Shiksha Mandal's

Bajaj College of Science, Wardha

Department of Chemistry

Revised Syllabus of M. Sc. Chemistry
Semester I
for Academic Autonomy

(Approved in BOS Meeting 8-September-2021)

Syllabus for M. Sc. Chemistry
Effective from 2021-22
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.

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.

M. Sc. Chemistry

Semester I

Paper – I [Code: PG- CHE (02)- S1-T1]

Inorganic Chemistry

60 h (4 h per week) :15 h per unit [L-T-P = 4-0-0] **80 Marks**

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. Describe the role of metal in biological system and their function.
5. 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 and carboranes.
4. Validate the role of bioinorganic chemistry in every day action.

Contents:-

Unit-I **15h**

A. Stereochemistry and Bonding in Main Group Compound: VSEPR-Shape of simple inorganic molecules and ions containing lone pairs, various stereochemical rules and resultant geometry of the compounds of non-transitional elements, shortcoming of VSEPR model. Bent's rule and energetics of hybridization.

B. Metal – Ligand Bonding:

Crystal Field Theory: Splitting of d-orbital in tetragonal, square planar and trigonal bipyramid complexes. Jahn-Teller effect, spectrochemical series, nephelauxetic effect. Limitations of crystal field theory. M. O. Theory for octahedral, tetrahedral & square planar complexes with and without π-bonding.

Unit-II **15h**

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 Cluster I **15h**

Boron hydrides: Classification, nomenclature, structure, bonding and topology of boranes, 4 digit coding (STYX) number for higher boranes and their utility, study of metalloboranes, carboranes and metallocarboranes with reference to preparation and structure. Wade's rule for boranes and carboranes.

Unit-IV: Bioinorganic Chemistry: **15h**

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 (Structure & functions): 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: Haemoglobin and myoglobin, its structure and functions.

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

Reference books:

1] S. F. A. Kettle, J. N. Murral & S. T. Teddler: Valency Theory
2] C. A. Coulson: Valency
3] J. E. Huheey: Inorganic Chemistry
4] F .A. Cotton & G. Wilkinson: Advanced Inorganic Chemistry 3rd, 5th& 6th Editions.
5] A. F. Willims: Theoretical Approach in inorganic chemistry.
6] A. Mannas Chanda: Atomic Structure and chemical Bonding
7] L. E. Orgel: An introduction to transition metal chemistry, Ligand field theory, 2nd Edition.
8] J. J. Logowski: Modern Inorganic Chemistry
9] B. Durrant and P. J. Durrant: Advanced Inorganic Chemistry
10] J. C. Bailar: Chemistry of co-ordination compounds.
11] W. L. Jolly: Modern Inorganic Chemistry
12] R. S. Drago: Physical methods in inorganic chemistry.
13] Waddington: Nonaqueous solvents.
14] Sisler: Chemistry of non-aqueous solvents.
15] A. K. Barnard: Theoretical Inorganic Chemistry
16] Emeleus and Sharpe: Modern Aspect of Inorganic Chemistry.
17] F. A. Cotton: Chemical Applications of Group theory.
18] Jones: Elementary Co-ordination chemistry.
19] B. N. Figgis: Introduction to Ligand field.
20] S. F. A. Kettle: Co-ordination chemistry.
21] M. C. Day and J. Selbin: Theoretical Inorganic Chemistry.

22] J. Lewin and Wilkins: Modern Co-ordination chemistry.
23] Gowarikar, Vishwanathan and Sheedar: Polymer science.
24] R. L. Dutta and A. Symal: Elements of magneto chemistry
25] P. Atkins: Inorganic Chemistry 4th Edition, Oxford University Press.
26] D. M .P. Mingos: Essential Trends in Inorganic Chemistry, Oxford University Press
27] Bertini, et al: Bioinorganic Chemistry (Viva)
28] Fenton, David E.: Bio coordination chemistry, Oxford
29] Selected Topics in Inorganic Chemistry by Wahid U Malik, Tuli, Madan.
30] A Logical Approach to Modern Inorganic Chemistry by Jagdamba Singh
31] Essentials of Bio Inorganic Chemistry by Monal Singh Neerja Gupta
32] Concise Coordination Chemistry by R. Gopalan , V. Ramalingam
33] Advanced inorganic chemistry Volume I by Madan malik Tuli Prakash S.Chand publication
34] Advanced inorganic chemistry Volume II Madan malik Tuli Prakash S.Chand publication

Semester I
Paper II [Code: PG- CHE (02)- S1-T2]
Organic Chemistry

60 h (4 h per week) :15 h per unit [L-T-P = 4-0-0] 80 Marks

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: : 15 h

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

B. Bonding other than covalent bonding: Hydrogen bonding, inclusion compounds, rotaxanes, catenanes, cyclodextrins, cryptands, crown ethers, Phase transfer catalyst, fullerenes.

C. Aromaticity: Benzenoid and non-benzenoid compounds, Huckel's rule, antiaromaticity, homoaromaticity, annulenes, azulenes, cyclopentadienyl anion, tropylium cation, tropone and tropolone.

