimetric and Spectrophotometric methods

i) Copper (II) and Nickel (II)
ii) Copper (II) and Zinc (II)
iii) Nickel (II)—Zinc (II) and
iv) Copper (II)—Iron (III)

III. Qualitative analysis of radicals:

Semi-micro Analysis of inorganic mixture of containing total of five radicals including interfering radicals (not more than one such radical in a mixture), rare earth (not more than two rare earths in a mixture) and combination of cations (minimum 8 mixtures).

Cations: Mercury (I, II), Pb, Ag, Bi (III), Cu (II), Cd (II), As (IV, V), Sb (IV, V), Sn (II, IV), Fe (III), Al (III), Cr (III), Ni (II), Co (II), Mn (II), Zn (II), Barium, Strontium, Calcium and Magnesium.

Interfering radicals: Phosphate, Oxalate, Fluoride and Borate.

Rare Earth: Tl, Mo, W, Se, Ti, Zr, Th, V, U, Ce.

(Spot Test for individual cations should be performed)

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

DSC IV (Practical)

PGCH1P2: Physical Chemistry Practical

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

Course Objectives

The most important objective of this course is to apply theoretical principles to conduct various physic-chemical studies of some systems. The students should learn to apply non-instrumental and instrumental techniques for better understanding of physical chemistry concepts.

Course Outcomes

After completing this course, the students will-

1) Learn the determination of important quantities of liquids such as volume contraction on mixing and activation parameters of viscous flow.
2) Understand the determination of the critical micelle concentration (CMC) of a given surfactant and molecular mass of a polymer.
3) Know how to determine heat of dilution and also study effect of impurity on CST in phenol-water systems.
4) Understand determination of distribution coefficient, know how to construct the phase diagrams of two components system, find the mutual solubility of glycerol-*m*-toluidine.
5) Be able to determine rate constant, equilibrium constant and order of various reactions.
6) Learn to employ conductometry, potentiometry and pH metry for different studies.

Contents:-

It is expected to perform minimum 14 experiments in a semester. In examination one experiment from non-instrumental section and one experiment from instrumental section should be asked.

A] Non-instrumental Experiments:

1) To study the variation of volume contraction with mole fraction of alcohol in alcohol - water system
2) To determine the activation parameters of viscous flow for a given liquid.
3) To determine the critical micelle concentration (CMC) of a given surfactant/ soap/ shampoo by surface tension measurements.
4) Determination of molecular mass of a polymer by viscometry method.
5) To determine integral heat of KNO_3, at two different conc. and calculation of heat of dilution.
6) Effect of 1% NaCl, 1% succinic acid, 0.5% naphthalene on CST in phenol-water systems.
7) Distribution of succinic acid in H_2O-benzene, H_2O-ether and comparison of distribution coefficient.
8) To construct the phase diagrams of two components system (phenol- urea, diphenyl-aminebenzophenone; α-naphtyl amine-phenol) forming compounds with congruent melting points.
9) To study the mutual solubility of glycerol-*m*-toluidine and to determine congruent points.

10) To study kinetics of hydrolysis of an ester by NaOH reaction.
11) To determine equilibrium constant of the equation $KI+I_2=KI_3$ by distribution method.
12) To study the kinetics of the reaction between potassium persulphate and potassium iodide.
13) Determination of order of reaction of oxidation of ethyl alcohol by acid dichromate.

B] Instrumental Experiments:

1) To titrate conductometrically monobasic and dibasic acids with NaOH and determine the strength of given acid.
2) To determine equivalent conductance of weak electrolyte at infinite dilution by Kohlrausch's method.
3) To determine the heat of reaction, equilibrium constant and other thermodynamic functions for the reaction $Zn + Cu^{2+} \rightarrow Zn^{2+} + Cu$ potentiometrically.
4) To determine the formal redox potential of $Fe^{2+} \rightleftharpoons Fe^{3+}$ and $Ce^{3+} \rightleftharpoons Ce^{4+}$ systems by titrating ferrous ammonium sulphate against ceric sulphate.
5) To determine the pH of a buffer solutions using a quinhydrone electrode.
6) To determine the strength of given $Cu^{2=}$ solution by potentiometrically titrating against EDTA (Complexometric titrations).

Reference books:

- J. B. Yadav, Practical Physical Chemistry
- Das and Behra, Practical Physical Chemistry
- Carl W. Garland, Joseph W. Nibler and David P. Shoemaker, Experiments in Physical Chemistry, Mc-Graw Hill, 8th Edition, 2009.
- Farrington Daniels, Joseph Howard Mathews, John Warren Williams, Paul Bender, Robert A. Alberty, Experimental Physical Chemistry, Mc-Graw Hill, Fifth Edition, 1956.
- John W. Shriver and Michael George, Experimental Physical Chemistry, Lab Manual and Data Analysis, the University of Alabama in Huntsville, Fall 2006
- Chondhekar T.K: Systematic Experiments In Physical Chemistry, Rajbog S.W., Aniali Pubn.
- Merits And Thomas: Advanced Analytical Chemistry
- Ewing, G. W. : Instrumental Methods Of Chemical Analysis, Mcgraw-Hill
- Khopkar S.M.:Basic Concept of Analytical Chemistry
- Wlehov G. J: Standard Methods Of Chemical analysis 6th Ed
- Braun:Instrumental Methods of Chemical Analysis

Shiksha Mandal's

Bajaj College of Science, Wardha

(An Autonomous Institution)

Department of Chemistry

Proposed Syllabus for Two Year M.Sc. Chemistry

ELECTIVE

Semester I courses

Syllabus under Autonomy

(Draft to be discussed and approved in BOS Meeting 08-July-2023 to be implemented from Academic Session 2023-24)

Shiksha Mandal's

Bajaj College of Science, Wardha

Syllabus of M.Sc. I Semester I

ELECTIVE - I

PGCH1E1: Bonding, Stereochemistry and Nucleophilic Substitutions

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

Course Objectives

To learn

1. Basic idea about important electronic effects in organic chemistry, reactive intermediate, aromaticity.
2. 3-D aspect of organic molecules such as optical activity of asymmetric and dissymmetric molecules.
3. aliphatic nucleophilic substitution reaction.
4. aromatic nucleophilic and electrophilic substitution reactions.

Course Outcomes

Students will gain an understanding of:

1. fundamental knowledge of reactive intermediate, chemical bonding & aromaticity.
2. 3-D aspects of organic molecules.
3. aliphatic nucleophilic substitution reaction.
4. aromatic nucleophilic and electrophilic substitution reactions.

