DEPARTMENT OF CHEMISTRY

COURSE STRUCTURE

for

M.Sc. (Chemistry)
Four Semesters (Two Year)

Programme

Based on

Choice Based Credit System (CBCS)
(As per Ordinanc-14)

I & II Semester 2020-21
III & IV Semester 2021-22

AWADHESH PRATAP SINGH UNIVERSITY, REWA (M.P.)

Semester Course of M.Sc. Chemistry

Programme	**:**	**M.Sc. Chemistry**
Programme Code	**:**	**13**
Duration	**:**	**4 Semester (Two Year)**

Chemistry Program Goals

1. To provide specific knowledge in chemistry that stresses scientific reasoning and analytical problem solving with a molecular perspective.
2. To provide students with the skills required to succeed, the chemical industry research and professional.
3. To expose the students to a breadth of experimental techniques using modern instrumentation.

Learning Objectives

1. Student will learn the broad knowledge of different field of chemistry.
2. The student will understand the advance knowledge of spectroscopy, thermodynamic principles, nature of chemical reactions and energy related problems.
3. The student will understand the interdisciplinary nature of chemistry and to integrate knowledge of mathematics, physics and other disciplines to a wide variety of chemical problems for industries and quality control.
4. The student will learn the laboratory skills needed to design, safely conduct and interpret chemical research.
5. The student will acquire a foundation of chemistry of sufficient breadth and depth to enable them to understand and critically interpret the advance chemical literature.
6. The student will develop the ability to effectively communicate scientific information and research results in written and oral formats.
7. The student will learn professionalism, including the ability to work in teams and apply basic ethical principles in life and profession. He/She will understand how to interpret the results and apply them in solving the problems.

PROGRAM OUTCOME (PO)

The following outcome reflects the terminal skills that all Master Post Graduates should be able to demonstrate program completion.

PO1: The chemistry course is designed to give core knowledge with the skills to critically assess and solve problems, related to chemical science.

PO2: The different papers sub-discipline such as organic, inorganic, physical and analytical chemistry give detail knowledge and applications in respective specialization.

PO3: The Masters students will have working knowledge of chemical instrumentation and laboratory techniques.

PO4: The training will the help students to design and conduct independent work in industry or academia.

PROGRAM SPECIFIC OUTCOME (PSO)

PSO1

- Understanding of fundamental and advanced concepts of Quantum Chemistry and coordination chemistry.
- Knowledge of fundamentals of inorganic spectroscopy, their interpretation and their applications.
- Study of various chemical reagents and their role in inorganic synthesis and inorganic analysis.

PSO2

- Basic knowledge of Organic chemistry
- Study of various reaction intermediates and reaction pathways.
- Understanding of various organic reactions, rearrangement, cross-coupling reactions and applications.

PSO3

- Basic understanding of basic area of physical chemistry.
- Knowledge of various theories of physical chemistry such as thermodynamics, electrochemistry and properties of solutions.
- Applications of physical chemistry in various fields.

PSO4

- Basic understanding of analytical chemistry.
- Knowledge of volumetric methods of analysis and gravimetric analysis.
- Study of spectro-analytical techniques and their applications to various chemical systems.

Eligibility: B.Sc. with Mathematics and Biology as a subject.

Age Limit: No age limit.

Admission Procedure: The admission will be done as per merit of qualifying examinations.

Vision of the University

To be the premier institution that offers teaching and learning programmes of the best quality, graduate students who excel and become leaders in the chosen profession contributing to the community, the nation and the world, and prepares individuals of the highest moral fibre. The vision of university is:

To create an ideal society and an intellectual environment that initiates, nourishes and perpetuates values of co-existence and to fulfill and achieve excellence. The university, under the dynamic leadership of our honourable Vice-chancellor is working on quite a few ambitious plans. The idea is to develop the university as a knowledge city.

M.Sc. CHEMISTRY
(FOUR SEMESTER COURSE)

SCHEME OF EXAMINATION
(CBCS Syllabus)
(Effective from 2020-21)

SEMESTER –I

Paper	**Course No.**	**Course**	**Credit**	**Marks**
Paper I	MCH-401	Inorganic Chemistry I	**4**	**100(60+40)**
Paper II	MCH-402	Organic Chemistry I	**4**	**100(60+40)**
Paper III	MCH-403	Physical Chemistry I	**4**	**100(60+40)**
Generic Elective				
Paper IV	MCH-404	(a) Mathematics for Chemists[1] (b) Biology for Chemists[2]	**4**	**100(60+40)**
Practical	Inorganic + Organic + Physical (2+2+2)		**6**	**50+50+50**
		Comprehensive viva voce	**4***	**100**
Total Marks			**26**	**650**

*Virtual Credit
[1] Strictly for the students without Mathematics in B.Sc.
[2] Strictly for the students without Biology in B.Sc.

SEMESTER –II

Paper	**Course No.**	**Course**	**Credit**	**Marks**
Paper V	MCH-405	Inorganic Chemistry II	**4**	**100(60+40)**
Paper VI	MCH-406	Organic Chemistry II	**4**	**100(60+40)**
Paper VII	MCH-407	Physical Chemistry II	**4**	**100(60+40)**
Generic Elective				
Paper VIII	MCH-408	Spectroscopy and Diffraction Methods	**4**	**100(60+40)**
Practical	Inorganic + Organic + Physical (2+2+2)		**6**	**50+50+50**
		Comprehensive viva voce	**4***	**100**
Total Marks			**26**	**650**

*Virtual Credit

SEMESTER– III

Paper	Course No.	Course	Credit	Marks
Paper–I	MCH-501	Application of Spectroscopy	**4**	**100(60+40)**
Paper–II	MCH-502	Photochemistry	**4**	**100(60+40)**
Discipline Elective (any one)				
Paper–III	MCH-503 MCH-504 MCH-505	Analytical Chemistry Heterocyclic Chemistry Electrochemistry	**4**	**100(60+40)**
Generic Elective (any one)				
Paper–IV	MCH-506 MCH-507	Industrial Chemistry Medicinal Chemistry	**4**	**100(60+40)**
Practical		Inorganic + Organic + Physical (2+2+2)	**6**	**50+50+50**
		Comprehensive viva voce	**4***	**100**
Total Marks			**26**	**650**

*Virtual Credit

SEMESTER– IV

Paper	Course No.	Course	Credit	Marks
Paper V	MCH-508	Organotransition Metal Chemistry	**4**	**100(60+40)**
Paper VI	MCH-509	Solid State Chemistry	**4**	**100(60+40)**
Discipline Elective (any one)				
Paper VII	MCH-510 MCH-511 MCH-512	Natural Product Organic synthesis Polymer Chemistry	**4**	**100(60+40)**
Generic Elective (any one)				
Paper VIII	MCH-513 MCH-514	Environmental Chemistry Computer-Aided Drug Discovery	**4**	**100(60+40)**
Practical		Inorganic + Organic + Physical (2+2+2)	**6**	**50+50+50**
		Comprehensive viva voce	**4***	**100**
Total Marks			**26**	**650**

*Virtual Credit

Grand Total Marks M.Sc. (Ist to IVth Sem) = **2600**

SEMESTER –I
Paper-I
MCH-401: INORGANIC CHEMISTRY-I

COURSE OBJECTIVES

To make the student conversant with

- The basic concept of Molecular Symmetry and Group Theory
- Stereochemistry and bonding in main group compounds
- Metal ligand equilibrium in solution
- Reaction mechanism of transition metal complexes
- Metal ligand bonding

Unit-I

Molecular Symmetry and Group Theory

Symmetry elements and symmetry operations, definition of group, subgroup and classes in a group. Conjugacy relation and classes. Point symmetry group. Schonfilies symbols, representations of groups by matrices (representation for the C_n, C_{nv}, C_{nh}, D_{nh} group to be worked out explicity). Character of a representation. The great orthogonality theorem (without proof) and its importance. Character tables and their use. Reducible representations and their reduction spectroscopy. Derivation of character table for C_{2v} and C_{3v} point group Symmetry aspects of molecular vibrations of H_2O molecule.

Unit-II

Stereochemistry and Bonding in Main Group Compounds

VSEPR, Walsh diagram (triatomic and penta-atomic molecules), dπ-pπ bond, Bent rule and Short comings of VSEPR model, energetics of hybridization, some simple reactions of covalently bonded molecules.

Unit-III

Metal-Ligand Equilibrium in Solution

Stepwise and overall formation constants and their interaction, trends in stepwise constant, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand. Chelate effect and its thermodynamic origin, determination of binary formation constants by potentiometry and spectrophotometry.

Unit-IV

Reaction Mechanism of Transition Metal Complexes

Energy profile of a reaction, reactivity of metal complex, inert and labile complexes, kinetic application of valence bond and crystal field theories, kinetics of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidences in favour of conjugate mechanism, anion reactions, reactions without metal ligand bond cleavage. Substitution reactions in square planar complexes, the trans effect, mechanism of the substitution reaction. Redox reaction, electron transfer reactions, mechanism of one electron transfer reactions, outer sphere type reactions, cross reactions and Marcus-Hush theory, inner sphere type reactions.

Unit-V

Metal-Ligand bonding

Limitation of crystal field theory, molecular orbital theory for bonding in octahedral, tetrahedral and square planar complexes, π-bonding and molecular orbital theory. John-Teller effect, Electronic spectra and transition metal complexes, spectroscopic term and microstates for the p^2 and d^2 configurations.

Books Suggested

1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
2. Inorganic Chemistry, J.E. Huhey, Harpes & Row.
3. Chemistry of the Elements. N.N. Greenwood and A. Earnshow, Pergamon.
4. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
5. Magnetiochemistry, R.L. Carlin, Springer Verlag.
6. Comprehensive Coordiantion Chemistry eds., G. Wilkinson, R.D. Gillars and J.A. Mc Cleverty,Pergamon.

7. J.E. House, Inorganic Chemistry, Elsevier, 2008.
8. D.K. Sriver, P.W. Alkins and C.H. Langford, Inorganic Chemistry, Oxford University, Pra 51, Oxford, 1994.

COURSE OUTCOMES

The students will be able to

- know the Symmetry elements and symmetry operations covers a wide area of research in theoretical chemistry.
- know the shape of the molecules and their point groups
- Demonstrate and understanding of VSEPR theory
- evaluate the stability of metal ligand complexes
- Get knowledge about reaction mechanism and metal ligand bonding

SEMESTER–I
Paper-II
MCH-402: ORGANIC CHEMISTRY-I

COURSE OBJECTIVES

To make the student learn about the

- Concepts of aromaticity
- The basic concepts in stereochemistry
- To understand principles of organic reaction mechanism, substitution, elimination, homo- and hetero bond addition reactions.

Unit-I

Nature and Bonding in Organic Molecules

Delocalized chemical bonding-conjugation, cross conjugation, resonance hyperconjugation, bonding in fullerences, tautomerism. Aromaticity in benzenoid and non-benzoid compounds, alternate and non-alternate hydrocarbons. Huckel's rule, energy. Level of π-molecular orbitals, annulenes, anti-aromaticity, homo-aromaticity, PMO approach. Bonds weaker than covalent-addition compounds, crown ether complexs and cryptands, inclusion compounds, catenanes and rotaxanes.

Unit-II

Stereochemistry

Strain due to unavoidable crowding Elements of symmetry, chirality, molecules with more than one chiral center, threo and ertythro isomers, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis, Asymmetric synthesis. Optical activity in the absence of chiral carbon (biphenyls, allenes and spirane chirallity due to helical shape. Stereochemistry of the compounds containing nitrogen, sulphur and phosphorus.

Unit-III

Conformational analysis and linear free energy relationship

Conformational analysis of cycloalkanes, decalines, effect of conformation on reactivity, conformation of sugars. Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes. The Hammett equation and linear free energy relationship, substituents and reaction constants, Taft equation.

Unit-IV

Reaction Mechanism : Structure and Reactivity

Type of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtir-Hammett principle. Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotopes effects.