D. Reactive intermediates: Generation, structure, stability and chemical reactions of carbocations, carbanions, free radicals, carbenes, nitrenes and benzyne / arynes.

Unit-II: 15 h

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: 15 h

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 SN^1, SN^2, mixed SN^1, SN^2, SET and SN^i 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: **15h**

A. Aromatic Nucleophilic Substitution

A general introduction to different mechanisms of aromatic nucleophilic substitution SNAr, SN^1, benzyne and SRN^1 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

1) Advanced Organic Chemistry –Reaction mechanism and structure. Jerry March, John Wiley
2) Advanced Organic Chemistry- 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) Stereochemistry of Organic Compounds- D. Nasipuri, New Age International
10) Stereochemistry of Organic Compounds- P. S. Kalsi, New Age International
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) Stereochemistry of Carbon Compounds- E. L. Eliel
15) Physical Organic Chemistry-J. Hine
16) Name Reaction in Organic chemistry –Surrey
17) Advanced Organic Chemistry – L. F. Fieser and M. Fieser.

18) Organic Chemistry Vol. I and II - I. L. Finar
19) Modern Organic Chemistry- J.D. Roberts and M. C. Caserio
20) The Search for Organic Reaction Pathways (Longmann), Peter Skyes
21) Organic Chemistry 5th Edition (McGraw Hill), S. H. Pine
22) Organic Chemistry (Willard Grant Press Botcon), John Mcmurry
23) A Textbook of Organic Chemistry- R. K. Bansal New Age International
24) New Trends in Green Chemistry –V. K. Ahluwalia and M. Kidwai, Anamaya publishers New Delhi
25) Organic Chemistry, J. Clayden, N. Greeves, S. Warren and P. Wothers, Oxford University Press
26) Organic Chemistry, 4th Edition, G Marc Loudon, Oxford University Press
27) Advanced Organic Chemistry by J. Singh
28) Organic Chemistry by V. K. Ahluwalia
29) A Logical Approach to Modern Organic Chemistry by Jagdamba Singh

Semester I
Paper III [Code: PG- CHE (02) - S1-T3]
Physical Chemistry

60 h (4 h per week) :15 h per unit [L-T-P = 4-0-0] 80 Marks

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 various terms, equations and their derivations important for understanding of systems with variable compositions.
3. To extend the study of Gibbs phase rule to more advanced one, two and three component systems
4. To understand the concept and methods of determination of molecular mass of macromolecules.
5. To learn advanced concepts and theories of chemical kinetics.

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. Understand various concepts related to systems with variable compositions such as chemical potential, fugacity etc.
3. Realize application of phase rule to study of some important one, two and three component systems.
4. Understand the concept of number and mass average molecular mass of macromolecules and their methods of determination.
5. Learn modern concepts and theories of reaction dynamics.

Contents:-

Unit-I

Classical Thermodynamics: 15h

A. Recapitulation of Laws of thermodynamics, Exact and inexact differentials, condition of exactness, Pfaff differential expression and equations, Applications of Pfaff 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

Systems of Variable Compositions: 15h

A. Importance of Partial Molar Properties, Chemical Potential, Gibbs Duhem Equation, Relationship of Chemical Potential with U, H and A; Effect of Temperature on Chemical Potential and Effect of Pressure on Chemical Potential, Chemical Potential of Pure Ideal Gas, Chemical Potential in an Ideal Gas Mixture, Thermodynamics of a Mixture of Ideal Gases (enthalpy and entropy).

B. Chemical Potential of Real Gases and Fugacity, Raoult's Law and Ideal Solution, Thermodynamics of Binary Solution with i) One Volatile Component ii) Two Volatile

Components, Chemical Potential in Non-ideal Solution, Excess function of Non-ideal Solution, Activity Coefficients of Nonelectrolytes, Debye-Huckel Theory, Limited and Extended Law (Derivation Expected).

Unit-III

Phase Equilibrium and Macromolecules: **15h**

A. Phase Equilibrium: Gibbs Phase rule and its derivation, calculation of degrees of freedom, reduced phase rule, one component systems (Helium, carbon), 1^{st} and 2^{nd} order phase transition, lambda line, two component systems forming solid solutions having congruent and incongruent melting point, partially miscible solid phase, three component systems, graphical presentation, influence of temperature, systems with 1, 2, 3 pairs of partially miscible liquids, transition points.

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

Unit-IV

Chemical Kinetics: **15h**

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, 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)

Reference books:

1] R. P. Rastogi and R. R. Mishra, An Introduction to Chemical Thermodynamics, Vikas Publication, Gorakhpur, 2010.
2] P. W. Atkins and D. Paula, Physical Chemistry, 8th Edition, Oxford University Press, 2010.
3] E. N. Yenemin, Fundamentals of Chemical Thermodynamics, MIR, Publications.
4] G. K. Vemulapalli, Physical Chemistry, Prentice – Hall of India, 1997.
5] S. Glasstone and De Van No Strand, Thermodynamics for Chemists, 1965.
6] S. M. Blinder, Advanced Physical Chemistry,
7] D. Mcquarie and J. Simon, Physical Chemistry – A Molecular Approach, University Press, 2000.
8] G. M. Barrow, Physical Chemistry, Tata Mc-Graw Hill, V edition 2003.
9] H. K. Moudgil, Text Book of Physical Chemistry, Pretice Hall of India, New Delhi, 2010.
10] G.M.Panchenkov and V.P.Labadev, “Chemical Kinetics and catalysis”, MIR Publishing.
11] E.A. Moelwyn- Hughes, “Chemical Kinetics and Kinetics of Solutions”, Academic.
12] K. J. Laidler, Chemical Kinetics, Third Edition (1987), Harper and Row, New York.
13] J. Raja Ram and J. C. Kuriacose, Kinetics and Mechanism of Chemical Transformations MacMilllan Indian Ltd., New Delhi (1993).
14] C. H. Bamford and C. F. H. Tipper, Comprehensive Chemical Kinetics, Vol 1., Elsevier Publications, New York, 1969.
15] C. H. Bamford and C. F. H. Tipper, Comprehensive Chemical Kinetics, Vol 2., Elsevier Publications, New York, 1969.
16] S. Glasstone, K. J. Laidler and H. Eyring, The Theory of Rate Processes, Mc-Graw Hill, New York, 1941.
17] A. Findley, The Phase Rule and its Applications, Longmans Green and Co., Mumbai.
18] Santosh Kumar Upadhyay, Chemical Kinetics and Reaction Dynamics, Springer 2006.
19] G. K. Agrawal, Basic Chemical Kinetics, Tata-Mc-Graw Hill, 1990.

20] N. B. Singh, N. S. Gajbhiye, S. S. Das, Comprehensive Physical Chemistry, New Age International, 2014.
21] K. L. Kapoor, Text Book of Physical Chemistry, Vol – I to Vol-VI, 2011.

e-References:-

e-PGPathshala (inflibnet.ac.in)

Semester I
Paper IV [Code: PG- CHE (02)- S1-T4]
Analytical Chemistry

60 h (4 h per week) :15 h per unit [L-T-P = 4-0-0] 80 Marks

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 Statistical analysis and validation
2. Understanding Separation Techniques, Chromatography, Ion exchange and Solvent extraction
3. Gaining knowledge of classical methods of analysis
4. Knowing Optical Methods of Analysis Spectrophotometry - Colorimetry and Flame photometry

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. Evaluate the analytical data in terms of statistics.
5. Understanding fundamentals of Separation techniques like Chromatography & solvent extraction.
6. 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.
7. Explain the theoretical principles of selected instrumental methods colorimetry & Spectrophotometry.

Contents:-

Unit-I

Introduction and Statistical Analysis: 15h

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

B. Statistical analysis and validation: 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. Significant figures and rules to determine significant figures. Calculations involving significant figures. 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. Application of Microsoft Excel in statistical analysis (statistical functions and spreadsheets in MS-Excel). Validation of newly developed analytical method. Certified reference materials (CRMs). Numerical problems.

Unit-II

Separation Techniques: 15h

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), Super Critical extraction, Applications.

Unit-III

Classical Methods of Analysis: **15h**

A. Volumetric analysis: General principle. Criteria for reactions used in titrations. Primary standards and secondary standards. Theory of indicators. Internal and external 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. Estimation of Calcium; Barium. Numerical problems.

C. Stoichiometry: Stoichiometric and sub-stoichiometric reactions and calculations.

Unit-IV

Optical Methods of Analysis-I: **15h**

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 λ_{max}. 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.

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

<u>Reference books</u>:

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

Semester I
Practical-I [Code: PG- CHE (02)- S1-P1]
Inorganic Chemistry

12 h per week [L-T-P = 0-0-8] 100 Marks

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 be also able to perform qualitative and quantitative analysis of different compounds and mixtures.
3. Appreciate the procedure for inorganic analysis.

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)

<u>Reference books</u>:

1] Synthesis and Characterization of Inorganic Compounds, W. L. Jolly, Prentice Hall.

2] Inorganic Experiments, J. Derck Woollins, VCH.

3] Practical Inorganic Chemistry, G. Marrand, B. W. Rockett, Van Nostrand.
4] A Text Book of Quantitative Inorganic Analysis, A. I. Vogel, IIIrd Edition
5] EDTA Titrations. F. Laschka
6] Instrumental Methods of Analysis, Willard, Merit and Dean (CBS, Delhi).
7] Inorganic Synthesis, Jolly
8] Instrumental Methods of Chemical Analysis, Yelri Lalikov
9] Fundamental of Analytical Chemistry, Skoog D.A. &West D.M Holt Rinehart &Winston Inc.
10] Experimental Inorganic Chemistry, W.G. Palmer, Cambridge.
11] Quantitative Analysis: Day and Underwood
12] Physical Methods In Inorganic Chemistry: R. S. Drago
13] General and Inorganic Chemistry: N. Akjmetov

Semester I

Practical -II [Code: PG- CHE (02)- S1-P2]

Physical Chemistry

12 h per week [L-T-P = 0-0-8] 100 Marks

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:

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

Shiksha Mandal's

Bajaj College of Science, Wardha

Department of Chemistry

Revised Syllabus of M. Sc. Chemistry
Semester II
for Academic Autonomy

(Approved in BOS Meeting 8-September-2021)