Contents:-

Unit-I

Chemical bonding, Aromaticity and Reactive Intermediates:

Chemical bonding: Recapitulation of delocalized chemical bonding, conjugation, resonance, hyperconjugation, cross conjugation, alternant and non-alternant hydrocarbons, tautomerism, Inductive effect.

A. **Bonding other than covalent bonding:** Hydrogen bonding, inclusion compounds, rotaxanes, catenanes, cyclodextrins, cryptands, crown ethers, Phase transfer catalyst, fullerenes.
B. **Aromaticity**: Benzenoid and non-benzenoid compounds, Huckel's rule, antiaromaticity, homoaromaticity, annulenes, azulenes, cyclopentadienyl anion, tropylium cation, tropone and tropolone.
C. **Reactive intermediates:** Generation, structure, stability and chemical reactions of carbocations, carbanions, free radicals, carbenes, nitrenes and benzyne / arynes.

Unit-II

A. **Stereochemistry:** Elements of symmetry, optical activity, chirality, enantiomers, diastereomers, meso compounds, stereochemical nomenclature (R-S, D-L, E-Z, threo-erythro), method of resolution, optical purity.

B. **Stereochemical principles:** prochirality, enantiotopic and diastereotopic atoms, groups and faces, stereochemistry of addition-elimination reactions, stereospecific and stereoselective synthesis, asymmetric synthesis, optical activity in biphenyls, spiranes, allenes.

C. **Conformational Analysis:** Conformational analysis of n-butane and cycloalkanes (5–8 membered rings), substituted cyclohexanes, mono substituted, disubstituted cyclohexanes, decalines, effect of conformation on reactivity.

Unit-III

A. Reaction mechanism: Types of mechanism, types of reaction, thermodynamics and kinetics requirements and control, thermodynamics vs kinetics control, Hammond's postulate, Curtin-Hammett principle, potential energy diagrams, transition states and intermediates, methods of determining mechanisms, Kinetic isotope effects, Hard and soft acids and bases.

B. Aliphatic nucleophilic substitution: The SN1, SN2, mixed SN1, SN2, SET and SNi mechanisms. Nucleophilicty, effect of leaving group, ambient nucleophiles and ambient substrates regiospecificity, substitution at allylic and vinylic carbon atoms

C. Neighbouring Group Participation: Concept of NGP, anchimetric assistance with mechanism, neighboring group participation by π and σ bonds, classical and non-classical carbocations, phenonium ions. Intramolecular displacement by hydrogen, oxygen, nitrogen, sulphur and halogen. Alkyl, cycloalkyl, aryl participation, participation in bicyclic system, migratory aptitude, carbocation rearrangement in NGP.

Unit IV

A. Aromatic Nucleophilic Substitution A general introduction to different mechanisms of aromatic nucleophilic substitution SNAr, SN1,benzyne and SRN1 mechanisms, arynes as reaction intermediate, Reactivity - effect of substrate structure, leaving group and attacking nucleophile. The Von Richter, Sommlet-Hauser and Smiles rearrangements

B. Aromatic electrophilic substitution The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The o/p ratio, ipso attack, orientation in benzene ring with more than one substituents, orientation in benzene ring with more than one substituents, orientation in other ring system. Reactions: nitration, halogenation, sulphonation, Friedel-Crafts alkylation and acylation, Vilsmeir-Hack reaction, Gatterman-Koch reaction, Pechman reaction, Reimer-Tieman reaction, Diazonium coupling.

C. Effect of Structure on reactivity: Resonance and field effects, Steric effect, Quantitative treatment: The Hammett equation and linear free energy relationship, substituent and reaction constants. Taft Equation

List of books

- Advanced Organic Chemistry –Reaction mechanism and structure. Jerry March, John Wiley
- Advanced Organic Chemistry- F.A. Carey and R. J. Sunberg, Plenum
- A Guidebook to Mechanism in Organic Chemistry-Peter Skyes, Longman
- Structure and Mechanism in Organic Chemistry-C.K. Gold, Cornell University Press

- Organic Chemistry, R.T. Morrison Boyd. Prentice Hall
- Modern Organic Chemistry-H.O. House, Benjamin
- Principal of Organic Chemistry-R.O.C. Norman and J.M. Coxon, Blackie Academic and Professional
- Reaction Mechanism in Organic Chemistry-S.M. Mukharji and S.P. Singh, Macmilan
- Stereochemistry of Organic Compounds- D. Nasipuri, New Age International
- Stereochemistry of Organic Compounds- P. S. Kalsi, New Age International
- Frontier Orbitals and Organic Chemical Reactions-I. Fleming
- Orbital Symmetry – R. E. Lehr and A. P. Marchand
- Reactive Intermediate in Organic Chemistry-N. S. Isaacs
- Stereochemistry of Carbon Compounds- E. L. Eliel
- Physical Organic Chemistry-J. Hine
- Name Reaction in Organic chemistry –Surrey
- Advanced Organic Chemistry – L. F. Fieser and M. Fieser

ELECTIVE - II

PGCH1E2: Polymer Chemistry I

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

Course Objectives

The main objectives of this course are

- To study basic concept, raw materials, nomenclature and classification of polymers along with types of polymerization with their mechanisms
- To understand concepts of polymer molar mass and important methods of determination.
- To realize important physical characteristics of polymers
- To learn about synthesis and application of some commercial and functional polymers

Course Outcomes

At the end of this course, students will-

- Be abreast with basic concept, raw materials, nomenclature and classification of polymers. of polymers.
- Understand types of polymerization with their mechanisms
- Realize concepts of polymer molar mass and important methods of determination.
- Gain an understanding of important physical characteristics of polymers
- Have the knowledge about synthesis and application of some commercial and functional polymers

Unit-I: Introduction to Polymer

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

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

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

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.

Reference books:

- 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.
- Contemporaty polymer chemistry: H.R. Alcock and F. W. Lambe, Prentice Hall.
- Principles of polymer Chemistry: Flory, Cornell Univ. press.
- Introduction to polymer chemistry: R. B. Seymour, McGraw Hill.
- Principles of polymerization: Odian.
- A first course in polymer chemistry: A. Strepikheyew, V. Derevistkay and G. Slonimasky, Mir Publishers, Moscow.