Unit-V

Aliphatic Nucleophilic Substitution

The S_N2, S_N1 mixed S_N1 and S_N2 and SET mechanism. The neighboring group mechanism, neighboring group participation by p and s bonds, anchimeric assistance. Classical and nonclassical carbocations, phenomium ions, norborynl systems, common carbocation rearrangements. Application of NMR spectroscopy in the detection of carbocations. The SN1 mechanism. Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis and ultrasound, ambident nucleophile, regioselectivity.

Books Suggested

1. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry, F.A. Carey and R.J. Sunderg, Plenum.
3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
4. Structure and Mechanism in Organic Chemistry, C.K. Ingold, Comell University Press.
5. Organic Chemistry, R.T. Morrison and R.N. Boyd, Prentice-Hall.
6. Modern Organic Reactions, H.O. House, Benjamin.
7. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic & Professionsl.
8. Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh, Macmillan.
9. Pericyclic Reactions, S.M. Mukherji, Macmillan, India
10. Stereochemistry of Organic Compounds, D.Nasipuri, New Age International.
11. Stereochemisty of Organic Compounds, P.S. Kalsi, New Age International.
12. Spectroscopic methods in Organic Chemistry, D.H. Williams, I. Fleming, Tata McGraw-Hill.
13. Application of Spectroscopy of Organic Compounds, J.R. Dyer, Prentice Hall.
14. Organic Chemistry, J. McMurry, Thomson Asia.
15. Organic Chemistry, W. Kemp, ELBS, Macmillan.

COURSE OUTCOMES

The students will be able to

- Acquire the skills for correct stereo-chemical assignment and interpretation in rather simple organic molecules.
- Understanding of Organic reaction, rearrangement and cross-coupling reaction with their mechanism and application.

SEMESTER –I
Paper-III
MCH-403: PHYSICAL CHEMISTRY-I

COURSE OBJECTIVES

To make the student conversant with

- The objective of the course is to know the application of quantum mechanics in physical models and experiments of chemical systems. The student will be able to calculate the Energy of the system including E_{HOMO}, E_{LUMO} and bond order.
- The main objective of the course is to provide fundamental concepts of thermodynamics effects and relationships. The course is to give knowledge of comprehensive and rigorous treatment of classical thermodynamics, thermodynamics relations. Explain the concept of partial molar properties fugacity and activity.

Unit-I

Introduction to Exact Quantum Mechanical Results
Schrödinger equation and the postulates of quantum mechanics. Discussion of solutions of the Schrödinger equation to some model systems viz., particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom and helium atom.

Unit-II
Approximate Methods
The variation theorem, linear variation principle. Perturbation theory (First order and nondegenerate). Applications of variation method and perturbation theory to the Helium atom.
Molecular Orbital Theory
Huckel theory of conjugated systems bond and charge density calculations. Applications to ethylene, butadiene, cyclopropenyl radical cyclobutadiene etc. Introduction to extended Huckel theory.

Unit-III
Angular Momentum
Ordinary angular momentum, generalized angular momentum, eigenfucntions for angular momentum, eigenvalues of angular momentum operator using ladder operators addition of angular momenta, spin, antisymmetry and Pauli exclusion principle.

Unit-IV
Classical Thermodynamics
Brief resume of concepts of laws of thermodynamics, free energy, chemical potential and entropies. Partial molar free energy, partial molar volume and partial molar heat content and their significance. Determinations of these quantities. Concept of fugacity and determination of fugacity. Non-ideal systems : Excess function s for non-ideal solutions. Activity, activity coefficient, Debye Huckel theory for activity coefficient fo electrolytic solutions; determination of activity and activity coefficients; ionic strength. Application of phase rule to three component systems; second order phase transitions.

Unit-V
Statistical Thermodynamics
Concept of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging. Canonical, grand canonical and micro-canonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers). Partition functions-translation, rotational, vibrational and electronic partition functions, Calculation of thermodynamic properties in terms of partition. Application of partition functions. Fermi-Dirac Statistics, distribution law and applications to metal. Bose-Einstein statistics distribution Law and application to helium.

Books Suggested

1. Physical Chemistry, P.W. Atkins, ELBS.
2. Introduction to Quantum Chemistyry, A.K. Chandra, Tata Mc Graw Hill.
3. Quantum Chemistry, Ira N. Levine, Prentice Hall.
4. Coulson's Valence, R.Mc Ween y, ELBS.
5. Chemical Kinetics. K.J. Laidler, McGraw-Hill.
6. Kinetics and Mechanism of Chemical Transformation J.Rajaraman and J. Kuriacose, Mc Millan.
7. Micelles, Theoretical and Applied Aspects, V. MOraoi, Plenum.
8. Modern Electrochemistry Vol. 1 and Vol II J.O.M. Bockris and A.K.N. Reddy, Planum.
9. Introduction to Polymer Science, V.R. Gowarikar, N.V. Vishwanathan and J. Sridhar, Wiley Eastern.
10. Introduction to Quantum Chemistry-R.K. Prasad, New Age Publication.
11. Thermodynamics for students of Chemistry, Shobanlal Nagin Chand Co. 1986.

COURSE OUTCOMES

- Students will be able to grasp fundamental concepts of operators, algebra of operators and quantum mechanical and Schrodinger wave equations for single and multi electron systems.

- Students will be able to grasp fundamental concepts of operators, algebra of operators and quantum mechanical and Schrodinger wave equations for single and multi electron systems.
- The student will be able to perform energy calculation for conjugated hydrocarbon systems.
- Students will also understand various thermodynamic relationship, the concept of free energy and partial molar quantities, activity and activity coefficients and determination.

SEMESTER– I
Paper-IV
MCH-404: (a) MATHEMATICS FOR CHEMISTS
(For students without Mathematics in B.Sc.)

COURSE OBJECTIVES

The objective of the course is to know the basics of the mathematics which are generally applied in chemistry viz., vectors and matrix algebra, differential and integral calculus, permutation and probability

Unit-I

Vectors

Vectors, dot, cross and triple products etc. gradient, divergence and curl, Vector Calculus.

Matrix Algebra

Addition and multiplication; inverse, adjoint and transpose of matrices.

Unit-II

Differential Calculus

Functions, continuity and differentiability, rules for differentiation, applications of differential calculus including maxima and minima (examples related to maximally populated rotational energy levels, Bohr's radius and most probable velocity from Maxwell's distribution etc.).

Unit-III

Integral calculus

Basic rules for integration, integration by parts, partial fractions and substitution. Reduction formulae, applications of integral calculus. Functions of several variables, partial differentiation, co-ordinate transformations (e.g. Cartesian to spherical polar).

Unit-IV

Elementary Differential equations

First-order and first degree differential equations, homogenous, exact and linear equations. Applications to chemical kinetics, secular equilibria, quantum chemistry etc. second order differential equation and their solutions.

Unit-V

Permutation and Probability

Permutations and combinations, probability and probability theorems average, variance root means square deviation examples from the kinetic theory of gases etc., fitting (including least squares fit etc with a general polynomial fit.

Books Suggested

1. The chemistry Mathematics Book, E.Steiner, Oxford University Press.
2. Mathematics for chemistry, Doggett and Suiclific, Logman.
3. Mathematical for Physical chemistry : F. Daniels, Mc. Graw Hill.
4. Chemical Mathematics D.M. Hirst, Longman.
5. Applied Mathematics for Physical Chemistry, J.R. Barante, Prentice Hall.
6. Basic Mathematics for Chemists, Tebbutt, Wiley.

7. Mathematics for Chemists, Bhupendra Singh, Pragati Prakashan.
8. Defferential Calulus/Integral Calculus, Dr. G. Prasad, Ppthishala Pvt. Ltd.
9. A Course in Vectors and their Applications: R. S. Mishra, Prakashan Kendra, Lucknow.

COURSE OUTCOMES

Basic mathematics is the back bone of modern chemistry. Students from biology background are also taking admission in the Program. Hence, the course is useful in understanding topics where mathematics is involved.

SEMESTER –I
Paper-IV
MCH-404 (b) BIOLOGY FOR CHEMISTS
(For students without Biology in B.Sc.)

COURSE OBJECTIVES

The Chemistry involved in biological processes is need of the time. Therefore, the main objective of the course is to know the basics of the biology which are generally applied in chemistry. The students will be able to understand the biological process through the course.

Unit-I

Cell Structure and Functions

Structure prokaryotic and eukaryotic cells, intracellular organelles and their functions, comparison of plant and animal cells. Ove4rview and their functions, comparison of plant and animal cells. Overview of metabolic processes-catabolism and anabolism. ATP – the biological energy currency. Origin of life-unique properties of carbon chemical evolution and rise of living systems. Introduction to bio-molecules, building blocks of biomacromolecules.

Unit-II

Carbohydrates

Conformation of monosaccharides, structure and functions of important derivatives of mono-saccharides like glycosides, deoxy sugars, myoinositol, amino sugars. Nacetylmuramic acid, sialic acid disaccharides and polysaccharides. Structural polysaccharides cellulose and chitin. Storage polysaccharides-starch and glycogen. Structure and biological function of glucosaminoglycans of mucopolysaccharides. Carbohydrates of glycoporteins and glycolipids. Role of sugars in biological recognition. Blood group substances. Ascorbic acid.

Unit-III

Lipid

Fatty acids, essential fatty acids, structure and function of triacylglycerols, glycerophospholipids, sphingolipids, cholesterol, bile acids, prostaglandins. Liproproteins-compositiion and function, role in atherosclerosis. Properties of lipid aggregates-micelles, bilayers, liposomes and their possible biological functions. Biological membranes. Fluid mosaic model of membrane structure. Lipid metabolism-boxidation of fatty acids.

Unit-IV

Amino-acids, Peptides and Proteins

Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing. Secondary structure of proteins. force responsible for holding of secondary structures. ahelix, -b-sheets, super secondary structure, triple helix structure of collagen. Tertiary structure of protein-folding and domina structure. Quaternary structure. Amino acid metabolism-degradation and biosynthesis of amino acids, sequence determination:

chemical/enzymatic/mass spectral, racemization/detection. Chemistry of oxytocin and tryptophan releasing hormone (TRH).

Unit-V

Nucleic Acids

Purine and pyrimidine bases of nucleic acids, base pairing via Hbounding. Structure of ribonucleic acids (RNA) and deoxyribonucleic acid (DNA), double helix model of DNA and forces responsible for holding it. Chemical and enzymatic hydrolysis of nucleic acids. The chemical basis for heredity, an overview of replication of DNA, transcription, translation and genetic code. Chemical synthesis of mono and trinucleoside.

Books Suggested

1. Principles of Biochemistry, A.L. Lehninger, Worth Publishers.
2. Biochemistry, L. Stryer, W.H. Freeman.
3. Biochemistry, J. David Rawan, Neil Patterson.
4. Biochemistry, Voet and Voet, John Wiley.
5. Outlines of Biochemistry E.E. Conn and P.K. Stumpf, John Wiley.

COURSE OUTCOMES

Basic knowledge of biology is also involved in chemistry related to real life problems which chemistry students must know. The students coming from Mathematics background are made aware o the basic knowledge required. Hence, the course is useful in understanding topics covered in this course.

SEMESTER –I
PRACTICAL
(Duration: 6 hrs in each branch)

Note- Practical examination of Inorganic/Organic/Physical will be conducts at the end of each semester during examination.

Inorganic Chemistry

COURSE OBJECTIVES

The students will learn

- The basics of quantitative estimation of metal complexes.
- To separate different ions by paper chromatography.
- The interpretation od IR spectra of metal complexes.

Experiment - 1	15
Experiment -2	15
Viva Voce	10
Record	10
Total	**50**

1. **Chromatographic Separations**
   (a) Cadmium and zinc
   (b) Zinc and magnesium
   (c) Lead and silver

2. **Complexometric titration**
   Estimation of Ca^{2+}, Mg^{2+} and Zn^{2+}

3. **Interpretation of IR spectra of some known inorganic complexes.**

Books Suggested

1. Synthesis and Characterization of Inorganic Compounds, W. L. Jolly, Prentice Hall.
2. Inorganic experiments, 3rd edition, J. D. Woollins, Wiley-VCHVerlag GmbH @Co.KGaA, 2012.
3. Foundations of College Chemistry in the Laboratory, M. Hein, J. N. Peisen and R. L. Miner, John Wiley and Sons, 2011.
4. In-house Laboratory Manual, Departmentof Chemistry, APSU Rewa.