Bajaj College of Science, Wardha (Autonomous College)

SUBJECT: CHEMISTRY

Syllabus of M.Sc. I Semester II

Paper V [Code: PG- CHE (02)-S2-T1]

Inorganic Chemistry

60 h (4 h per week): 15 h per unit [L-T-P = 4-0-0] 80 Marks

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

A. Metal – Ligand Equilibria in Solution: 15h

Stepwise and overall formation constants; trends in stepwise formation constants; factors affecting stability of metal complexes with reference to nature of metal ion, ligand, chelate effect and thermodyanamic origin. Determination of formation constant by: (1) spectrophotometric method (Job's and Mole ratio method) (2) Potentiometric method (Irving - Rossotti Method)

B. 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, various types of acid hydrolysis, factors affecting acid hydrolysis, stereochemistry of intermediates in SN^1 and SN^2, Base hydrolysis, Conjugate base (SN^1CB) mechanism, Essential requirements for SN^1CB mechanism, Direct and indirect evidences in favor of conjugate mechanism, anation reaction, reaction without metal ligand bond breaking.

Unit-II

Reaction mechanism of transition metal complexes –II: **15h**

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 (Electrostatic polarization theory; pi bonding theory), 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: **15h**

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, 18 electron rule, synthesis and structures.

B. Metal nitrosyls

Nitrosylating agents for synthesis of metal nitrosyls, EAN rule. 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. Application of Dinitrogen and dioxygen complexes. Application of Wilkinson’s catalyst and Vaska’s compound.

Unit-IV: Cluster II **15h**

Metal-Metal Bond:

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:

1] S. F. A. Kettle, J. N. Murral & S. T. Teddler: Valency Theory
2] C. A. Coulson: Valency
3] J. E. Huheey: Inorganic Chemistry
4] F .A. Cotton & G. Wilkinson: Advanced Inorganic Chemistry 3rd , 5th & 6th Editions.
5] A. F. Willims: Theoretical Approach in inorganic chemistry.
6] A. Mannas Chanda: Atomic Structure and chemical Bonding
7] L. E. Orgel: An introduction to transition metal chemistry, Ligand field theory, 2nd Edition.
8] J. J. Logowski: Modern Inorganic Chemistry
9] B. Durrant and P. J. Durrant: Advanced Inorganic Chemistry
10] J. C. Bailar: Chemistry of co-ordination compounds.
11] W. L. Jolly: Modern Inorganic Chemistry
12] R. S. Drago: Physical methods in inorganic chemistry.
13] Waddington: Nonaqueous solvents.
14] Sisler: Chemistry of non-aqueous solvents.
15] A. K. Barnard: Theoretical Inorganic Chemistry
16] Emeleus and Sharpe: Modern Aspect of Inorganic Chemistry.
17] F. A. Cotton: Chemical Applications of Group theory.
18] Jones: Elementary Co-ordination chemistry.
19] B. N. Figgis: Introduction to Ligand field.
20] S. F. A. Kettle: Co-ordination chemistry.
21] M. C. Day and J. Selbin: Theoretical Inorganic Chemistry.
22] J. Lewin and Wilkins: Modern Co-ordination chemistry.
23] Gowarikar, Vishwanathan and Sheedar: Polymer science.
24] R. L. Dutta and A. Symal: Elements of magneto chemistry
25] P. Atkins: Inorganic Chemistry 4th Edition, Oxford University Press.
26] D. M .P. Mingos: Essential Trends in Inorganic Chemistry, Oxford University Press
27] Bertini, et al: Bioinorganic Chemistry (Viva)

28] Fenton, David E.: Bio coordination chemistry, Oxford
29] Selected Topics in Inorganic Chemistry by Wahid U Malik, Tuli, Madan.
30] A Logical Approach to Modern Inorganic Chemistry by Jagdamba Singh
31] Essentials of Bio Inorganic Chemistry by Monal Singh, Neerja Gupta
32] Concise Coordination Chemistry by R. Gopalan , V. Ramalingam
33] Advanced inorganic chemistry Volume I by Madan, Malik, Tuli Prakash S. Chand publication
34] Advanced inorganic chemistry Volume II Madan, Malik, Tuli Prakash S. Chand publication

Semester II
Paper VI [Code: PG- CHE (02)- S2-T2]
Organic Chemistry

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

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: **15h**

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: **15h**

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: **15h**

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: **15h**

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

Semester II
Paper VII [Code: PG- CHE (02) - S2-T3]
Physical Chemistry

60 h (4 h per week): 15 h per unit [L-T-P = 4-0-0] **80 Marks**

Course Objectives

1. To recapitulate fundamentals of quantum chemistry and extending the study to derivations of wave functions for particle in three dimensional box and hybrid orbitals.
2. To study various electrochemical processes, thermodynamic quantities, potentials and different types of fuel cells.
3. To revise the fundamentals of solid state and understand the nature as well thermodynamics of crystal defects and nonstoichiometry.
4. To get introduced to fundamentals of Statistical Thermodynamics.
5. To study important adsorption isotherms as well as important aspects of micelles.