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

Department of Chemistry

Proposed Syllabus for Two Year M.Sc. Chemistry

Research Methodology (RM)

Semester I Course

Syllabus under Autonomy

(Draft discussed and approved in BOS Meeting 08-July-2023 to be implemented from Academic Session 2023-24)

Shiksha Mandal's

Bajaj College of Science, Wardha (Autonomous)

Department of Chemistry

M.Sc. I Semester I, NEP-2023-24

PGCH1RM: Research methodology

[4 Credits]

Course Objectives

1. Gain a comprehensive understanding of research methodology and its fundamental concepts.
2. Acquire skills in data collection, analysis, and interpretation using various statistical techniques.
3. Develop the ability to critically evaluate and select appropriate research methods for different types of research.
4. Enhance proficiency in technical writing, research reporting, and adherence to research ethics and academic integrity.

Course Outcomes

After learning research methodology course, students will be able to:

1. Identify and describe the characteristics of different types of research, including basic, applied, and patent-oriented research.
2. Apply descriptive and inferential statistical analysis techniques to analyze and interpret research data and its importance in research, and apply appropriate research methods.
3. Apply scientific thinking and problem identification techniques in the research process.
4. Develop skills in technical writing, research reporting, and the proper structure and organization of research documents and gain awareness of research ethics, academic integrity, and the importance of avoiding plagiarism and academic malpractice

Syllabus:

Module 1: Research basics and perception of research

1.1 Definition, General and specific characteristics of research, types of research (basic, applied and patent oriented).

1.2 Steps of Action (basic) research, objectives of basic research, characteristics of investigators.

1.3 Scientific thinking- characters, steps in process of scientific thinking, Steps in problem identification, criteria for selecting problem, and sources of scientific problems.

1.4 Review of literature- meaning, need, and objectives, structure of review of literature, sources of literature collection, Simple rules of structuring (writing) literature review.

Module 2: Statistical analysis for Chemists

2.1 Errors in chemical analysis. Classification of errors- systematic and random, additive, and proportional, absolute and relative. Accuracy and precision. Mean, median, average deviation and standard deviation.
2.2 Significant figures and rules to determine significant figures. Calculations involving significant figures.
2.3 Confidence limit, correlation coefficient and regression analysis. Comparison of methods: F-test and t-test. Rejection of data based on Q-test. Least squares method for deriving calibration graph.
2.4 Application of Microsoft Excel in statistical analysis (statistical functions and spreadsheets in MS-Excel). Certified reference materials (CRMs). Numerical problems.

Module 3: Scientific Writing and Presentation

3.1 Scientific writing. Types of scientific publications- magazines, journals, reviews, news-letters, structure of scientific paper.
3.2 Report Writing, different steps in report writing, types of reports, layout of research paper.
3.3 Research indicators & Metrics: Impact Factor, CiteScore, h-Index, i10-Index, Citation Index, references/bibliography, structuring the thesis, use of software in thesis writing.
3.4 Intellectual Property Rights (IPR): Introduction to IPR (Patents, Trademarks, Geographical indicators, Copyright, and neighboring rights), concept and theories, kinds of IPR, Advantages and disadvantages of IPR.

Module 4: Use of tools / techniques for Research

4.1 Methods to search required information effectively, Various reference styles, Reference Management Software like Zotero/Mendeley, preparation of bibliography database.
4.2 Software/tools: MS Word, MS Excel, Graph and chart preparation, MS Power Point, OriginLab (For plotting graph), ChemSketch, ChemDraw.
4.3 Research ethics, Academic integrity, Plagiarism, types, detection of plagiarism using software.

Reference/ Books:

1) Shanti Mishra, & Alok, S. (2011). Handbook of Research Methodology: A Compendium for Scholars & Researchers. Educreation Publishing.
2) Singh, Y. kumar. (2006). Fundamentals of Research Methodology and Statistics. New Age International Publishers.
3) Walliman, N. (2010). Research Methods The Basics. Routledge Taylor and Francis Group.
4) Research Methodology- C. R. Kothari
5) Best and Kahn, Research Methodology, PHI Limited
6) Design of Experience: Statistical Principles of Research Design and Analysis, by Robert O. Kuehl Brooks/cole.

7) Patrick Carey, Katherine T. Pinard, Ann Shaffer, Mark Shellman, New Perspectives Microsoft Office 365 and Office 2019 Introductory, 2020.

Assignments based on Research Methodology course

Instructions:

These assignments can enhance the professional skills needed to pursue a career in research/teaching. Therefore, each PG department should identify 10 assignments from the list below. Continuous evaluation will occur throughout the semester. Performance on the assignment will be graded for 40 marks.

1. **Navigate and use Google, Google Scholar, SciHub, PubMed, Web of Science, Elicit and ScienceDirect effectively to search for research papers, perform searches and retrieve relevant research papers.**
   [Suggestion/Working hours:- Dedicate a few hours each week to practice searching on these databases to continually refine your skills.]

2. **Write accurately references in APA format for various types of sources, including books, journal articles, websites, and conference papers and gain a comprehensive understanding of the Zotero platform, including its interface, features, and capabilities for managing bibliographic information.**
   [Suggestion/Working hours- Invest time in exploring and understanding the features of Zotero(https://www.zotero.org/) through guided tutorials and hands-on experience and gain proficiency in using Zotero to input, organize, and format references, and effectively manage bibliographic data]

3. **How to read research paper and develop a thorough understanding of the three-pass approach for effective note-taking from research readings.**

4. **Review and analyze collected references systematically to identify at least three prospective research problems or gaps in your domain.**
   [Suggestion/Working hours:- Review a minimum of 20 relevant references in your domain to gain a comprehensive understanding of current research trends and gaps. Dedicate focused time each week to systematically review references and refine your problem identification skill]

5. **Write at least three research objectives and three hypotheses that are well-defined, focused, and aligned with the research problem.**
   [Suggestion/Working hours:-Within one month, be able to formulate clear and relevant research objectives or hypotheses for the given research problem. Seek feedback from mentors or advisors to refine your research objectives or hypotheses and ensure their relevance and clarity.]