COURSE OUTCOMES

The students will be able to

- Estimate the metals from metal complexes.
- Separate and analyze different metal ions using paper chromatography.
- Identify the different groups present in the complexes.

Physical Chemistry

COURSE OBJECTIVES

To introduce experiments in chemical kinetics and equilibrium chemistry.

Experiment – 1	15
Experiment -2	15
Viva Voce	10
Record	10
Total	**50**

1. **Chemical Kinetic**s
   (a) Determination of velocity constant of the hydrolysis of methyl acetate catalysed by an acid (say HCl, H_2SO_4, etc.).
   (b) Determination of velocity constant of saponification of ethyl acetate with sodium hydroxide.
   (c) Determination of velocity of the reaction between potassium persulphate and potassium iodide.
2. **To determine the distribution coefficient of benzoic acid between toluene and water at room temperature.**

3. **To determine equilibrium constant for the reaction between iodide and iodine by the method of distribution.**

Books Suggested

1. An introduction to Statistical Thermodynamics, T. A. Hill, Dover Publications Inc., 1987.
2. Chemical Kinetics, K. J. Laidler, Pearson Education, 3rd edition, 2011.
3. Findley's Practical Physical Chemistry, B. P. Levitt, Longman.
4. Practical Physical Chemisry, A. M. James and F. E. Prichard, Longman.

COURSE OUTCOMES

Students will obtain hands on experience on chemical kinetics and equilibrium parameters.

Organic Chemistry

COURSE OBJECTIVES

To introduce organic synthesis, purification and identification of organic compounds using physiochemical techniques.

Experiment - 1	15
Experiment -2	15
Viva Voce	10
Record	10
Total	**50**

1. **Qualitative Analysis**
   Separation, purification and identification of compounds of ternary mixture (one liquid and one solid) using TLC and columns chromatography, chemical tests. IR spectra to be used for functional group identification.

2. **Organic Synthesis**
   Acetylation : Acetylation of cholesterol and separation of cholesteryl acetate by column chromatography. Oxidation : Adipic acid by chromic acid oxidation of cyclothexaneol Grignard reaction : Synthesis of triphenylmethanol from benzoic acid Aromatic electrophilic sustitutions : Synthesis of p-nitroaniline and pbromoaniline. Aldol condensation Dibenzal acetone from benzaldehyde. Synthesis of different Schiff bases using salicylaldehyde and amines, Synthesys of different dithiocarbamates. The Products may be characterized by Spectral Techniques.

3. **Qualitative analysis of Bi-functional compounds**
   (a) Anthranilic acid
   (b) p-aminobenzoic acid
   (c) Resorcinol
   (d) Acetamide
   (e) α/β-naphthole

Books Suggested

1. Laboratory Manual in Organic Chemistry, R. K. Bansal, Wiley, 2006.
2. Vogel's Textbook of Practical Organic Chemistry, ELBS.
3. Practical Organic Chemistry, F. G. Mann and B. C. Saunders, Orient Longman.
4. Experimental Organic Chemistry Vol 1 and 2, P. R; Singh, D. S. Gupta and K. S. Bajpai, Tata McGraw Hill.

COURSE OUTCOMES

Ensures the students to understand acquire knowledge and have hands on experience in organic synthesis and analysis by using physiochemical techniques.

SEMESTER –II
Paper-V
MCH-405: INORGANIC CHEMISTRY-II

COURSE OBJECTIVES

The complexes of transition metals are very important topics of applied chemistry. Even in Medicinal chemistry these complexes play important role. The main objective of the course is to provide fundamental concept of

- The electronic spectral studies of transition metal complexes.
- Magnetic properties of transition metal complexes.
- Metal π-complexes and metal clusters.

- Optical rotatory dispersion (ORD) and circular dichroism (CD).

Unit-I

Electronic Spectral Studies of Transition Metal Complexes

Spectroscopic ground states, correlation. Orgel and Tanabe-Sugano diagrams for transition metal complexes (d1-d9 states), Selection rule for electronic spectroscopy. Intensity of various type electronic transitions. Calculations of 10Dq, B and β parameters, charge transfer spectra.

Unit-II

Magnetic Properties of Transition Metal Complexes

Anomalous magnetic moments, Quenching of Orbital contribution. Orbital contribution to magnetic moment, magnetic exchange coupling and spin crossover.

Unit-III

Metal π-Complexes

Metal carbonyl, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls; preparation, bonding structure and important reaction of transition metal nitrosyl, dinitrogen and dioxgen complexes; tertiary phosphine as ligand, Wilkinson's catalyst.

Unit-IV

Metal Clusters

Synthesis, reactivity and bonding

Borane Chemistry

Higher boranes, carboranes, metalloboranes and metallo-carboranes compounds with metal metal multiple bonds.

Unit-V

Optical Rotatory Dispersion and Circular Dichroism

Linearly and circularly polarized lights; optical rotatory power and circular birefringence, elipticity and circular dichroism; ORD and Cotton effect, Faraday and Kerr effects; Assignment of electronic transitions; applications of ORD and CD for the determination of (i) absolute configuration of complexes and (ii) isomerism due to non-planarity of chelate rings.

Books Suggested :

1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
2. Inorganic Chemistry, J.E. Huhey, Harpes & Row.
3. Chemistry of the Elements. N.N. Greenwood and A. Earnshow, Pergamon.
4. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
5. Magnetiochemistry, R.L. Carlin, Springer Verlag.
6. Comprehensive Coordiantion Chemistry eds., G. Wilkinson, R.D. Gillars and J.A. Mc Cleverty,Pergamon.

COURSE OUTCOMES

- Student will be able to understand the spectroscopic ground states of d^1 to d^9 systems.
- They will gain the knowledge of magnetic moment and magnetic exchange coupling of transition metal complexes.
- Student will get the basic idea about metal-π complexes and metal clusters.

SEMESTER –II
Paper-VI
MCH-406: ORGANIC CHEMISTRY-II

COURSE OBJECTIVES

Understanding of chemical reaction and their mechanism is essential part of chemistry. This course is introduced for the detailed study of aromatic electrophilic substitution, aromatic nucleophilic substitution, free radical reactions, addition reactions, addition to carbon-hetero multiple bonds, elimination reactions. This course also imparts knowledge on different classes of pericyclic reactions.

Unit-I

Aromatic Electrophilic Substitution

The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles. Diazonium coupling, Vilsmeir reactiion, Gatterman-Koch reaction

Aromatic Nucleophilic Substitution

The SNAr SN^1, benzyne and SN^1 mechanism, Reactivity effect of substrate structure, leaving group and attacking nucleophile. The Von Richte. Sommelet-Hauser, and Smiles rearrangements.

Unit-II

Free Radical Reactions

Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. Reactivity in the attacking radicals. The effect of solvents on reactivity. Allylic halogenation (NBS), oxidation of aldehydes to carboyxlic acids, autooxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts, Sandmeyer reaction. Free radical rearrangement. Hunsdiecker reaction.

Unit III

Addition Reactions

Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio-and chemoselectivity, orientation and reactivity. Addition to cyclopropane ring. Hydrogenation of double and triple bounds, hydrogenation of aromatic rings. Hydroboration, Michael reaction, sharpless asymmetric epoxidation.

Unit-IV

Addition to Carbon-Hetero Multiple bonds

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acid esters and nitriles. Addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and usaturated carbonyl compounds. Witting reaction. Mechanism of condensation reactions involving enolates-Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions. Hydrolysis of esters and amides, ammonolysis of esters.

Elimination Reactions

The E2, E1 and E1 cB mechanisms and their spectrum. Orientation of the double bond. Reactitivty-effects of substrate structures, attacking base, the leavign group and the medium. Mechanism and orientation in pyrolytic elimination.

Unit-V

Pericyclic Reactions

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene
and allyl system. Classification of periycyclic reactions. Woodward-Hoffmann correlatino diagrams. FMO and PMO approach. Electrocyclic reactions-conrotatory and disrotatory motions, 4n 4n+2 and allyl systems. Cycloadditions-antarafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3 dipolar cycloadditions and cheleotrpic reactions. Sigmatropic rearrangements-suprafacial and antarafacial

shifts of H, sigmatropic involving carbon moieties, 3,3- and 5,5 sigmatropic rearrangements. Claise n, Cope and aza-Cope rearrangements. Fluxional tautomerism. Ene reaction.

Books Suggested

1. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.
2. Organic Chemistry, R.T. Morrison and R.N. Boyd, Prentice-Hall.
3. Modern Organic Reactions, H.O. House, Benjamin.
4. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie.
5. Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh, Macmillan.
6. Pericyclic Reactions, S.M. Mukherji, Macmillan, India.
7. Stereochemisty of Organic Compounds, P.S. Kalsi, New Age International.
8. Spectroscopic Methods in Organic Chemistry, D.H. Williams, I. Fleming, Tata McGraw-Hill.
9. Organic Chemistry, P.Y. Bruice, Pearson Education Asia.

COURSE OUTCOMES

- The student will be able to know the different types of organic reactions.
- Students will also understand the stereochemical aspects of different classes of pericyclic reactions.

SEMESTER–II
Paper-VII
MCH-407: PHYSICAL CHEMISTRY-II

COURSE OBJECTIVES

- Students will gain knowledge of chemical dynamics and non-equilibrium thermodynamics.
- Student will understand different aspects of the surface chemistry
- Student will develop skills to solve problems relating to molecular weights of macromolecules.
- The students will understand advance knowledge of electrochemistry.

Unit-I

Chemical Dynamics

Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation and the activated complex theory; ionic reactions, kinetic salt effects, steady state kinetics, kinetic and thermodynamic control of reactions, treatment of unimolecular reactions. Dyamic chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogenbromine and hydrogen-chlorine reactions) and homogenous catalysis, kinetics of enzyme reactions, general features fo fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis ad the nuclear magnetic resonance method, dynamics of unimolecular reactiosn (Lindemann Hinshelwood and Rice-Ramsperger-Kassel- Marcus (RRKM) theories for unimolecular reactions).

Unit-II

Surface Chemistry

Adsorption

Surface tension, capillary action, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, estimation of surface area (BET equation), Surface films on liquids (Electro-kinetic phenomenon).

Micelles

Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization-phase separation and mass action models, solublization, micro emulsion, reverse micelles.

Unit-III

Macromolecules

Polymer-definition, types of polymers, electrically conducting, fire resistant, liquid crystal polymers, kinetics of polymerization, mechanism of polymerization. Molecular mass, number and mass average molecular mass, molecular mass determination (Osmometry, viscometry, diffusion and light scattering methods), sedimentation, chain configuration of macromolecules, calculation of average dimension of various chain structures.

Emulsions

Theories of emulsification, coagulation, slow and rapid coagulation. Kenitics of coagulation. Von Smoluchouski equation and its verification.

Unit-IV

Non Equilibrium Theromodynamics

Thermodynamic criteria for non-equilibrium states, entropy production and entropy flow,
entropy balance equations for different irreversible processes (e.g., heat flow, chemical reaction etc.) transformations of the generalized fluxes and forces, non equilibrium stationary states, phenomenological equations, microscopic reversibility and Onsager's reciprocity relations, electrokinetic phenomena, diffusion, electric conduction.

Unit-V

Electrochemistry

Electrochemistry of solutions. Debye-Huckel-Onsager treatment and its extension, ion solvent interactions. Debye-Huckel-Jerum mode. Thermodynamics of electrified interface equations. Derivation of electro capillarity, Lippmann equations (surface excess), methods of determination. Structure of electrified interfaces. Overpotentials, exchange current density, derivation of Butler Volmer equation, Tafel plot. Quantum aspects of charge transfer at electrodes-solution interfaces, quantization of charge transfer, tunneling. Semiconductor interfaces-theory of double layer at semiconductor, electrolyte solution interfaces, structure of double layer interfaces. Effect of light at semiconductor solution interface. Polarography theory, Ilkovic equation; half wave potential and its significance.