Course Outcomes

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

1. Derive the wave functions for particle in three dimensional box and hybrid orbitals: understand the concept of degeneracy and solve related numericals.
2. Understand faradic-nonfaradic processes, thermodynamics of cell, electrochemical potentials and some important fuel cells.
3. Learn the basics of solid state chemistry and gain some understanding of crystal defects and nonstoichiometry.
4. Know the important concepts of statistical thermodynamics with preliminary idea of Maxwell Boltzmann, Bose Einestein, Fermi Dirac statistics.
5. Derive important adsorption isotherms as well as realize some important aspects of micelles.

Contents:-

Unit-I

Quantum Chemistry: **15h**

Recapitulation, Postulates of Quantum Mechanics, Operator algebra, Commutator of operators and Numericals. Eigen values, Eigen functions and Numericals. Normalized, orthogonal wave functions and Numericals. Particle in three dimensional box, degeneracy of energy levels, Quantum mechanical principles of Hybridization, Construction of wave functions for sp, sp^2 and sp^3 hybrid orbitals. Treatment of linear harmonic oscillator and rigid rotor. Approximate methods. Solving Electronic Schrödinger equation for Hydrogen atom

Unit-II

Electrochemistry **15h**

Introduction and over view of Electrochemical Processes, Electrochemical Cell and Reactions, Faradic and Nonfaradiac Processes, Basic Electrochemical Thermodynamics, Free Energy and cell EMF, Half Reaction and Reduction Potentials, Formal Potentials, Reference Electrodes, Measurements of Potential Differences, Electrochemical Potentials, Fermi Level and Absolute Potentials, Liquid Junction Potential. Electrochemical devices: Alkaline fuel cells, Phosphoric acid fuel cells, High temperature fuel cells.

Unit-III

Solid State Chemistry: **15h**

A. Introduction: Introduction to crystals, Unit Cell and lattice parameters, Symmetry elements in crystals, Absence of fivefold axis, Space groups, The Bravais Lattices, Miller Indices, Bragg's Equation, seven crystal system, Packing in crystals, Hexagonal Closest Packing (HCP) Cubic Closest Packing (CCP), Voids, packing fraction, Numericals.

B. Crystal Defects and Non-stiochiometry: Perfect and imperfect crystals, point defects, line and plane defects. Thermodynamics of Schottky and Frenkel defect formation, colour centers, non-stiochiometry and defects. Numericals.

Unit-IV

Statistical Thermodynamics and Surface Chemistry: **15h**

A. **Statistical thermodynamics:** Lagrange's Method of Undetermined Multipliers (Conditional Maximization), Stirling Approximation, Concept of Distribution, Thermodynamic Probability and most probable distribution, Maxwell Boltzmann, Bose Einestein, Fermi Dirac statistics, comparison between three statistics.
B. **Surface Chemistry:** Adsorption definition, Thermodynamics of adsorption, Langmuir adsorption isotherm, Langmuir constant and Gibbs energy of adsorption, Langmuir adsorption with lateral interaction, BET adsorption isotherm, adsorption on heterogeneous surface, the potential theory of Polanyi.
C. **Micelles:** Micellization, Hydrophobic Interaction, Critical Micellar Concentration (CMC), factors affecting CMC of surfactants, thermodynamics of micellzation - mass action models, micellar solubilization, Numericals.

Reference books:

1] Ira .N. Levine, Quantum Chemistry, 5th edition (2000), Pearson educ., Inc.New Delhi
2] A.K.Chandra, Introductory Quantum Chemistry, 4th edition (1994), Tata Mcgraw Hill, New Delhi.
3] M.W.Hanna, "Quantum Mechanics in Chemistry", Benjamin
4] L. Pualing and E. B. Wilson, Introduction to Quantum Mechanics with Applications to Chemistry, McGraw Hill, New York (1935).
5] R. K. Prasad, Quantum Chemistry, New Age International, Delhi.
6] R. K. Prasad, Quantum Chemistry through problems and solutions, New Age International, New Delhi, 2009.
7] B. C. Reed, Quantum Mechanics, Jones and Bartlett, New Delhi, 2010.
8] S. Glasstone, An Introduction to Electrochemistry, East-West Press Pvt. Ltd., New Delhi, 2004.
9] H. K. Moudgil, Text Book of Physical Chemistry, Pretice Hall of India, New Delhi, 2010.
10] S. O. Pillai, Solid State Physics, New Age International, New Delhi, 2102.
11] N. B. Hanny, Treaties in Solid State Chemistry,
12] M. C. Day and J Selbin, Theoretical Inorganic Chemistry, Reinhold Pub. Corp., New York,
13] M. C. Gupta, Statistical Thermodynamics, New Age International.
14] K. Huang, Statistical Mechanics, Wiley, New Delhi, 2003.
15] Andrew Maczek, *Statistical Thermodynamics*, Oxford University Press Inc., New York (1998).
16] C.Kittel, "Introduction to solid state Physics",Wiley
17] L.V.Azaroff, "Introduction to solids", McGraw Hill
18] L. E. Smart and E. A. Moore, Solid State Chemistry-An Introduction, CRC Tylor and Fransis, 2005.
19] C. N. R. Rao and Gopalakrishnan, "New Directions in Solid State Chemistry" Second Edition, Cambridge University Press.
20] Anthony R. West, "Solid State Chemistry and its Applications" Wiley India Edition