6. **Create a graph (line/bar/pie) using Microsoft Excel. Prepare publication ready graph and write legend for the graph and table.**

7. **Understand structure of scientific poster. Write well-structured scientific poster that effectively communicates research findings, adheres to design principles, and captures audience attention.**

8. **Understand structure of oral presentation and demonstrate the ability to deliver a clear and engaging oral presentation, incorporating effective communication techniques, and supporting visual aids.**

9. **Find out how to use the chosen plagiarism detection tool step by step to check a paper for possible instances of plagiarism. Attain the ability to use the chosen plagiarism detection tool proficiently, including uploading documents, interpreting plagiarism reports, and understanding similarity scores.**

10. **Write one page research proposal. Write research proposal in the format of any funding agency.**

11. **Write minireview article.**

12. **Write short communication with one table and one figure.**

13. **Write scientific blog.**

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 II courses

Syllabus under Autonomy

(Draft discussed and approved in BOS Meeting 08-July-2023 to be implemented from Academic Session 2023-24)

Shiksha Mandal's

Bajaj College of Science, Wardha

Syllabus of M.Sc. I Semester II

DSC V (Theory)

PGCH2T1: Organic Chemistry

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

Course Objectives

To learn

1. various addition reactions across C-C, C-O and C-N multiple bonds.
2. basic concepts in molecular rearrangement & elimination reaction.
3. types and mechanism of free radical reactions.
4. principles and advantages of green chemistry.

Course Outcomes

Students will gain an understanding of:

1. various addition reactions across C-C, C-O and C-N multiple bonds.
2. basic concepts in molecular rearrangement & elimination reaction.
3. types and mechanism of free radical reactions.
4. principles and advantages of green chemistry.

Contents:-

Unit-I Addition reactions:

A. Addition to carbon-carbon multiple bond: Mechanistic and stereochemical aspects of addition reaction involving electrophiles, nucleophiles and free radicals, regio and chemoselectivity, Orientation and stereochemistry, Addition to cyclopropanes, Hydrogenation of double bond and triple bonds. Hydrogenation of aromatic rings, hydroboration..

B. Addition to carbon-hetero atom multiple bond: Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters, and nitriles, Addition of Grignard reagents, organozinc and organolithium reagents to carbonyls and unsaturated carbonyl compounds, Wittig reaction, Mechanisms of condensation reactions involving enolates- Aldol, Knoevengel, Claisen, Mannich, Benzoin, Perkin, Stobbe reaction, Michael reaction and Robinson annulations. Hydrolysis of esters and amide

Unit-II Molecular rearrangements:

A. Molecular rearrangements: Classification and General mechanistic treatment of electrophilic, nucleophilic and free radical moleculer rearrangement. Mechanism and synthetic applications of Wagner-Meerwin, Pinacol-Pinacolone, Tiffenev-Demjnov ring expansion,

benzil-benzilic acid, Favorski, Baeyer Villiger, Wolff, Arndt-Eistert synthesis, Curtius Lossen, Beckman, Hoffman, Schmidt rearrangement.

B. Elimination reactions: E1, E2, E1CB mechanisms, orientation and stereochemistry in elimination reaction, Saytzeff and Hoffman's rule, Effect of substrate structure, attacking base, leaving group and medium, competition between elimination and substitution, syn eliminations, pyrolytic elimination.

Unit-III Free radical reactions:

Generation of free radicals, types and mechanism of free radical reactions, free radical substitution mechanism at an aromatic substrate, aliphatic substrate, reactivity at a bridgehead position, Neighbouring group assistance, reactivity for aliphatic and aromatic substrates, reactivity in attacking radicals, effect of solvent on reactivity, Halogenation at an alkyl carbon, allylic carbon (NBS), hydroxylation at an aromatic carbon by means of Fenton's reagent. Auto-oxidation, chlorosulphonation (Reed Reaction) Coupling of alkynes and arylation of aromatic compounds by diazonium salts, Sandmeyer reaction, Free radical rearrangement: Hunsdiecker reaction, Iododecarboxylation, Barton reaction, Hoffmann-Loefler-Freytag reaction.

Unit-IV Green chemistry:

Twelve basic principles of green chemistry, calculation of atom economy of rearrangements, addition, substitution and elimination reaction with suitable examples, Case study of Bhopal gas tragedy and Seveso disaster, Synthesis involving basic principles of green chemistry-paracetamol, Ibuprofen, hydroquinone, adipic acid, ε-caprolactum, styrene, urethanes, Free radical bromination, Multi-component reactions (Biginelli, Ugi and Passerini reaction), Prevention or minimization of hazardous products, choice of solvents. Sonochemistry, microvave induced reactions, polymer supported reagents, reactions in aqueous medium, zeolites and ionic liquid supported reaction, Solvent free reactions, electrochemical reactions, Biocatalysts in Organic synthesis.

Reference books:

1) Advanced Organic Chemistry –Reaction mechanism and structure. Jerry March, John Wiley
2) Advanced Organic Chemistry- Part-A- F.A. Carey and R. J. Sunberg, Plenum
3) A Guidebook to Mechanism in Organic Chemistry-Peter Skyes, Longman
4) Structure and Mechanism in Organic Chemistry-C.K. Gold, Cornell University Press
5) Organic Chemistry, R.T. Morrison Boyd. Prentice Hall
6) Modern Organic Chemistry-H.O. House, Benjamin
7) Principal of Organic Chemistry-R.O.C. Norman and J.M. Coxon, Blackie Academic and Professional
8) Reaction Mechanism in Organic Chemistry-S.M. Mukharji and S.P. Singh, Macmilan
9) Advanced Organic Chemistry – L. F. Fieser and M. Fieser.
10) Organic Chemistry Vol. I and II - I. L. Finar
11) Frontier Orbitals and Organic Chemical Reactions-I. Fleming
12) Orbital Symmetry – R. E. Lehr and A. P. Marchand
13) Reactive Intermediate in Organic Chemistry-N. S. Isaacs
14) A Textbook of organic chemistry- R.K. Bansal
15) Some Modern Methods of Organic Synthesis-W. Carruthers
16) Advance Organic Chemistry Part-B-F. A. Caray and R. J. Sundberg Plenum Press

17) Modern Synthetic Reaction. H. O. House and W. A. Benjamin
18) Designing Organic Synthesis-S. Warren
20) Organic Reaction and their Mechanism-P. S. Kalsi
21) New trends in green chemistry –V.K. Ahluwalia and M. Kidwai, Anamaya publishers New Delhi

DSC VI (Theory)

PGCH2T2: Analytical Chemistry

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

Course Objectives

The primary objective of this course is to acquire basic concepts, principles, and techniques of modern analytical chemistry that would empower students with an analytical mind set and the abilities to solve diverse analytical problems in an efficient and quantitative way that conveys the importance of accuracy and precision of the analytical results. The Course is aimed at-

1. Studying Introduction to analytical chemistry.
2. Gaining knowledge of classical methods of analysis.
3. Understanding Separation Techniques, Chromatography, Ion exchange and Solvent extraction.
4. Knowing Electroanalytical Methods of Analysis – conductometry & Potentiometry.
5. Knowing optical methods of Analysis – Spectrophotometry and Colorimetry

Course Outcomes

1. Express the role of analytical chemistry in science.
2. Explain the fundamentals of analytical chemistry and steps of a characteristic analysis.
3. Compare & express qualitative and quantitative methods.
4. Understanding fundamentals of Separation techniques like Chromatography & solvent extraction.
5. Explain the theoretical principles and important applications of classical analytical methods within titration (acid/base titration, complexometric titration, redox titration, precipitation titration), and various techniques within gravimetric methods.
6. Realize the theoretical principles of electroanalytical & optical techniques conductometry, Potentiometry, Spectrophotometry and Colorimetry

Content

Unit-I

Introduction to analytical chemistry: Types of analysis-qualitative and quantitative. Classification of analytical methods- classical and instrumental, basis of their classification with examples.