Books Suggested

1. Physical Chemistry, P.W. Atkins, ELBS.
2. Introduction to Quantum Chemistry, A.K. Chandra, Tata Mc Graw Hill.
3. Quantum Chemistry, Ira N. Levine, Prentice Hall.
4. Coulson's Valence, R.Mc Ween y, ELBS.
5. Chemical Kinetics. K.J. Laidler, McGraw-Hill.
6. Kineties and Mechanism of Chemical Transformation J.Rajaraman and J. Kuriacose, Mc Millan.
7. Micelles, Theoretical and Applied Aspects, V. MOraoi, Plenum.
8. Modern Electrochemistry Vol. 1 and Vol II J.O.M. Bockris and A.K.N. Reddy, Planum.
9. Introduction to Polymer Science, V.R. Gowarikar, N.V. Vishwanathan and J. Sridhar, Wiley Eastern.
10. Physical Chemistry, P.C. Rakshit.
11. Quantum Chemistry, Eyring and Kimball.

COURSE OUTCOMES

- Students will be able to explain the process taking place in any chemical reaction.
- The basics of non-equilibrium thermodynamics will also be understood.
- Students will be able to have understanding about surface chemistry and its applications.
- Students will be able to solve the problems related to molecular weights of macromolecules.
- Students will understand the advance electrochemistry.

SEMESTER –II
Paper-VIII

MCH-408: Spectroscopy and Diffraction Methods

COURSE OBJECTIVES

The objective of this course is to give basic principles and applications of modern spectroscopic techniques (Nuclear Magnetic Resonance Spectroscopy, Nuclear Quadrupole Resonance Spectroscopy and Electron Spin Resonance Spectroscopy) and Diffraction Techniques (X-ray Diffraction, Electron Diffraction and Neutron Diffraction).

Unit-I

Nuclear Magnetic Resonance Spectroscopy

Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurements, factors, influencing chemical shift, deshielding, spin-spin interactions, factors influencing coupling constant "j" Classification (AXB, AMX, ABC, A2B2 etc.). spin decoupling; basic ideas about instrument, NMR studies of nuclei other than protin-13C, 19F and ^{31}P. FT NMR, advantages of FT NMR.

Unit II

Nuclear Quadrupole Resonance Spectroscopy

Quadrupole nuclei, quadrupole moments, electric field gradient, coupling constant, splitting, General principles and Instrumentation, Applications.

Unit-III

Electron Spin Resonance Spectroscopy

Basic principles, zero field splitting and Kramer's degeneracy, factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants, some representative examples of esr spectra of Cu^{2+} and $V(O)^{2+}$ complexes, spin Hamiltonian, spin densities and Mc Connell relationship, measurement techniques, applications.

Unit-IV

X-ray Diffraction

Bragg condition, Miller indices, Laue Method, Bragg method, Debye Scherrer method of X-ray structural analysis of crystals, index reflections, identification of unit cells from systematic absences in diffraction pattern, Structure of simple lattices and X-ray intensities, structure factor and its relation to intensity and electron density, phase problem. Description of the procedure for an X-ray structure analysis, absolute configuration of molecules.

Unit-V

Electron Diffraction

Scattering intensity vs. scattering angle, Wierl equation, measurement technique, elucidation of structure of simple gas phase molecules. Low energy electron diffraction and structure of surfaces.

Neutron Diffraction

Scattering of neutrons by solids measurement techniques, Elucidation of structure of magnetically ordered unit cells.

Books suggested

1. Modern Spectroscopy, J.M. Hollas, John Viley.
2. Applied Electron Spectroscopy for chemical analysis d. H. Windawi and F.L. Ho, Wiley Interscience.
3. NMR, NQR, EPr and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Harwood.
4. Nuclear Qudrupole Resonance Spectroscopy, T.P. Das and E.L. Hann, Academic Press, New York and London, 1958.
5. Physical Methods in Chemistry, R.S. Drago, Saunders College.
6. Chemical Applications of Group Theory, F.A. Cotton.
7. Introduction to Molecular Spectroscopy, G.M. Barrow, Mc Graw Hill.
8. Basic Principles of Spectroscopy, R. Chang, Mc Graw Hill.

9. Theory and Application of UV Spectroscopy, H.H. Jaffe and M. Orchin, IBHOxford.
10. Introduction to Photoelectron Spectroscopy, P.K. Ghosh, John Wiley.
11. Introduction to Magnetic Resonance. A Carrington and A.D. Maclachalan, harper & Row.

COURSE OUTCOMES

- The Knowledge of modern spectroscopy such as NMR, NQR and ESR, symmetry of structure etc. and their applications is useful in understanding the different inorganic and organic molecules.
- Student will able to solve the molecular structures using different diffraction techniques.

SEMESTER –II
PRACTICAL
(Duration: 6 hrs in each branch)

Inorganic Chemistry

COURSE OBJECTIVES

The students will learn estimation of metal ions (gravimetrically and volumetrically) and inorganic synthesis.

Experiment - 1	15
Experiment -2	15

Viva Voce	10
Record	10
Total	**50**

1. **Separation and estimation of two metal ions**
   (a) Estimation of copper and nickel both by gravimetric method.
   (b) Estimation of barium gravimetrically and copper volumetrically methods.
   (c) Estimation of copper and zinc in a mixed solution of both by gravimetric methods.
   (d) Estimation of nickel and zinc in a mixed solution of both by gravimetric methods.

2. **Preparation and synthesis of metal complexes**
   (a) $VO(acac)_2$
   (b) $Ni(acac)_2$
   (c) $K_3[Fe(C_2O_4)_3]$
   (d) Prussian Blue, Turnbull's Blue.
   (e) $Co(NH_3)_6]$ $[Co(NO_2)_6]$
   (f) $Hg[Co(SCN)_4]$
   (g) $[Cu(NH_3)_4]SO_4.H_2O$
   (h) $[Ni(NH_3)_6]Cl_2$
   (i) $Ni(dmg)_2$

3. **Interpretation of Electron Paramagnetic Resonance (epr) spectra of some paramagnetic complexes.**

Books Suggested

1. Synthesis and Technique in Inorganic Chemistry: A Laboratory Manual, 3rd edition, G. S. Girolami, T. B. Rauchfuss and R. J. Angelici, University Science Books, 1999.
2. Advanced Practical Chemistry, R. Mukhopadyay and P. Chatterjee, Books & Allied (P) Ltd., 2007.
3. Quantitative Chemical Analysis, 6th edition, J. Mendham, R. C. Denney, M. J. K. Thomas David and J. Barnes, Prentice Hall, 2000.
4. Analytical Chemistry, S. M. Khopker, New Age International Ltd., Dew Delhi.

COURSE OUTCOMES

The students will be able to understand estimation of metal ions and synthesizing inorganic complexes.

Physical Chemistry

COURSE OBJECTIVES

To make the students expertise in electrochemistry and interpretation of thermodynamic, kinetic and QSAR parameters.

Experiment - 1	15
Experiment -2	15
Viva Voce	10
Record	10
Total	**50**

1. **Determination of composition of a mixture of weak and strong acids by conductor metric titration of following acids:**

(a) HCl and CH_3COOH
(b) HNO_3 and CH_3COOH
(c) H_2SO_4 and CH_3COOH

2. **Determination of composition of a mixture of weak and strong acids by pH metric titration of followings acids:**
   (a) HCl and CH_3COOH
   (b) HNO_3 and CH_3COOH
   (c) H_2SO_4 and CH_3COOH

3. **Theoretical interpretation of Thermodynamic parameters, kinetic parameters and QSAR parameters.**

Books Suggested

1. Experimental Physical Chemistry, V. D. Athawale, New Age International, 2007.
2. Practical Physical Chemistry, B. Viswanathan and P.S. Raghavan, Viva Books Pvt. Ltd., 2005.
3. Experimental Physical Chemistry, R. C. Das and B. Behera, Tata McGraw Hill.
4. Practical Physical Chemistry, A. M. James and F. E. Prichard, Longman.

COURSE OUTCOMES

Students will be able to

- Determine the composition of mixtures of two acids using conductometric and pH-metric methods.
- Difference thermodynamics, kinetic and QSAR parameters.

Organic Chemistry

COURSE OBJECTIVES

To make the students conversant with

- Identification of hydroxyl groups in organic compounds.
- Estimation amines and phenols.
- Oil sample estimation.
- Determination of water quality parameters.
- Multistep synthesis.

Experiment - 1	15
Experiment -2	15
Viva Voce	10
Record	10

Total	**50**

1. **Quantitative Analysis**
   Determination of the percentage or number of hydroxyl groups in an organic compound by acetylation method. Estimation of amines/phenols using bromate bromide solution/or acetylation method. Determination of iodine and Saponification values of an oil sample. Determination of DO, COD and BOD of water sample.

2. **Multistep preparation**
   (a) m-nitro aniline from nitrobenzene
   (b) Hippuric acid from glycine
   (c) Aspirin from salicylic acid
   (d) p-bromo aniline from aniline
   (e) phthalamide from phthlic acid

3. **Interpretation of some IR and NMR spectra of some known compounds.**

Books Suggested

1. Experiments and techniques in Organic Chemistry, D. Pasto, C. Johnson and M. Miller, Prentice Hall.
2. Organic Chemistry-Lab Manual, N. S. Gnanapragasam, G. Ramamurthy and S. Viswanathan Co. Pvt. Ltd., 1998.
3. Vogel's Practical Organic Chemistry, A. I. Vogel, A. R. Tatchell, B. S. Furnis, A. J. Hannaford and P. W. G. Smith, 5th edition, Pearson education Ltd., 1996.
4. Handbook of Organic Analysis-Qualitative and Quantitative, H. Clarke and A. Arnold.

COURSE OUTCOMES

At the end of semester, the students will be able to

- Identify the hydroxyl groups in organic compounds.
- Estimate amines and phenols.
- Determine water quality parameters from water samples.

SEMESTER –III
Paper-I
MCH-502: APPLICATION OF SPECTROSCOPY

COURSE OBJECTIVES

The paper of application of spectroscopy is introduced for the detailed studies of fundamental concepts, tools and techniques used behind UV-visible, infra red, Raman, NMR, Mössbauer and Mass Spectrometric methods for structural determination of molecules.

Unit-I

Ultraviolet and Visible spectroscopy

Various electronic transitions (185-800 nm) Beer-Lambert law, effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes, Fieser Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic compounds. Steric effect in biphenyls. Electronic Spectral Studies for d^1- d^9 systems in octahedral, tetrahedral and square planar complexes with some representative examples of electronic spectra with some representative examples of electronic spectra.

Unit-II

Infrared and Raman Spectroscopy

Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ether's, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (ketone's, aldehyde's, esters, amides, acids, anhydride's, lactones, lactams and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and fermi resonance. Infrared and Raman spectra of AB_3, AB_4, AB_5 and AB_6, mode of bonding of ambidentate ligands, nitrosyl, ethylenediamine and diketonato complexes, application of resonance Raman spectroscopy and its applications.

Unit-III

Nuclear Magnetic Resonance Spectroscopy – I

General introduction and definition, Chemical shift, spin – spin interaction, shielding and deshilding mechanism, mechanism of measurement of chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, and amides & mercapto).

Nuclear Magnetic Resonance Spectroscopy – II

Chemical exchange, effect of deuteration, Complex spin – spin interation between two, three, four and five nuclei (I order spectra) Stereochemistry, hindered rotation, Karplus curve-variation of coupling constant with disordered angle, NMR shift reagents, solvent effects, Nuclear overhauser effect (NOE).