21] D. K. Chakravorty, Solid State, New Age International.
22] Modern Electrochemistry, Volume 1 and 2, J.O.M Bokris and A.K.N, Reddy Plenum Press N.Y. (1970)
23] Electrochemical Methods second edition, A.J. Bard and L.R. Faulkner, John Wiley and Son (2001).
24. Physics and Chemistry of Interface, second edition, Hans-Jurgen Butt, Karlheunz Graf, Micael Kappl, Willey VCH (2006), ISBN-13 978-3-527-40629-6
25] Physical Chemistry of Surface, A.W. Admson, fifth edition, Wiley Interscience Publiation (1990)
26] Surfactant Science and Technology, second edition, Drew Myers, VCH Publishers (1992)
27] Principles of Colloids and Surface Chemistry, P.C. Hiemenz Marcel and Dekker, N.Y. (1977)

e-References:-

e-PGPathshala (inflibnet.ac.in)

Semester II
Paper VIII [Code: PG- CHE (02)- S2-T4]
Analytical Chemistry

60 h (4 h per week): 15 h per unit [L-T-P = 4-0-0] **80 Marks**

Course Objectives

The aim of this course is to provide students with a broad understanding of the principles and applications of analytical chemistry.

1. Students are first provided with an introduction into sample collection and preparation.

This course will cover advanced separation techniques:

2. Gas chromatography, HPLC & Super critical fluid Chromatography.

Finally, students will also be introduced to basic and commonly used instrumental methods of chemical analysis:

3. atomic absorption spectroscopy
4. some electroanalytical methods.

Course Outcomes

After the successful completion of this course, students will -

1. Be able to plan for sampling and understand how different sampling methods can be used in speciation studies.
2. Be familiar with Stoichiometric and sub-stoichiometric reactions and calculations.
3. Understand the theoretical principles of modern separation techniques Gas chromatography & HPLC.
4. Get introduced to new separation method Supercritical fluid chromatography.
5. Get knowledge of the theoretical principles of modern analytical techniques AAS.
6. Realize the theoretical principles of electroanalytical techniques Polarography & Ampereometry.

Unit-I

Sampling and Quantification: **15h**

A. Sampling and sample treatment: Criteria for representative sample. Techniques of sampling of gases (ambient air and exhaust gases), liquids (water and milk samples), solids (soil and coal samples) and particulates. Hazards in sampling. Safety aspects in handling hazardous chemicals. Sample dissolution methods for elemental analysis: Dry and wet ashing, acid digestion, fusion processes and dissolution of organic samples.

B. Detection and quantification: Concepts and difference between sensitivity, limit of detection and limit of quantification, role of noise in determination of detection limit of analytical techniques. Units in chemical analysis and their interconversion.

Unit-II

Modern separation techniques: **15h**

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

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

C. Supercritical fluid chromatography: Introduction and applications.

Unit-III

Optical methods of analysis-II: 15h

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

B. **Inductively coupled plasma-atomic emission spectroscopy:** Principle, atomization and excitation. Plasma source and sample introduction. Instrumentation. Comparison of Flame photometry with ICP-AES & AAS. Applications.

Unit-IV

Electrochemical methods of analysis-II: 15h

A. Polarography: Principle of DC polarography. Instrumentation in polarography. Advantages and limitations of DME. Types of currents- residual current, migration current, diffusion current, limiting current, adsorption current, kinetic current and catalytic current. Ilkovic equation-diffusion current constant and capillary characteristics. Derivation of equation of polarographic wave and half wave potential. Experimental determination of half wave potential. Reversible, quasi reversible and irreversible electrode reactions. Polarographic maxima and maximum suppressor. Oxygen interference and deaeration. Introduction to pulse, a.c. and oscillographic techniques and their advantages. Applications of polarography in determination of dissolved oxygen, metal ion quantification and speciation, simultaneous determination of metal ions, analysis of organic compounds. Limitations of polarography.

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

<u>Reference books</u>:

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] Sample Pre-treatment and Separation: R. Anderson (John Wiley and Sons)
6] Stoichiometry: B. I. Bhatt and S.M. Vora, 2nd Edition (Tata Mc-Graw Hill publication)
7] Instrumental Methods of Chemical Analysis: Braun (Tata McGraw-Hill)
8] Advanced Analytical Chemistry: Meites and Thomas (McGraw-Hill)
9] Instrumental Methods of Analysis: G. Chatwal and S. Anand (Himalaya Publishing House)
10] Analytical Chemistry: Problems and Solution, S. M. Khopkar (New Age International Publication)
11] Basic Concepts in Analytical Chemistry: S. M. Khopkar (New Age International Publication)
12] Advance Analytical Chemistry: Meites and Thomas: (Mc Graw Hill)
13] An Introduction to Separation Science: L. R. Shyder and C. H. Harvath (Wiley Interscience)
14] Fundamental of Analytical Chemistry: S. A. Skoog and D. W. West
15] Instrumental Methods of Chemical Analysis: G. W. Ewing
16] Polarography: Koltoff and Ligane
17] Electroanalytical Chemistry: Sane and Joshi (Quest Publications)