Classical Methods of Analysis:

a) Volumetric analysis: General principle. Criteria for reactions used in titrations. Primary standards and secondary standards. Theory of indicators. Types of titrations with examples- Acid-base, precipitation, redox and complexometric. Titration curves for monoprotic and polyprotic acids and bases. Indicators used in various types of titrations. Masking and demasking agents.

b) Gravimetric analysis: General principles and conditions of precipitation. Concepts of solubility, solubility product and precipitation equilibria. Steps involved in gravimetric analysis. Purity of precipitate: Co-precipitation and post-precipitation.

Fractional precipitation. Precipitation from homogeneous solution. Particle size, crystal growth, colloidal state, aging and peptization phenomena. Ignition of precipitates.

Unit-II

Separation Techniques:

a) Chromatography: Definition and Classification. Techniques used in Paper, Thin Layer and Column chromatography. Applications in qualitative and quantitative analysis.

b) Ion exchange: Principle and technique. Types of ion exchangers. Ion exchange equilibria. Ion exchange capacity. Effect of complexing ions. Zeolites as ion-exchangers. Applications.

c) Solvent extraction: Principle and techniques. Distribution ratio and distribution coefficient. Factors affecting extraction efficiency: Ion association complexes, chelation, synergistic extraction, pH. Numericals based on multiple extractions. Role of chelating ligands, crown ethers, calixarenes and cryptands in solvent extraction. Introduction to Solid phase extraction (SPE) and Microwave assisted extraction (MAE), Applications.

Unit-III

Electroanalytical Method-I

Conductometry: Concepts of electrical resistance, conductance, resistivity and conductivity. Specific, molar and equivalent conductance and effect of dilution on them. Measurement of conductance. Kohlrausch's law, Applications of conductometry in determination of dissociation constant, solubility product. Conductometric titrations. High frequency titrations. Numerical problems.

Potentiometry: Circuit diagram of simple potentiometer. Indicator electrodes: hydrogen electrode, quinhydrone electrode, antimony electrode and glass electrode. Reference electrodes: Calomel electrode and Ag/AgCl electrode. Theory of potentiometric titrations. Acid-base, redox, precipitation and complexometric titrations. Nernst equation, standard electrode potential, Determination of cell potential, n, Kf and Ksp. pH titrations. Buffers and buffer capacity. pH of buffermixtures based on Henderson-Hasselbalch equation.

Unit-IV

Optical Methods of Analysis-I:

a) Spectrophotometry and Colorimetry: Principle of colorimetry. Beer's law, its verification, and deviations. Instrumentation in colorimetry and spectrophotometry (single and double beam). Sensitivity and analytical significance of molar extinction coefficient and λmax. Comparison method, calibration curve method and standard addition method for quantitative estimation. Role of organic ligands in spectrophotometric analysis of metal ions. Ringbom plot and Sandell's sensitivity. Photometric titrations. Determination of pK value of indicator. Simultaneous determination. Composition and stability constant of complex by Job's and mole ratio methods. Derivative spectrophotometry. Numerical problems.

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

DSC VII (Practical)

PGCH2P1: Organic Chemistry Practical

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

Course Objectives

To learn the purification techniques (solvents & reagents), qualitative analysis of two component mixture & organic preparation of single step & two step synthesis.

Course Outcomes

Students will gain an understanding of:

1) Separation and analyze the different component mixtures of simple organic compounds.
2) Purification, Crystallization, and different Distillation processes.
3) How to calculate a limiting reagent, yield, and percent yield
4) Synthesis using substitution and condensation reactions.
5) Single step & multistep synthesis.

Contents:-

I. Purification techniques (Demonstrations):

a) Purification of solvents and reagents using techniques like crystallization, distillation, steam distillation, vacuum distillation etc.

b) Chromatography: TLC, Column, paper

c) Solvent extraction using soxhlet extractor

II. Qualitative Analysis:

Two component mixture separation using chemical and physical techniques and using solvents.

(8 mixtures minimum)

III. Organic Preparations (minimum 8 preparations):

Spectral characterization of prepared compounds wherever possible**:**

1. Single step preparation

a) Aldol condensation: Benzaldehyde →Dibenzal acetone (chalcone)

b) Benzophenone → benzhydrol

c) Nitrobenzene → m-di-nitrobenzene

d) m-di-nitrobenzene → m-nitroaniline

e) Methyl acetoacetate → 5-methyl-isoxazol-3-ol

f) Ethyl acetoacetate → 4-aryl-6-methyl-3,4-dihydro-2(1H)-pyrimidinone ester

g) Ethyl acetoacetate→Diethyl 1,4-dihydro-2,6-dimethyl-4-phenylpyridine-3,-5dicarboxylate

h) Sulphanilic acid → Methyl orange

i) p-nitroaniline → p-red

2. Two step preparation

a) Acetanilide → p-nitroacetanilide → p-nitroaniline

b) Aniline → 2,4,6-tribromo aniline → 2,4,6-tribromoacetanilide

c) Nitrobenzene → m-dinitrobenzene → m-nitroaniline

d) benzophenone→ benzophenoneoxime→ Benzanilide

e) Chlorobenzene→ 2,4-dinitrochlorobenzene → 2,4-dinitrophenylhydrazine

f) Glycine → Benzoyl glycine(hippuric acid) → 4-benzilidene-2-phenyl oxazole

Reference Books:-

- A Textbook of Practical Organic Chemistry, 4th Edn., A. I. Vogel, ELBS.
- Laboratory Techniques in Organic Chemistry, V. K. Ahluwalia, Pooja Bhagat, Renu Agrawal, I. K. International
- Practical Organic Chemistry: Qualitative Analysis, Ane's Student Edition, S. P. Bhutani, Aruna Chhikara, Ane Books India
- Advanced Practical Organic Chemistry, John Leonard, Barry Lygo, Garry procter, CRC Press, Special Indian Edition
- Organic Chemistry – A Lab Manual, Pavia, Lampman, Kriz, Engel, Cengage learning
- Practical Organic Chemistry, F. G. Mann and B. C. Saunders, English language Book Society
- Organic Chemistry: Laboratory Course book, Dr. P. V. Tekade, Selective and Scientific books, New Delhi

DSC VIII (Practical)

PGCH2P2: Analytical Chemistry Practical

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

Section (A):

I. Classical methods and separation techniques: Calibration, validation, and computers

1) Calibration of pipette and burette.
2) Statistical analysis of data.
3) Use of MS-Excel in statistical analysis of data and curve fitting.