Unit-IV

Mössbauer Spectroscopy

Basic principles, spectral parameters and spectrum display. Application of the technique to the studies of (1) bonding and structures of Fe^{+2} and Fe^{+3} compounds including those of intermediate spin, (2) Sn^{+2} and Sn^{+4} compounds nature of M-L bond, coordination number, structure and (3) detection of oxidation state and in equivalent MB atoms.

Unit V

Mass Spectrometry

Introduction ion production E1, C1 FD, ESI and FAB, factors affecting fragmentation, ion analysis, ion abundance Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak. Me Lafferty rearrangement. Nitrogen rule. High resolution mass spectrometry. Structure elucidation of simple molecules using UV – Visible, IR, NMR and mass spectral techniques.

Books Suggested

1. Physical Methods for Chemistry, R.S. Drago, Saunders Compnay.
2. Structural Methods in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H. Rankin and S. Cradock, ELBS.
3. Infrared and Raman Spectral : Inorganic and Coordination Compounds K. Nakamoto, Wiley.
4. Progress in Inorganic Chemistry vol., 8, ed., F.A. Cotton, vol., 15 ed. S.J. Lippard, Wiley.
5. Transition Metal Chemistry ed. R.L. Carlin vol. 3 dekker.
6. Inorganic Electronic Spectroscopy, A.P.B. Lever, Elsevier.
7. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, .V. Parish, Ellis Haywood.
8. Practical NMR Spectroscopy, M.L. Martin. J.J. Deepish and G.J. Martin, Heyden.
9. Spectrometric Identification of Organic Compounds, R.M. Silverstein, G.C. Bassler adn T.C. Morrill, John Wiley.
10. Introduction to NMR spectroscopy, R.J. Abraham, J. Fisher and P. Loftus, Wiley.
11. Application of Spectroscopy of Organic Compounds, J.R. Dyer Prentice Hall.
12. Spectroscopic Methods in Organic Chemistry D.H. Williams, I. Fleming, Tata McGraw-Hill.

COURSE OUTCOMES

After studying this course the student will be able to

- Understand the basics of UV-visible, infra red, Raman, NMR, Mössbauer and Mass Spectrometric techniques.
- Solve numerical and experimental graphs of all of the above techniques.
- Cover wide area of research in above spectroscopic methods.

SEMESTER –III
Paper II
MCH-501: PHOTOCHEMISTRY

COURSE OBJECTIVES

- To provide the students the basics of photochemistry and reaction mechanism.
- To impart the knowledge of photochemistry of carbonyl compounds and different type of photochemical reactions.

Unit-I

Photochemical Reactions

Interaction of electromagnetic radiation with matter, types of excitations, fate of excited molecule, quantum yield, transfer of excitation energy, actinometry.

Unit -II

Determination of Reaction Mechanism

Classification, rate constants and life times of reactive energy state determination of rate constants of reactions, Effect of light intensity on the rate of photochemical reactions, Types of photochemical reactions-photo dissociation, gas-phase photolysis.

Unit -III

Photochemistry of Alkene

Intramolecular reactions of the olefinic bond-geometrical isomerism, cyclisation reactions, rearrangement of 1,4- and 1,5-dienes.

Photochemistry of Aromatic Compounds

Isomerisations, additions and substitutions.

Unit -IV

Photochemistry of Carbonyl Compounds

Intramolecular reactions of carbonyl compounds-saturated, cyclic and acyclic, α, β, γ unsaturated and α, β, unsaturated compounds, cyclohexadienones, Intermolecular cyloaddition reactions-dimerisations and oxetane formation.

Unit-V

Miscellaneous Photochemical Reactions.

Photo-Fries reactions of annelids, Photo-Fries rearrangement, Barton reaction, Singlet molecular oxygen and its reactions, Photochemical formation of smog, Photodegration of polymers, Photochemistry of vision.

Books Suggested

1. Fundamentals of Photochemistry, K.K. Rothagi-Mukheriji, Wiley-Eastern.
2. Essentials of Molecular Photochemistry, A Gilbert and J. Baggott, Blackwell Scientific Publication.
3. Molecular Photochemistry, N.J. Turro, W.A. Benjamin.
4. Introductory Photochemistry, A. Cox and t. Camp, McGraw Hill.
5. Photochemistry, R.P. Kundall and A. Gilbert. Thomson Nelson.
6. Organic Photochemistry, J. Coxon and B. Halton, Cambridge University Press.
7. Photochemistry and Pericyclic reactions, J. Singh and J. Singh, New Age International, New Delhi.
8. Modern Molecular Photochemistry, N.J. Turro, University Science Book, California.

COURSE OUTCOMES

The students able to

- Get the knowledge of photochemical reactions and mechanism of photochemical reactions.
- Gain the knowledge of photochemistry of alkenes, aromatic compounds and carbonyl compounds along with miscellaneous photochemical reactions.

SEMESTER –IV
DISCIPLINE ELECTIVE
Paper III
MCH-503: Organotransition Metal Chemistry

COURSE OBJECTIVES

Organotransition metal chemistry is the study of chemical compounds containing at least one chemical bond between a carbon atom of an organic molecule and a transition metal. This paper is introduced for the detailed studies of transition metal organometallic compounds, organotransition metal catalysts and basic ideas of fluxional organometallic compounds.

Unit -I

Alkyls and Aryls of Transition Metals

Types, routes of synthesis, stability and decomposition pathways organocopper in organic synthesis.

Compounds of Transition Metal-Carbon Multiple Bonds

Alkylidenes, alkylidynes, low valent carbenes and carbynes-synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions on the ligands, role in organic synthesis.

Unit -II

Transition Metal π-Complexes

Transition metal π-Complexes with unsaturated organic molecules, alkenes, alkynes, allyl, diene, dienyl, arene and trienyl complexes, preparation, properties, nature of bonding and structural features. Important reactions relating to nucleophilic and electrophilic attack on ligands and to organic synthesis.

Unit -III

Transition organometalic compounds

Transition metal compounds with bonds to hydrogen, boron, silicon

Unit -IV

Homogeneous Catalysis

Stoichiometric reactions for catalysis, homogeneous catalytic hydrogenation, Zeigler- Natta polymerization of olefins, catalytic reactions involving carbon monoxide such as hydrocarbonylation of olefins (oxoreaction), explanation reactions, activation of C-H bond.

Unit -V

Fluxional Organometallic Compounds

Flexionality and dynamic equilibrium in compounds such as η^2 olefine, η^3-allyl and dienyl complexes.

Books Suggested

1. Principles and Application of Organotransition Metal Chemistry, J.P. Collman, L.S. Hegsdus, J.R. Norton and R.G. Finke, University Science Books.
2. The Organometallic Chemistry of the Transition Metals, R.H. Crabtree. John Wiley.
3. Metallo-organic Chemistry, A.J. Pearson, Wiley.
4. Organometallic Chemistry, R.C. Mehrotra and A. Singh New Age International.

COURSE OUTCOMES

On completion of the course students will be able to

- Acquire understanding of various classes of organotransition metal compounds- alkyl and aryls of transition metals, transition metal complexes of carbenes and carbynes and transition metal pi-complexes.
- Have understanding of catalysis reactions involving organotransition metal compounds and basics of fluxional organometallic compounds.
- Develop ideas for further research in the field of organotransition metal chemistry.

SEMESTER –III
DISCIPLINE ELECTIVE
Paper III
MCH-504: Heterocyclic Chemistry

COURSE OBJECTIVES

To provide knowledge on

- Heterocycles and non-aromatic heterocycles.
- Synthesis and characterization of various natural compounds of biological importance.
- heterocyclic compounds of biological and pharmaceutical importance.

Unit-I

Nomenclature of Heterocycles

Replacement and systematic nomenclature (HantzsMCH-Widman system) for monocyclic fused and bridged heterocycles.

Aromatic Heterocycles

General chemical behaviour of aromatic heterocycles, classification (structural type), criteria of aromaticity (bond lengths, ring current and chemical shifts in 1H NMRspectra. Empirical resonance energy, delocalization energy and Dewar resonance energy, diamagnetic susceptibility exaltations). Heteroaromatic reactivity and tautomerism in aromatic heterocycles.

Unit-II

Non-aromatic Heterocycles

Strain-bond angle and torsional strains and their consequences in small ring heterocycles. Conformatino of six-membered heterocycles with reference to molecular geometry, barrier to ring inversion, pyramidal inversino and 1,3-diaxial interaction. Stereo-electronic effects anomeric and related effects, Attractive interactions-hydrogen bonding and intermolecular nucleophilic lectrophilic interactions. Heterocyclic Synthesis Princples of heterocyclic synthesis involing cyclization reactions and cycloaddition reactions.

Unit-III

Small Ring Heterocycles

Three-membered and four-membered heterocycles-synthesis and reactions of azirodines, oxiranes, thiranes, azetidines, oxetanes and thietanes.

Benzo-Fused Five-Membered Heterocycles

Synthesis and reactions including medicinal applications of benzopyrroles, bezofurans and benzothiophenes.

Unit-IV

Meso-ionic Heterocycles

General classification, chemistry of some important meso-ionic heterocycles of type-A and B and their applications.

Six-Membered Heterocycles with one Heteroatom
Synthesis and reactions of pyrylium salts and pyrones and their comparison with pyridinium & thiopyrylium salts and phridones. Synthesis and reactions of quionlizinium and benzopyrylium salts, coumarins and chromones.

Unit-V
Six Membered Heterocycles with Two or More Heteroatoms Synthesis and reactions of diazones, triazines, tetrazines and thiazines. Seven-and Large-Membered Heterocycles Synthesis and reactions of azepines, oxepines, thiepines, diazepines thiazepines, azocines, diazocines, dioxocines and dithiocines.

Heterocyclic Systems Containing P, As, Sb and B
Heterocyclic rings containing phosphorus : Introduction, nomenclature, synthesis and characteristics of 5- and 6-membered ring systemsphosphorinaes, phosphorines, phospholanes and phospholes. Heterocyclic rings containing As and Sb: Introduction, synthesis and characteristics of 5- and 6-membered ring system. Heterocyclic rings containing B : Introduction, synthesis reactivity and spectral characteristics of 3- 5- and 6- membered ring system.

Books Suggested

1. Heterocyclic Chemistry Vol. 1-3, R.R. Gupta, M. Kumar and V.Gupta, Springer Verlag.
2. The Chemistry of Heterocycles, T. Eicher and S. Hauptmann, Thieme.
3. Heterocyclic chemistry J.A. Joule, K. Mills and g.F. Smith, Chapman and Hall.
4. Heterocyclic Chemistry, T.L. Gilchrist, Longman Scietific Techinal.
5. Contemporary Hetrocyclic Chemistry, G,.R. Newkome and W.W. Paudler, Wiley-Inter Science.
6. An Introductiion to the Heterocyclic Compounds, R.M. Acheson, Johnwiely.
7. Comprehensive Heterocyclic Chemistry, A.R. Katrizky and C.W. Rees, eds. Pergamon Press.

COURSE OUTCOMES

- Students will achieve insight on isolation, characterization and synthesis of various natural compounds of biological importance.
- Students will acquire knowledge on different heterocylic compounds.

SEMESTER –III
DISCIPLINE ELECTIVE
Paper III
MCH-505: Electrochemistry

COURSE OBJECTIVES

The objective of this course is

- To introduce students to conversion and storage of electrochemical energy
- To introduce students to give the basic idea about corrosion and stability of the metals.
- To introduce students to how different kinetic parameters for quasi and irreversible or evaluated etc.

Unit-I
Conversion and Storage of Electrochemical Energy Present status of energy Consumption
Pollution problem. History of fuel cells, Direct energy conversion by electrochemical means. Maximum intrinsic efficiency of an electrochemical converter. Physical interpretation of the Carnot efficiency factor in electrochemical energy converters. Power outputs. Electrochemical Generators (Fuel Cells): Hydrogen

oxygen cells, Hydrogen Air cell, Hydrocarbon air cell, Alkane fuel cell, Phosphoric and fuel cell, direct NaOH fuel cells, applications of fuel cells.