Semester II
Practical-III [Code: PG- CHE (02)- S2-P1]
Organic Chemistry

12 h per week [L-T-P = 0-0-8] 100 Marks

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:-

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

Semester II
Practical-IV [Code: PG- CHE (02)- S2-P2]
Analytical Chemistry

12 h per week [L-T-P = 0-0-8] 100 Marks

Course Objectives

Analytical measurements are aimed at obtaining qualitative and quantitative information about the composition and structure of various materials that have relevance to both fundamental understanding as well as applications towards improving the quality of life. Here students develop an understanding of the broad role of the chemist in measurement and problem solving for analytical tasks. Also experience some scientific methods employed in analytical chemistry.

Course Outcomes

1. Performing classical analytical experiments, and make observations and assessments of important factors that could affect the analytical result.
2. Use of digital tools MS-Excel to present chemical analytical work.
3. Understanding of methods for calibration and sampling applied to quantitative analysis.
4. Understanding the application of analytical methods based on titrations, separations, electrochemical measurements, and spectroscopy at an introductory level.

Contents:-

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:-

- Svehla, G. *Vogel's Qualitative Inorganic Analysis*, Pearson Education, 2012.
- Mendham, J. *Vogel's Quantitative Chemical Analysis*, Pearson, 2009.
- Willard, H. H., *Instrumental methods of analysis*, Wiley, 1988
- Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011)
- Das R. C., Behra B., Experimental Physical Chemistry, Tata McGraw Hill.
- Yadav J. B., Advanced Practical Physical Chemistry, Goel Publishing House.
- Alexander Findlay, Levitt B. P., Findlay's Practical Physical Chemistry, Longman, London
- http://nsdl.niscair.res.in
- http://ocw.mit.edu

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- Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011)
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INCHARGE
Department of Chemistry
Bajaj College of Science
WARDHA

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

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

Course Code: PG–CHEM(02)-S3-T1-SP1

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

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

Unit-I

Photochemistry: 15L

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

Unit-II

Pericyclic Reactions: 15L

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

Unit-III

Oxidation and Reduction: 15L

a) Oxidation:

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

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

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

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

b) Reduction:

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

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

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

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

Unit-IV

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

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

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

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

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

<u>Reference books</u>:

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

Course Code: PG–CHEM(02)-S3-T2-SP2

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

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

Unit-I

Terpenoids and Porphyrins: 15L

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

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

Unit-II

Alkaloids and Prostaglandins: 15L

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

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

Unit-III

Steroids and Plant Pigments: 15L

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

Biosynthesis of steroids (lanosterol)

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

Biosynthesis of flavonoids: Acetate pathway and Shikimic acid pathway

Unit-IV

Carbohydrates, amino acids, proteins and peptides: 15L

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

Chemistry of starch and cellulose.

B] Amino acids, protein and peptides: Amino acids, structural characteristics, acid-base property, stereochemistry of amino acids, optical resolution, Strecker synthesis, peptide and proteins structure of peptide and protein, primary, secondary, tertiary and quaternary structure. Reaction of polypeptide, structure determination of polypeptide, Solid phase peptide synthesis, end group analysis.

Reference books:

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

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

8 h per week **100 Marks**

[A] Quantitative Analysis

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

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

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

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

[C] QUALITATIVE ANALYSIS

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

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

Course Code: PG –CHEM(02)-S3-T3-EL1

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

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

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

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

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

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

Unit-II: Water **15 h**

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

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

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

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

Unit IV: Air **15 h**

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

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

Course Code: PG –CHEM(02)-S3-P2

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

8h per week **Marks-100**

WATER ANALYSIS

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

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

AIR ANALYSIS

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

SOIL ANALYSIS

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

Reference books:

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

Course Code: PG –CHEM(02)-S3-T3-EL1

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

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

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

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

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

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

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

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

Unit IV: Commercial polymers **15h**

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

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

Course Code: PG –CHEM(02)-S3-P2

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

8h per week **Marks-100**

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

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

Reference books:

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

Course Code: PG–CHEM(02)-S3-T3-EL1

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

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

UNIT-I: **15 h**

Drug Design

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

UNIT-II: **15 h**

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

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

B] Diuretics: Introduction, mode of action, loop diuretics. Synthesis of Bumetanide, Frusemide, Ethacrynic acid, clorexolone Quinethazone.

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

UNIT-III: **15 h**

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

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

UNIT-IV: **15 h**

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

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

Course Code: PG –CHEM(02)-S3-P2

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

8 h per week **Marks-100**

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

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

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

<u>Reference books</u>:

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

Course Code: PG –CHEM(02)-S3-T4

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

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

Unit-I

Symmetry properties of molecules and group theory: 15L

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

Unit-II

Microwave and Mössbauer Spectroscopy: 15L

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

B] Mössbauer spectroscopy:

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

Unit-III

Infrared and Raman Spectroscopy: 15L

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

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

Unit-IV

Diffraction techniques: 15L

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

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

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

Reference books:

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

OR

Course Code: PG –CHEM(02)-S3-T4

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

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

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

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

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

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

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

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

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

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

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

Industrial applications of alloys.