II. Volumetry

1) Determination of Na_2CO_3 in washing soda.
2) Determination of NaOH and Na_2CO_3 in a mixture.
3) Estimation of nickel in given solution by direct complexometric titration with EDTA using bromopyrogallol red.
4) Estimation of nickel in given solution by complexometric back-titration with EDTA.
5) Estimation of chloride in given solution by Mohr's titration.
6) Estimation of chloride in given solution by Volhard's titration.
7) Determination of volume strength of commercial hydrogen peroxide by redox titration with $KMnO_4$.
8) Estimation of phenol/ aniline by bromination method.
9) Estimation of glucose.
10) Estimation of acetone.
11) Estimation of formaldehyde.
12) Estimation of Mn in the presence of Fe using masking phenomenon (ferromanganese alloy).

III. Gravimetry

1) Estimation of barium as barium sulphate.
2) Estimation of calcium as calcium oxalate/ calcium carbonate/ calcium oxide.

IV. Separation techniques

1) Qualitative separation of metal ions by paper chromatography for 2/3 components.
2) Determination of ion-exchange capacity of resin.
3) Separation of ions by ion exchange.

Section (B): Instrumental techniques

I. 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

II. 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:

- Quantitative analysis: Day and Underwood (Prentice-Hall of India)
- Vogel's Text Book of Quantitative Inorganic Analysis-Bassett, Denney, Jeffery and Mendham (ELBS)
- Analytical Chemistry: Gary D. Christian (Wiley, India).
- Instrumental Methods of Analysis: Willard, Merrit, Dean, Settle (CBS Publishers, Delhi, 1986)
- Instrumental Methods of Chemical Analysis: Braun (Tata McGraw-Hill)
- Advanced Analytical Chemistry: Meites and Thomas (McGraw-Hill)
- Instrumental Methods of Analysis: G. Chatwal and S. Anand (Himalaya Publishing House)
- Analytical Chemistry: Problems and Solution- S. M. Khopkar (New Age International Publication)
- Basic Concepts in Analytical Chemistry: S. M. Khopkar (New Age International Publication)
- Advance Analytical Chemistry: Meites and Thomas: (Mc Graw Hill)
- An Introduction to Separation Science: L. R. Shyder and C. H. Harvath (Wiley Interscience)
- Fundamentals of Analytical Chemistry: S. A. Skoog and D. W. West
- Instrumental Methods of Chemical Analysis: G. W. Ewingeriments In Physical Chemistry, Rajbog S.W., Aniali Pubn.
- Merits And Thomas: Advanced Analytical Chemistry

- Ewing, G. W. : Instrumental Methods Of Chemical Analysis, Mcgraw-Hill
- Khopkar S.M.:Basic Concept of Analytical Chemistry
- Wlehov G. J: Standard Methods Of Chemical analysis 6th Ed
- Braun:Instrumental Methods of Chemical Analysis

Shiksha Mandal's

Bajaj College of Science, Wardha

(An Autonomous Institution)

Department of Chemistry

Proposed Syllabus for Two Year M.Sc. Chemistry

ELECTIVE

Semester II courses

Syllabus under Autonomy

(Draft to be discussed and approved in BOS Meeting 08-July-2023 to be implemented from Academic Session 2023-24)

Shiksha Mandal's

Bajaj College of Science, Wardha

Syllabus of M.Sc. I Semester II

ELECTIVE - I

PGCH2E1: Reaction Mechanism, π-Complexes and Clusters

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

Course Objectives

1. Analyse the reactivity of transition metal complexes.
2. Analyse the reaction pathways of complex formation understand its reaction mechanism.
3. Study the preparation, structures and properties of metal carbonyls and metal nitrosyls and the chemistry of dioxygen and dinitrogen complexes.
4. Understand the classification of metal clusters containing metal-metal bonds.
5. Learn about the isopolyacids and heteropolyacids and their structures.

Course Outcomes

The learner will gain knowledge of:

1. Reaction mechanism governing the substitution reaction substitution and electron transfer reactions in transition metal complexes.
2. Structure and bonding in metal carbonyls and metal nitrosyls.
3. Occurrence of metal-metal bonds in metal clusters and its significance.

Contents:-

Unit-I Reaction mechanism of transition metal complexes-I:

Energy profile of reaction, reactivity of metal complexes, inert and labile complexes, kinetics of octahedral substitution: Acid hydrolysis, factors affecting acid hydrolysis, stereochemistry of intermediates in SN^1 and SN^2, Base hydrolysis, Conjugate base mechanism, Direct and indirect evidences in favour of conjugate mechanism, anation reaction, reaction without metal-ligand bond breaking.

Unit-II Reaction mechanism of transition metal complexes –II:

Substitution reaction in square planar complexes: trans effect, cis effect, steric effect, solvent effect, effect of leaving group, effect of charge, effect of nucleophile, effect of temperature. Trans effect theories, use of trans effect, mechanism of substitution reaction of Pt(II) Complexes, electron transfer reactions. Types of electron transfer reaction, conditions of electron transfer and mechanism of one electron transfer reaction, outer sphere and inner sphere mechanism, two electron transfer reactions, complementary and non-complementary reaction , tunneling effect, cross reactions.

Unit-III Metal π-Complexes:

a) Metal carbonyls

Structure and bonding, vibrational spectra of metal carbonyls for bonding and structure elucidation, important reaction of metal carbonyls. Metal carbonyl clusters with reference to classification, EAN rule, synthesis and structures.

b) Metal nitrosyls

Nitrosylating agents for synthesis of metal nitrosyls, vibrational spectra, and X-ray diffraction studies of transition metal nitrosyls for bonding and structure elucidation, important reactions of transition metal nitrosyls, structure and bonding. Dinitrogen and dioxygen complexes. Wilkinson's catalyst and Vaska's compound.