Electrochemical Energy Storage
Properties of Electrochemical energy storage : Measure of battery performance, Charging and discharging of a battery, Storage Density, Energy Density. Classical Batteries: (i) Lead Acid (ii)Nickel-Cadmium, (iii) Zinc manganese dioxide. Modern Batteries: (i) Zinc-Air (ii) Nickel-Metal Hydride, (iii) Lithium Battery, Future Electricity storers: Storage in (i) Hydrogen, (ii) Alkali Metals, (iii) Non aqueous solutions.

Unit-II
Corrosion and Stability of Metals
Civilization and Surface mechanism of the corrosion of the metals; Thermodynamics and the stability of metals, Potential -pH (or Pourbaix) Diaphragmsl; uses and abuses, Corrosion current and corrosion potential -Evans diagrams. Measurement of corrosion rate: (i) Weight Loss method, (ii) Electrochemical Method.

Inhibiting Corrosion
Cathodic and Anodic Protection. (i) Inhibition by addition of substrates to the electrolyte environment, (ii) by charging the corroding method from external source, anodic Protection, Organic inhibitors, The fuller Story Green inhibitors.

Passivation
Structure of Passivation films, Mechanism of Passivation, Spontaneous Passivation Nature's method for stabilizing surfaces.

Unit-III
Bioelectrochemistry
bioelectrodics, Membrane Potentials, Simplistic theory, Modern theory, Electrical conductance in biological organism: Electronic, Protonic electrochemical mechanism of nervous systems, enzymes as electrodes.

Kinetic of Electrode Process
Essentials of Electrode reaction. Current Density, Overpotential, Tafel Equation, Butler Volmer equation. Standard rate constant (K) and Transfer coefficient (a), Exchange Current.

Irreversible Electrode processes
Criteria of irreversibility, informatino from irreversible wave.

Unit-IV
Methods of determining kinetic parameters for quasi-rversible and irreversible waves
Koutecky's methods, Meits Israel Method, Gellings method.

Electrocatalysis
Chemical catalysts and Electrochemical catalysts with special reference to purostates, porphyrin oxides of rare earths. Electrocatalysis in simple redox reactions, in reaction involving adsorbed species. Influence of various parameters.

Unit-V
Potential Sweep Method
Linear sweep Voltammetry, Cyclic Voltammetry, theory and applications. Diagnostic criteria of cycli voltammetry. Controlled current microelectrode techniques : comparison with controlled potentials methods, chronopotentiometry, theory ad applications.

Bulk Electrolysis Methods

Controlled potential coulometry, Controlled Coulometry, Electroorganic synthesis and its important applications. Stripping analysis : anodic and Cathodic modes, Pre electrolysis and Stripping steps, applications of Stripping Analysis.

Books Suggested

1. Modern Electrochemistry Vol. I, IIa, Vol. IIB J'OM Bockris and A.K.N. Reddy, Plenum Publication, New York.
2. Polarographic Techniques by L. Meites, Interscience.
3. "Fuel Cells : Thjeir electrochemistry". McGraw Hill Book Company, New York.
4. Modern Polarographic Methods by A.M. Bond, Marcell Dekker.
5. Polarography and allied techniques by K. Zutshi, New age International publicatin. New Delhi.
6. "Electroaalytical Chemistry by Basil H. Vessor & Galen W. ; Wiley Interscience.
7. Electroanalytical Chemistry by Basil H. Vessor & alen w. ; Wiley Interscience.
8. Topics in pure and Applied Chemistry, Ed. S. K. Rangrajan, SAEST Publication, Karaikudi (India)

COURSE OUTCOMES

- Students to understand the concept of electrochemistry and it's various theories.
- Students will be able to determine various parameters / properties using different techniques, the knowledge of which helps them to use in different fields.

SEMESTER –III
GENERIC ELECTIVE
Paper IV
MCH-506: INDUSTRIAL CHEMISTRY

COURSE OBJECTIVES

The course provides an introduction to

- Industrial Gases and Inorganic Chemicals.
- To impart basic knowledge of Petroleum Chemistry.
- To learn how to make Glasses, Ceramics and Cements.
- To learn the manufacturing of Sugar, Papers, Leathers and Fertilizers.

Unit I

Industrial Gases and Inorganic Chemicals

Industrial Gases

Large scale production, uses, storage and hazards in handling of the following gases: oxygen, nitrogen, argon, neon, helium, hydrogen, acetylene, carbon monoxide, chlorine, fluorine, sulphur dioxide and phosgene.

Inorganic Chemicals

Manufacture, application, analysis and hazards in handling the following chemicals: hydrochloric acid, nitric acid, sulphuric acid, caustic soda, common salt, borax, bleaching powder, sodium thiosulphate, hydrogen peroxide, potash alum, chrome alum, potassium dichromate and potassium permanganate.

Industrial Metallurgy

Preparation of metals (ferrous and nonferrous) and ultra pure metals for semiconductor technology.

Unit II

Fuel Chemistry

Review of energy sources (renewable and non-renewable). Classification of fuels and their calorific value.

Petroleum and Petrochemical Industry

Composition of crude petroleum, Refining and different types of petroleum products and their applications. Fractional Distillation (Principle and process), Cracking (Thermal and catalytic cracking), Reforming Petroleum and non-petroleum fuels (LPG, CNG, LNG, bio-gas, fuels derived from biomass), fuel from waste, synthetic fuels (gaseous and liquids), clean fuels. Petrochemicals: Vinyl acetate, Propylene oxide, Isoprene, Butadiene, Toluene and its derivatives Xylene.

Lubricants
Classification of lubricants, lubricating oils (conducting and non-conducting) Solid and semisolid lubricants, synthetic lubricants. Properties of lubricants (viscosity index, cloud point, pore point) and their determination.

Unit III
Silicate Industries
Glass
Glassy state and its properties, classification (silicate and non silicate glasses). Manufacture and processing of glass. Composition and properties of the following types of glasses: Soda lime glass, lead glass, armoured glass, safety glass, borosilicate glass, fluorosilicate, coloured glass, photosensitive glass.

Ceramics
Important clays and feldspar, ceramic, their types and manufacture. High technology ceramics and their applications, super conducting and semi conducting oxides, fullerenes carbon nanotubes and carbon fiber.

Cements
Classification of cement, ingredients and their role, Manufacture of cement and the setting process, quick setting cements.

Unit IV
Sugar
Intruduction , Raw materials, Manufacture of sugar from Cane sugar, Cane sugar refining, By-products from sugar industries and their uses.

Pulp & paper
Various types of Pulps, Manufacture of pulps, Papers, Polymer modified papers, Board and structural materials.

Unit V
Leather
Introduction, Animal skins, Manufacture of leather, Byproducts, Chemicals used in leather industries.

Fertilizers
Introduction, Classification, Manufacturing of; Urea, Ammonium nitrate, Normal super phosphate & Triple super phosphate.

Books Suggested

1. E. Stocchi: Industrial Chemistry, Vol-I, Ellis Horwood Ltd. UK.
2. S. S. Dara: A Textbook of Engineering Chemistry, S. Chand & Company Ltd. New Delhi.
3. A. K. De, Environmental Chemistry: New Age International Pvt, Ltd, New Delhi.
4. O. P. Vermani, A. K. Narula: Industrial Chemistry, Galgotia Publications Pvt. Ltd., New Delhi.
5. P. C. Jain, M. Jain: Engineering Chemistry, Dhanpat Rai & Sons, Delhi.
6. P. C. Jain, M. Jain: Engineering Chemistry, Dhanpat Rai & Sons, Delhi.
7. Plastic Additives Technology Hand Book: Himadri Panda, Engineers India Research Institute.
8. Chemical process principales: part 1 & II – O.A / Hougen, K.M Watson RA Ragatz (CBS).

COURSE OUTCOMES

At the completion of this course, students should be able to

- Understand the basic concepts of Industrial Gases and Fuel Chemistry.
- Understand the manufacturing of Glasses, Ceramics, Cements, Sugar, Papers, Leathers and Fertilizers.

SEMESTER –III
GENERIC ELECTIVE
Paper IV
MCH-507: Medicinal Chemistry

COURSE OBJECTIVES

The objective of this course is

- Topic of Medicinal Chemistry due to its wide applications in our daily life. Medicinal Chemistry is an important discipline at the intersection of chemistry, especially synthetic organic chemistry, and pharmacology and various other biological specialties, where they are involved with design, chemical synthesis and development for market of pharmaceutical medicines.

Unit-I

Structure and activity

Relationship between chemical structure and biological activity (SAR). Receptor Site Theory. Approaches to drug design. Introduction to combinatorial synthesis in drug discovery. Factors affecting bioactivity. QSAR-Free-Wilson analysis, Hansch analysis, relationship between Free-Wilson analysis and Hansch analysis.

Unit-II

Pharmacodynamics

Introduction, elementary treatment of enzymes stimulation, enzyme inhibition, sulfonamides, membrane active drugs, drug metabolism, xenobiotics, biotransformation, significance of drug metabolism in medicinal chemistry.

Unit-III

Antibiotics and antibacterials

Introduction, Antibiotic β-Lactam type - Penicillins, Cephalosporins, Antitubercular. Streptomycin, Broad spectrum antibiotics . Tetracyclines, Anticancer – Dactinomycin (Actinomycin D)

Unit-IV

Antifungal

Polyenes, Antibacterial - Ciprofloxacin, Norfloxacin, Antiviral . Acyclovir .

Antimalarials: Chemotherapy of malaria. SAR. Chloroquine, Chloroguanide and Mefloquine

Unit-V

Non-steroidal Anti-inflammatory Drugs

Diclofenac Sodium, Ibuprofen and Netopam.

Antihistaminic and antiasthmatic agents

Terfenadine, Cinnarizine, Salbutamol and Beclomethasone dipropionate.

Books Suggested

1. Introduction to medicinal chemistry, A. Gringuage, Wiley-VCH.
2. Wilson and Gisvold's Text Book of Organic Medicinal and Pharmaceutial Chemistry, Ed. Robert F. Dorge.
3. An Introduction to Drug Design, S.S. Pandeya and J. R. Dimmock, New Age International.
4. Burger's Medicinal Chemistry and Drug Discovery, Vol-I (Chapter 9 and Chapter 14), Ed. M.E. Wolff, John Wiley.
5. Goodman and Gilman's Pharmacoloical Basis of Therapeutics, Mc-GRaw- Hill.
6. The organic Chemistry of Drug Design and Drug Action, R.B. Silverman, Academic Press.
7. Strategies for Organic Drug Synthesis and Design, D.Ledinicer, John Wiley.
8. Principals of Medicinal Chemistry W.O. Foye.
9. Medicinal Chemistry; The role of organic chemist in Drug Research, S.M. Roberts and B. J. Pricer.

COURSE OUTCOMES

- Understand Drug metabolism and mechanism pathway.
- Recognize and comment on different synthetic strategies and methods for stereocontrol when faced with synthetic drugs.
- Understood different system of human body. Application of drug molecules.
- To learn theories and principle related to medicinal chemistry.

SEMESTER –III
PRACTICAL
(Duration: 6-8 hrs in each branch)

Inorganic Chemistry

COURSE OBJECTIVES

The students will learn

- Separation of metals using chromatographic techniques.
- Complexometric titration.
- Estimation of Ca^{2+}, Mg^{2+} and Zn^{2+} using flame photometers.

Experiment - 1	15
Experiment -2	15
Viva Voce	10
Record	10
Total	**50**

1. **Chromatographic seperations and estimation**
   (a) Paper chromatography-separation of nickel, manganese, cobalt and zinc. Determination of R_f values.
   (b) Separation and estimation of permagnate and dichromate ions by absorption chromatography.
2. **Quantitative analysis**

Estimation of metal complexes by different techniques

a. Cu-EDTA (Volumetrically)
b. Cu-NH_4CNS (Gravimetrically)
c. Ni-DMG (Gravimetrically)
d. Oxalate-$KMnO_4$ (Volumetrically)

3. **Paper chromatography**

Separation of cations by Paper Chromatography of following cations

(a) Ag(I), Pb(II) and Hg_2(II)
(b) Hg(II), Cu(II) and Pb(II)
(c) Ni(II), Co(II) and Zn(II)
(d) Ni(II), Co(II) and Cu(II)

Books Suggested

1. A handbook of Analytical Inorganic Chemistry, International Scientific Publishing Academy, India, 2005.
2. Synthesis and Characterization of Inorganic Compounds, W. L. Jolly, Prentice Hall.
3. Vogel's Textbook of Quantitative Analysis, revised, J. Bassett, R. C. Denney, G. H. Jeffery and J. Mendham, ELBS.
4. A collection of Inorganic General Chemistry Experiments, A. J. Elias, Universities Press, Sangam Books Ltd., 2002.