Reference books:

1] Quantitative analysis: Day and Underwood (Prentice-Hall of India)

2] Vogel's Text Book of Quantitative Inorganic Analysis-Bassett, Denney, Jeffery and Mendham (ELBS)

3] Analytical Chemistry: Gary D. Christian (Wiley, India).

4] Instrumental Methods of Analysis: Willard, Merrit, Dean, Settle (CBS Publishers, Delhi, 1986)

5] Instrumental Methods of Chemical Analysis: Braun (Tata McGraw-Hill)

6] Advanced Analytical Chemistry: Meites and Thomas (McGraw-Hill)

7] Instrumental Methods of Analysis: G. Chatwal and S. Anand (Himalaya Publishing House)

8] Analytical Chemistry: Problems and Solution- S. M. Khopkar (New Age International Publication)

9] Basic Concepts in Analytical Chemistry: S. M. Khopkar (New Age International Publication)

10] Advance Analytical Chemistry: Meites and Thomas: (Mc Graw Hill)

11] An Introduction to Separation Science: L. R. Shyder and C. H. Harvath (Wiley Interscience)

12] Fundamentals of Analytical Chemistry: S. A. Skoog and D. W. West

13] Instrumental Methods of Chemical Analysis: G. W. Ewing

Bajaj College of Science, Wardha (Autonomous College)

SUBJECT: CHEMISTRY

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

Course Code: PG–CHEM(02)-S4-T1-SP1

Paper–XIII : 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 annulation, Methods of ring synthesis, Linear and convergent synthesis.

Reference books:

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

Course Code: PG–CHEM(02)-S4-T2-SP2

Paper–XIV: 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 methods of application dying mechanism, methods of dying, such as direct dying, vat dying, dispersive dying, formation of dye in fibre, dying with reactive dyes, study of quinoline yellow, cyamine dye, ethyl red, methylene blue, Alizarin, cyamine-green, fluorescein, cosin, erythrosine, Rhodomines and Indigo.

B] Pharmaceutical chemistry:

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

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

Reference books:

1] Textbook of Polymer Science, F. W. Billmeyer Jr, Wiley
2] Polymer Science, V. R. Gowarikar, N. V. Viswanathan and J. Sreedhar, Wiley-Eastern
3] Functional Monomers and Polymers, K. Takemoto, Y. Inaki and R. M. Ottanbrite
4] Bioorganic Chemistry: A Chemical Approach to Enzyme Action, Hermann Dugas and C. Penny, Springer-Verlag
5] Understanding Enzymes, Trevor Palmer, Prentice Hall
6] Enzyme Chemistry: Impact and Applications, Ed. Collin J. Suckling, Chapman and Hall
7] Enzyme Structure and Mechanism, A. Fersht, W. H. Freeman
8] Introduction to Medicinal Chemistry, A. Gringuage, Wiley-VCH
9] Wilson and Gisvold's Text Book of Organic Medical and Pharmaceutical Chemistry, 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

Course Code: PG –CHEM(02)-S4-P1
Practical –VII: Special Organic Chemistry Practical II [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).

<u>Course Code:</u> PG –CHEM(02)-S4-T3-EL2

Paper–XV: Elective II - Environmental Chemistry II [L-T-P = 4-0-0]

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

Unit-I: **15 h**

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

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

Sources, types and consequences, classification of wastes- domestic, industrial, municipal, hospital, nuclear and agricultural. Impact of solid waste on environment, human and plant health; effect of solid waste and industrial effluent discharge on water quality and aquatic life.
Solid waste Management: Different techniques used in collection, storage, transportation and disposal of solid waste (domestic, industrial and agricultural).

Unit-III: **15 h**

Waste water treatment & management: Wastewater Treatment: Primary, Secondary and Advanced treatment methods. Common effluent treatment plant. Drinking water treatment, Coagulation and flocculation, Sedimentation and Filtration, Disinfection and Softening. 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-IV: **15 h**

Soil analysis: Physical properties – texture, bulk density, permeability chemical properties—Ion exchange capacity, soil pH and micro and macro nutrient availability.
Analysis of constituents such as nitrogen, phosphorous, potassium and microconstituents (Zn and Cu)

Air pollution analysis— Sampling of aerosols and gaseous pollutants and their effects, SO_2, NO_2, CO, CO_2, particulates-SPM, RSPM, High Volume Sampler, Fabric Filters, Cyclones (direct and Reverse), ESP, ozone layer.

<u>Reference books</u>:

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

<u>Course Code:</u> PG –CHEM(02)-S4-T3-EL2

Paper–XV: Elective II - 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.

<u>Reference books</u>:

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

Course Code: PG –CHEM(02)-S4-T3-EL2

Paper–XV: Elective II - 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

Course Code: PG –CHEM(02)-S4-T4

Paper–XVI: 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:

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

B] Mass spectrometry:

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

Unit III: **15 h**

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 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)

<u>Reference books</u>:

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

Course Code: PG –CHEM(02)-S4-T4

Paper–XVI: **(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

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