Unit-IV Metal cluster:

Occurrence of metal-metal bonds, Classification of metal cluster: binuclear, trinuclear, tetranuclear, pentanuclear, and hexanuclear with reference to halide, oxide, alkoxide and acetate clusters. Isopoly, heteropoly acids and their anions.

Reference books:

- S. F. A. Kettle, J. N. Murral & S. T. Teddler: Valency Theory
- C. A. Coulson: Valency
- J. E. Huheey : Inorganic Chemistry
- F .A. Cotton & G. Wilkinson: Advanced Inorganic Chemistry 3rd, 5th& 6th Editions.
- F. Willims: Theoretical Approach in inorganic chemistry.
- Mannas Chanda: Atomic Structure and chemical Bonding
- L. E. Orgel: An introduction to transition metal chemistry, Ligand field theory, 2nd Edition.
- J. J. Logowski: Modern Inorganic Chemistry
- B.Durrant and P.J.Durrant: Advanced Inorganic Chemistry
- J. C. Bailar: Chemistry of co-ordination compounds.
- W. L. Jolly: Modern Inorganic Chemistry
- R. S. Drago: Physical methods in inorganic chemistry.
- Waddington: Nonaqueous solvents.
- Sisler: Chemistry of non-aqueous solvents.
- K. Barnard: Therotical Inorganic Chemistry
- Emeleus and Sharpe: Modern Aspect of Inorganic Chemistry.
- F. A. Cotton: Chemical Applications of Group theory.
- Jones: Elementary Co-ordination chemistry.
- N. Figgis: Introduction to Ligand field.
- S. F. A. Kettle: Co-ordination chemistry.
- M. C. Day and J. Selbin: Theoretical Inorganic Chemistry.
- J. Lewin and Wilkins: Modern Co-ordination chemistry.
- Gowarikar, Vishwanathan and Sheedar: Polymer science.
- R. L. Dutta and A. Symal: Elements of magneto chemistry

- P. Atkins: Inorganic Chemistry 4th Edition, Oxford University Press.
- D.M.P.Mingos: Essential Trends in Inorganic Chemistry, Oxford University Press
- Bertini, et al: Bioinorganic Chemistry (Viva)
- Fenton, David E.: Biocoordination chemistry, Oxford

ELECTIVE - II

PGCH2E2: Polymer Chemistry II

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

Course Objectives

- To reinforce the basic concepts of polymer chemistry including polymerization processes and techniques, polymer architectures, configuration and conformation of polymers etc.
- To learn the spectroscopic, thermal and thermochemical techniques for characterization of polymers.
- To study briefly few examples of biomedical, inorganic, coordination and diene based polymers

Course Outcomes

On successful completion of this course, student should

- Understand the important basic concepts of polymer chemistry
- Know the types and techniques of polymerization processes
- Gain knowledge about important polymer characterization techniques

Know synthesis and application of some important biomedical, inorganic, coordination and diene based polymers

Course Contents

Unit-I: Polymerization

Importance, basic concepts, raw materials for polymers, concept of functionality, comparison of chain and step-growth, examples of polymerization reactions (polyadditions, polycondensations) constitution of polymers, homopolymers and copolymers, polymer architectures (graft copolymers, star-branched, hyperbranched and dendrimers), configuration and conformation of polymers, coil formation, mobility in polymers, glass transition temperature, rubber elasticity, molecular weight distribution.

Unit-II: Techniques of Polymerization

Techniques of polymerization-suspension, emulsion and bulk polymerization, coordination, polymerization mechanism of Ziegler Natta polymerization, stereospecific polymerization, interfacial polycondensation, mechanism of polymerization.

Unit III: Characterization of Polymers

Spectroscopic techniques: Fundamentals, experimental and applications to polymers of the following techniques: UV-visible spectroscopy, IR and Raman spectroscopy, Nuclear Magnetic (proton, carbon), resonance spectroscopy, NMR of polymers in the solid state, two dimensional NMR spectroscopy, pyrolysis GC-MS.
Thermal methods-TGA, DTA, DSC,
Thermomechanical and X-ray diffraction study, Block and Graft copolymers, random, block, graft co-polymers, methods of copolymerization.

Unit IV: Specific Polymers

A) **Biomedical polymers**: Contact lens, dental polymers, artificial heart, kidney and skin.
B) **Inorganic polymers**: Synthesis and application of silicon, phosphorous and sulphur

containing polymers.

C) **Coordination polymers**: Synthesis and applications of coordination polymers.
D) **Diene-based polymers**: Polyisoprene, polybutadiene.

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.

Bajaj College of Science, Wardha (Autonomous College)

SUBJECT: CHEMISTRY

Syllabus of M.Sc. II/Semester III

CH 301: Paper 9 (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 $(COCl)_2$, 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.

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

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

CH 302: Paper 10 (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 tepenoids: myrecene, linalool, geraniol, α-terpeneol, limonene, camphor, α-pinene, β-pinene, farnesol, β-bisabolene and squelene

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, ends group analysis.

<u>Reference books</u>:

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

CH 305: Practical-V (Organic Chemistry Practical) [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 Amine 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)

CH-303: Paper 11 (Elective- 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, types of ecosystems.
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: Water **15 h**

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.

Unit-III: 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.

Unit-IV: **15 h**

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.

CH-306: 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 types 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

CH-303: Paper 11 (Elective- 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.

CH-306: 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.

CH-303: Paper 11 (Elective- 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.

CH-306: 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

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 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

CH-304: Paper 12 (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, group frequencies, 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. 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

CH-304: Paper 12 (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

Bajaj College of Science, Wardha (Autonomous College)

SUBJECT: CHEMISTRY

Syllabus of M.Sc. II/Semester IV

CH 401: Paper 13 (Special I-Organic Chemistry) [L-T-P = 4-0-0]

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

Unit-I **15L**

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 **15L**

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 Ist and IInd generation catalyst, reaction mechanism and application in the synthesis of homo and heterocyclic compounds.