COURSE OUTCOMES

The students will be able to

- Separate metals using chromatographic techniques.
- Estimate metal ions complexometrically.
- Estimate metals using flame photometric.

Physical Chemistry

COURSE OBJECTIVES

To introduce experiments in chemical kinetics and equivalent conductivity.

Experiment - 1	15
Experiment -2	15
Viva Voce	10
Record	10
Total	**50**

1. **Chemical Kinetics (determination of strength of two acids)**

(a) Determination of relative strengths of HCl and H_2SO_4 (k_1 / k_2) for the hydrolysis of methyl acetate.
(b) Determination of relative strengths of HNO_3 and H_2SO_4 (k_1 / k_2) for the hydrolysis of methyl acetate.

2. **Determination of Equivalence conductance of following strong electrolyte**
   (a) KCl
   (b) NaCl
   (c) $AgNO_3$
   (d) HCl
   (e) KNO_3

Books Suggested

1. Experimental Physical Chemistry: A. M. Halpern, G. C. McBane and W. H. Freeman, A Laboratory Prescribed Book, 3rd ed., 2006.
2. Senior Practical Physical Chemistry, B. D. Khosla, R. Chand and Co., New Delhi, 2007.
3. Practical Physical Chemistry, A. M. James and F. E. Prichard, Longman.
4. Findley's Practical Physical Chemistry, B. P. Levitt, Longman.

COURSE OUTCOMES

The students will be able to

- Determine the strength of two acids.
- Determine equivalence conductance of electrolytes.
- Calculate different electrochemical parameters.

Organic Chemistry

COURSE OBJECTIVES

The students will learn

- To determine vitamin C in drugs and in fruits.
- To separate and identify the sugars from given mixtures of glucose, fructose and sucrose.
- To interpretate ^{1}H and ^{13}C NMR spectroscopy of known samples.

Experiment - 1	15
Experiment -2	15
Viva Voce	10
Record	10
Total	**50**

1. **Quantitative analysis**

Determination of vitamin C in drug formulations and in fruits.

2. **Paper Chromatography**
   Separation and identification of the sugars present in the given mixture of glucose, fructose and sucrose by paper chromatography and determination of R_F values.

3. **Interpretation of ions of ^{1}H and ^{13}C NMR spectra of known organic compounds.**

Books Suggested

1. The Systematic Identification of Organic Compounds, R. L. Shriner and D. Y. curlin.
2. A Practical text book by Singh and Yadav, Pragati Prakashan.
3. Practical Organic Chemistry, F. G. Mann and B. C. Saunders, Orient Longman.
4. Experiments and techniques in Organic Chemistry, D. Pasto, C. Johnson and M. Miller, Prentice Hall.

COURSE OUTCOMES

Students will be able

- To identify vitamin C.
- To separate and identify the sugars.
- To interpretate the NMR spectra.

SEMESTER –IV
Paper-V
MCH-508: NATURAL PRODUCT

COURSE OBJECTIVES

To provide knowledge on various natural products of biological importance.

Unit-I

Terpenoids and Carotenoids

Calcifications, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Structure determination, stereochemistry, biosynthesis and synthesis of the following representative molecules: Citral, Geraniol α-Terpeneol, Menthol, Farnesol, Zingiberence, Santonin, Phytol, Abietic acid and β-Carotene.

Unit-II

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, synthesis and biosynthesis of the following: Ephedrine, (+)- Coniine, Nicotine, Atropine, Quinine and Morphine.

Unit-III

Steroids

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

Unit-IV

Plant Pigments

Occurrence, nomenclature and general methods of structure determination. Isolation and synthesis of Apigenin, Luteolin Quercetin, Myrcetin, Quercetin 3-glucoside, Vitexin, Diadzein, Aureusin, Cyanidin-7arabinoside, Cyanidin, Hirsutidin, Biosynthesis of flavonoids: Acetate pathway and Shikimic acid pathway.

Prophyrins

Structure and synthesis of Haemoglobin and Chlorophyll.

Unit V

Prostaglandis

Occurrence, nomenclature, classification, biogenesis and physiological effects. Synthesis of PGE2 and PGF2a.

Pyrethroids and Rotenones

Synthesis and reactions of Pyrethroids and Rotenones. (For structure elucidation, emphasis is to be placed on the use of spectral parameters wherever possible).

Books Suggested

1. Natural Products : Chemistry and Biological Significance, J. Mann, R.S. Davidson, J.B. Hobbs, D.V. Banthrope adn J.B. Harbome, Longman, Esses.
2. Organic Chemistry : Vol. 2 1L. Finar, ELBS
3. Stereoselective Synthesis : A Practical Approach, M. Norgradi, VCH.
4. Rodd's Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier.
5. Chemistry, Biological and Pharmacological Properties of Medicinal Plants from the Americas, Ed. Kurt Hostettmann, M.P. Gupta and A. Marston. Harwood Academic Publishers.
6. Introduction to Flavonoids, B.A. Bohm. Harwood Academic Publishers.
7. New Trends in Natural Product chemistry, Ataaur Rahman and M.L. Choudhary, Harwood Academic Publishers.
8. Insecticides of Natural Origin, Sukh Dev, Harwood Academic Publishers.

COURSE OUTCOMES

Students will achieve insight on various natural products of biological importance.

SEMESTER –IV
Paper-VI
MCH-509: SOLID STATE CHEMISTRY

COURSE OBJECTIVES

- The students will obtain required knowledge for understanding material science problems. Initially, they will study the structure of solids and get introduced with the importance of chemical and physical bonds, crystal (dis)order and defects for materials properties.
- They will get insight into electronic structure of crystals and compare it with the electronic structure of nanomaterials – to understand the 'nano' prefix.

- The students will understand high temperature phase equilibria and learn thermodynamic and kinetic treatments of phase transitions.

Unit-I
Solid State Reactions
General principles, experimental procedure, co-precipitation as a precursor to solid state reactions, kinetics of solid state reactions.

Unit-II
Crystal Defects and Non-Stoichiometry
Perfect and imperfect crystals, intrinsic and extrinsic defects-point defects, line and plane defects, vacancies-Schottky detects and Frenkel defects. Thermodynamics of Schottky and Frenkel defect formation, colour centres, non-stoichiometry defects.

Unit-III
Electronic Properties and Band Theory
Metals insulators and semiconductors, electronic structure of solid band theory band structure of metals, insulators and semiconductors, Intrinsic and extrinsic semiconductors, doping semiconductors, p-n junctions, super conductors. Optical properties-Application of optical and electron microscopy. Magnetic Properties-Classification of materials : Effect of temperature calculation of magnetic moment, mechanism of ferro and anti ferromagnetic ordering super exchange.

Unit-IV
Organic Solids
Electrically conducting solids. organic charge transfer complex, organic metals, new superconductors.

Unit-V
Liquid Crystals:
Types of liquid crystals: Nematic, Smectic, Ferroelectric, Antiferroelectric, Various theories of LC, Liquid crystal display, New materials.

Books Suggested.

1. Solid state chemistry and its applications, A.R. West, Student Edition Wiley.
2. Principles of the Solid State, H.V. Keer, Wiley Eastern.
3. Solid State Chemistry, N.B. Hannay.
4. Solid State Chemistry, D.K. Chakrabarty, New Wiley Eastern.
5. Solid State Chemistry, S.K. Joshi and R.A. Mashelker, World Scientific, Singapore.

COURSE OUTCOMES

To obtain the knowledge on design and development of materials with pre-required properties based on understanding the structure of solids in its influence on physico-chemical properties, understanding of phase relations, chemical synthesis, reaction kinetics as well as characterization methods.

SEMESTER –IV
DISCIPLINE ELECTIVE
Paper VII
MCH-510: Analytical Chemistry

COURSE OBJECTIVES

The objective of this course is

- To study concepts and theories behind basic methods and techniques used in analytical chemistry. This theory can be used to solve many rigorous problems of universe.

- To prepare the students for further research in analytical methods of chemistry.

Unit-I

Introduction

Role of analytical chemistry Classification of analytical methods classical and instrumental. Types of instrumental analysis. Selecting an analytical method. Neatness and cleanliness. laboratory operations and practices. Analytical balance. Techniques of weighing, errors. Volumetric glassware cleaning and calibration of glassware. Sample Volumetric glassware cleaning and Calibration of glassware. Sample preparationdissolution and decompositions. Gravimetric techniques. Selecting and handling or reagents. Laboratory notebooks. Safety in the analytical laboratory.

Errors and Evaluation

Definition of terms in mean and median. Precision-standard deviation, relative standard deviation. Accuracy-absolute error, relative error. Types of error in experimental data determinate (systematic), indeterminate (or random) and gross. Sources of error and the effects upon the analytical results. Methods for reporting analytical data. Statistical evaluation of data-indeterminate errors. The uses of statistics.

Unit-II

Food analysis

Moisture, ash, crude protein, fat crude fiber, carbohydrates, calcium, potassium, sodium and phosphate. Food adulteration-common adulterants in food, contamination of foods stuffs. Microscopic examination of foods for adulterants. Pesticide analysis in food prodcuts. Extraction and purification of sample. HPLC. Gas chromatography for organophosphates. Thin-layer chromatography for identification of chlorinated pesticides in food products.

Unit-III

Analysis of Water Pollution

Origin of Waste water, types, water pollutants and their effects. Sources of water pollution-domestic, industrial, agricultural soil and radioactive wastes as sources of pollution. Objectives of analysis-parameter for analysis-colour, turbidity, total solids, conductivity, acidity, alakalinity, hardness, chloride, sulphate, fluoride, silica, phosphates and different forms of nitrogen, Heavy metal pollution-public health significance of cadmium, chromium, copper, lead, zinc, managanese, mercurry and arsenic. General survey of instrumental technique for the analysis of heavy metals in aqueous systems. Measurements of DO, BOD, and COD. Pesticides as water pollutants and analysis. Water pollution laws and standards.

Unit-IV

Analysis of soil, Fuel, Body Fluids and Drugs

Analysis of Soil, moisture pH total nitrogen, phosphorus, silica, lime, magnesia, manganese, sulphur and alkali salts.

Fuel analysis : liquid and gas. Ultimate and proximate analysis-heating valuesgrading of coal. Liquid fuels-flash point, aniline point, octane number and carbon residue. Gaseous fuels-produced gas and water gas-calorific value.

Unit-V

Clinical Chemistry and Drug analysis

Composition of blood-collection and preservation of samples. Clinical analysis. Serum electrolytes, blood glucose, blood urea nitrogen, uric acid, albumin, globulins, barbiturates, acid and alkaline phosphates. Immunoassay: principles of radio immunoassay (RIA) and applications. The blood gas analysis trace elements n the body. Narcotics and dangerous drug. Classification of drugs. Screening by gas and thin-layer chromatography and spectrophotometeric measurements.

Books Suggested

1. Analytical Chemistry, G.D. Christian, J.Wicy.
2. Fundamentals o analytical Chemistry. D.A. Skoog. D.M. West and F.J. Hooler, W.B. Saunders.