Unit-III **15L**

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 **15L**

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 annelation, 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

CH 402: Paper 14 (Special II-Organic Chemistry) [L-T-P = 4-0-0]

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

Unit-I: Enzyme chemistry 15L

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 15L

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 B_6, Ondansetron, Serotonin, Indometacin, Cyanamid, fentiazac, trimethoprim, papaverine

Unit-III **15L**

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 of nucleic 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 **15L**

A] Dyes: General Introduction, classification on the basis of structure and methos 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, Ed Robert 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

CH 405: Practical-VII (Organic Chemistry Practical) [L-T-P = 0-0-8]

8 h per week **100 Marks**

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

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-one Butanoic 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).

CH-403: Paper 15 (Elective- Environmental Chemistry-II) [L-T-P = 4-0-0]

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

Unit-I: Water Pollution **15 h**

Pollutants, Types of pollutants, sources of water pollution, sampling, preservation and storage of water sample, physico –chemical, organoleptic and chemical analysis of water, electro-analytical, optical (UC-visible spectrophotometry, AAS, flame photometry, XRF, ICPAES) & chromatographic (GC and HPLC) techniques.

Historical development of detergents, chemistry of soaps and detergents.

Unit-II: Air Pollution **15 h**

Natural versus polluted air, 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.

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

Unit-III: Solid waste pollution **15 h**

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-IV: **15 h**

Soil Pollution: 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. Methodology of waste water disposal on land in India. Control of soil pollution.

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

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

CH-403: Paper 15 (Elective- Polymer Chemistry-II) [L-T-P = 4-0-0]

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

Unit-I: Polymerization **15h**

Importance, basic concepts, raw materials for polymers, concept of functionality, comparison of chain and step-growth, examples of polymerization reactions (polyadditions, polycondensations) constitution of polymers, homopolymers and copolymers, polymer architectures (graft copolymers, star-branched, hyperbranched and dendrimers), configuration and conformation of polymers, coil formation, mobility in polymers, glass transition temperature, rubber elasticity, molecular weight distribution.

Unit-II: Techniques of polymerization **15h**

Techniques of polymerization-suspension, emulsion and bulk polymerization, coordination, polymerization mechanism of Ziegler Natta polymerization, stereospecific polymerization, interfacial polycondensation, mechanism of polymerization.

Unit III: Characterization of polymers **15h**

Spectroscopic techniques: Fundamentals, experimental and applications to polymers of the following techniques: UV-visible spectroscopy, IR and Raman spectroscopy, Nuclear Magnetic (proton, carbon), resonance spectroscopy, NMR of polymers in the solid state, two dimensional NMR spectroscopy, pyrolysis GC-MS.
Thermal methods-TGA, DTA, DSC,
Thermomechanical and X-ray diffraction study, Block and Graft copolymers, random, block, graft co-polymers, methods of copolymerization.

Unit IV: Specific polymers **15h**

A) Biomedical polymers: Contact lens, dental polymers, artificial heart, kidney and skin.
B) Inorganic polymers: Synthesis and application of silicon, phosphorous and sulphur containing polymers.
C) Coordination polymers: Synthesis and applications of coordination polymers.
D) Diene-based polymers: Polyisoprene, polybutadiene.

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.

CH-403: Paper 15 (Elective- Medicinal Chemistry-II) [L-T-P = 4-0-0]

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

UNIT-I: **15 h**

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

B] Statastical method: For sampling and interpretation of results, Statastic 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: **15 h**

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: **15 h**

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.

UNIT-IV: **15 h**

A) Anthelminitics and antiamoebic drugs: Introduction to Helminthiasis, Anthelminitics, drugs used in cestode infection, drugs used in trematode infection, origin of antiamoebic drug, drugs used in nematode infection. Synthesis of: Clioquinol, Iodoquinol, Haloquinol, Dichlorphen, Niclosamide.

Anti-inflammatory drugs: Introduction, etiology of inflammatory diseases. The inflammatory response, biochemical response. Synthesis of: Phenyl butazone and its derivatives, pyrazolone derivatives, pyrole and indole acetic acid derivatives.

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 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

CH-404: Paper 16 (Spectroscopy – II (Core Subject Centric)) [L-T-P = 4-0-0]

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

Unit I: **15 h**

A] Ultraviolet and visible spectroscopy: Natural line width, line broadening, transition probability, 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: Nuclear magnetic Resonance Spectroscopy **15 h**

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 III: **15 h**

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 IV: **15 h**

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 (^{1}H 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-CN Banwell
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

OR

CH-404: Paper 16 (Foundation Course-II) Applied Analytical Chemistry–II [L-T-P = 4-0-0]

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

Unit-I: Water treatment **15h**

Hardness of water and types of hardness. Problems due to hardness. Removal of hardness by lime- soda process, Zeolite process and synthetic ion-exchange resins. Principle, instrumentation and comparison of these three processes. Numericals based on hardness removal. Desalination of sea- water.

Unit-II: Polymer chemistry and leather analysis **15h**

Polymer chemistry: Definition, classification, co-polymers, conducting polymers, determination of acid value, saponification value, iodine value, molar mass by end group analysis- amide and hydroxyl, molecular weight by viscosity method, glass transition temperature of polymers, TGA and DTA studies of polymers.

Analysis of leather: Determination of moisture, acid, free sulphur, total ash, chromic oxide in leather, tensile strength and stretch of leather.

Unit-III: Metallurgy **15h**

Ores and minerals, General principles of extraction of metals from ores. Steps involved in metallurgical extraction. Purification and concentration of ores. Extraction of crude metal from concentrated ore-pyrometallurgy, hydrometallurgy and electrolytic processes. Refining of metal. Thermodynamic aspects of metallurgical processes and Ellingham diagram. Furnaces in metallurgy. Metallurgy of Cu, Ag, Au, Al and Fe.

Unit-IV: Clinical analysis **15h**

General composition of blood, Collection and storage of blood samples, Estimation of chloride, calcium, sodium, potassium and bicarbonate in blood sample. Qualitative tests for reducing sugar. Estimation of blood glucose, urea, uric acid, blood urea-nitrogen, total serum protein,

serum albumin, serum creatinine, serum phosphate, serum bilirubin, serum cholesterol. Radioimmunoassay (RIA).

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. Chemistry for Environmental Engineering and Science: C N Sawyer, P L McCarty and G F Parkin
5. Vogel's Text Book of Quantitative Inorganic Analysis-Bassett, Denney, Jeffery and Mendham (ELBS)
6. Analytical Chemistry: Gary D. Christian (Wiley India).
7. Instrumental Methods of Analysis: Willard, Merrit, Dean, Settle (CBS Publishers, Delhi, 1986)
8. Water analysis : J. Rodier
9. A Text book of Inorganic Analysis : A.I.Vogel