3. Analytical Chemistry-Principles. J.H. Kennedy. W.B. Saunders.
4. Analytical Chemistry-Principles and Techniques. LG. Hargis. Prentice Hall.
5. Principles of Instrumental analysis D.A. Skoog and J.L. Loary, W.B. Saunders.
6. Principles of Instrumental Analysis D.A. Skoog W.B. Saunders.
7. Quantitative Analysis, R.A. Day, Jr. and A.L. Underwood, Prentice Hall.
8. Environmental Solution, S.M. Khopkar, Wiley Eastern.
9. Basic Concepts of Analysis Chemistry, S.M. Khopkar, Wiley Eastern.
10. Handbook of Instrumental Techniques for Analytical Chemistry, F. Settle, Prentice Hall.

COURSE OUTCOMES

After studying this course the student will be able to

- Understand the basic of this course and think & develop new ideas and concepts in analytical chemistry.
- Know about electroanayltical, thermoanalytical, radiochemical, chromatographic and spectral techniques.

SEMESTER –IV
DISCIPLINE ELECTIVE
Paper VII
MCH-511: Organic Synthesis

COURSE OBJECTIVES

To provide the knowledge on

- Advances in organic synthesis- applications of selective name reactions and catalysts used in synthetic organic laboratories.
- Cover wide area of research in organic chemistry.

Unit-I

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 reaction, amine synthesis, Protection of groups, chemo region and stereo selectivity.

Unit-II

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, a-b- unsaturated carbonyl compounds, control in carbonyl condensations, 1,5-difunctionalised compounds. Micheal addition and Robinson annelation.

Unit-III

Oxidation

Introduction, Different oxidative processes. Hydrocarbons-alkenes, aromatic rings, saturated C-H groups (activated and unactivated) Alcohols, diols, aldehyde's, ketones, ketals and carboxylic acids, amines, hydrazines, and sulphides. Oxidations with ruthenium tetraoxide, iodobenzene diacetate and thallium. (III) Nitrate.

Reduction

Introduction, Different reductive processes. Alkanes, alkenes, alkynes, and aromatic rings. Carbonyl compounds-aldehydes, ketones, acids and their derivatives. Epoxides. Nitro, nitroso, azo and oxime groups. Expoxide, Nitro, Nitroso, azo and oxime groups. Hydrogenolysis.

Unit IV

Organometallic Reagents

Principle, preparations, properties and applications of the following in organic synthesis with mechanistic details. Group I and II metal organic compounds Li, Mg, Hg, Cd, Zn and Ce Compounds.

Unit V

Synthesis of some complex molecules

Application of the above in the synthesis of following compounds: Canphor, longifoline, cartisone, reserpine, vitamin D, juvabion, aphidicolin and fredericamycin. A

Books Suggested

1. Designing Organic Synthesis, S. Warren. Wiley.
2. Organic Synthesis-Concept, Methods and Starting Materials, J. Fuhrhop.
3. Some Modern Methods of Organic Synthesis. W. carruthers, Cambridge Univ. Press.
4. Modern Synthetic Reactions H.O. House, W.A Benjamin.
5. Advanced Organic Chemistry : Reactions, Mechanisms and Structure, J. March. Wiley.
6. Principles, of Organic Chemistry Part B. F.a. Carey and R.J. Sundberg, Plenum Press.

COURSE OUTCOMES

Organic synthesis– reactions and catalysts is the backbone of organic chemistry and will train students to develop ideas for further research in the field of synthetic organic chemistry.

SEMESTER –IV
DISCIPLINE ELECTIVE
Paper VII
MCH-512: Polymers

COURSE OBJECTIVES

To make the student conversant with the

- Basic concepts of polymers, molecular weight and its distribution.
- Kinetics and mechanism of Addition, Coordination and Condensation polymerization.
- Various polymerization techniques.
- Various mechanical and electrical testing methods.
- Effect of polymer structure on mechanical, electrical and optical properties.

Unit-I

Basics

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 copolymerization. Polymerization conditions and polymer reactions. Polymerization in homogeneous and heterogeneous systems.

Unit-II

Polymer Characterization

Polydispersion-average molecular weight concept. Number, weight and viscosity average molecular weights. Polydispersity and molecular weight distribution. The practical significance of molecular weight. Measurement of molecular-weights. End-group, viscosity, light scattering, osmotic and ultracentrifugation methods.

Unit-III

Analysis and testing of polymers

Chemical analysis of polymers, spectroscopic methods, X-ray diffraction study. Microscopy. Thermal analysis and physical testing-tensile strength. Fatigue, impact. Tear resistance, Hardness and abrasion resistance.

Unit-IV

Inorganic Polymers

A general survey and scope of Inorganic Polymers special characteristics, classification, homo and hetero atomic polymers. Structure, Properties and Applications of

a. Polymers based on boron-borazines, boranes and carboranes.
b. Polymers based on Silicon, silicone's polymetalloxanes and polymetallosiloxanes, silazanes.

Unit V

Structure, Properties and Application of

a. Polymers based on Phosphorous-Phosphazenes, Polyphosphates
b. Polymers based on Sulphure-Tetrasulphur tetranitride and related compounds.
c. Co-ordination and metal chelate polymers.

Books Suggested

1. Inorganic Chemistry, J.E. Huheey, Harper Row.
2. Developments in Inorganic polymer Chemistry, M.F. Lappert and G.J. Leigh.
3. Inorganic polymers- N.H. Ray.
4. Inorganic polymers, Graham and Stone.
5. Inorganic Rings and Cages : D.A. Armitage.
6. Textbook of Polymers Science, F.W. Billmeyer Jr. Wiley.
7. Contemporary Polymer Chemistry, H.R. Al cock and F.W. Lambe, Prentice Hall.

COURSE OUTCOMES

- The students will become familiar with the basic concepts of polymers, mechanism and kinetics of polymerization, polymerization techniques and molecular weight determination.
- This knowledge would help the students to synthesize polymers and mechanism involved in it.
- It will enable the students to interpret their experimental data using the characterization techniques and structure-property relationship for their final semester research project.

SEMESTER –IV
GENERIC ELECTIVE
Paper VIII
MCH-513: ENVIRONMENTAL CHEMISTRY

COURSE OBJECTIVES

Objective f this course is

- To provide the systematic study of Atmospheric and Tropospheric Photochemistry.

- To help in understanding the causes of environmental pollution and can open up new methods for environmental pollution control.
- To make the students to learn about the environmental ecosystem, waste water handling and analysis.

Unit-I

Atmospheric Chemistry

Atmospheric layers, Vertical temperature profile, heat/radiation budget of the earth atmosphere systems. Properties of troposphere, thermodynamic derivation of lapse rate. Temperature inversion. Calculation of Global mean temperature of the atmosphere. Pressure variation in atmosphere and scale height. Biogeochemical cycles of carbon, nitrogen, sulphure, phosphorus oxygen. Residence times. Sources of trace atmospheric constituents: nitrogen oxides, sulphuredioxide and other sulphure compounds, carbondioxides, chlorofluorocarbons and other halogen compounds, methane and other hydrocarbons.

Tropospheric Photochemistry

Mechanism of Photochemical decomposition of NO_2 and formation of ozone. Formation of oxygen atoms, hydroxyl, hydroperoxy and organic radicals and hydrogen peroxide. Reactions of hydroxyl radicals with methane and other organic compounds. Reaction of OH radicals with SO_2 and NO_2. Formation of Nitrate radical and its reactions. Photochemical smog meteorological conditions and chemistry of its formation.

Unit-II

Air Pollution

Air pollutants and their classifications. Aerosols-sources, size distribution and effect on visibility, climate and health.

Acid Rain

Definition, Acid rain precursors and their aqueous and gas phase atmospheric Oxidation reactions. Damaging effects on aquatic life, plants, buildings and health. Monitoring of SO_2 and NO_2. Acid rain control strategies.

Stratospheric Ozone Depletion

Mechanism of Ozone formation, Mechanism of catalytic ozone depletion, Discovery of Antarctic Ozone hole and Role of chemistry and meteorology. Control Strategies.

Green House Effect

Terrestrial and solar radiation Spectra, Major green house gases and their sources and Global warming potentials. Climate change and consequences.

Urban Air Pollution

Exhaust emissions, damaging effects of carbon monoxide. Monitoring of CO. Control strategies.

Unit-III

Aquatic Chemistry and Water Pollution

Redox chemistry in natural waters. Dissolved oxygen, biological oxygen demand, chemical oxygen demand, determination of DO, BOD and COD. Aerobic and anaerobic reactions of organic sulphure and nitrogen compounds in water acid-base chemistry of fresh water and sea water. Aluminum, nitrate and fluoride in water. Petrification. Sources of water pollution. Treatment of waste and sewage. Purification of drinking water, techniques of purification and disinfection.

Unit IV Environmental Toxicology

Toxic heavy metals

Mercury, lead, arsenic and cadmium. Causes of toxicity. Bioaccumulation, sources of heavy metals. Chemical speciation of Hg, Pb, As, and Cd. Biochemical and damaging effects.

Toxic Organic Compound
Pesticides, classification, properties and uses of organochlorine and ionospheres pesticides detection and damaging effects.

Polychlorinated biphenyls
Properties, use and environmental continuation and effects.

Polynuclear Aromatic Hydrocarbons
Source, structures and as pollutants.

Unit-V
Soil and Environmental Disasters
Soil composition, micro and macronutrients, soil pollution by fertilizers, plastic an metals. Methods of re-mediation of soil. Bhopal gas tragedy, Chernobyl, three mile island, Minimtata Disease, Sevoso (Italy), London smog.

Books Suggested

1. Environmental Chemistry, Colin Baird, W.H. Freeman Co. New York, 1998.
2. Chemistry of Atmospheres, R.P. Wayne, Oxford.
3. Environment Chemistry, A.K. De, Wiley Eastern, 2004.
4. Environmental Chemistry, S.E. Manahan, Lewis Publishers.
5. Introduction to atmospheric Chemistry, P.V. Hobbs, Cambridge.

COURSE OUTCOMES
- Students will be able to have applied understanding of Atmospheric and Tropospheric Photochemistry.
- Students understanding the principles of water and air analysis.
- The course is also useful in understanding various aspects of Environmental Toxicology and Environmental Disasters.

SEMESTER –IV
GENERIC ELECTIVE
Paper VIII
MCH-514: COMPOTER-AIDED DRUG DISCOVRY

COURSE OBJECTIVES
The objective of this course is
- To provide theoretical knowledge about the use of computer in drug discovery.
- To understand the correlation of drug activity with structure of molecules.
- To understand the statistical tools applicable in Hansch analysis and regression analysis.
- Theoretically understanding the drug interaction with receptor.

Unit I
General information about drugs
Measuring drug activity, drug absorption, lipophilicity, pharmacokinetics factors, distribution of drugs, protein binding of drugs. Rational approaches to lead Discovery based on traditional medicine random screening non random screening lead Discovery based on drug metabolism and clinical observation.

Unit II
SAR vs Quantitative Structure-Activity Relationship

History and development of USA yaar types of physical chemical parameters experimental and theoretical approaches for the determination of physical chemical parameters such as partition Coefficient and its substitution constant and taps study constant hansch analysis free Wilson analysis 3D, QSAR approaches like COMFA and COMSIA.

Unit III

Topological modeling

Molecular graphs, atom connectivity, different types of matrices: distance matrix, adjacency matrix, Deutore matrix, Randic Connectivity indices, Kier and Hall valence connectivity indices Wiener index, Path Numbers, Sz index, Sadhana index, PI index , Balaban index for simple molecules : Derivatives of Benzene, Biphenyl, Quinolines, Acridines etc.

Unit IV

Regression analysis

Statistical parameters: R, F, SE, Pogliani quality factor, testing of models, Cross validation parameters, univariate and multivariate modelling. Computer softwares for modeling, Degree of freedom, de novo constants. Outliers.

Virtual screening techniques drug like Ne screaming concept of pharmacophore mapping and pharmacophore based screening molecular Docking

Unit V

Molecular Modeling

Introduction to molecular mechanics energy minimization methods and conformational analysis Global conformational minima determination introduction to bioinformatics kemo Informatics. Introduction to bioinformatics chemoinformatics.

Books Suggested

1. Medicinal chemistry: ASHUTOSH KAR, New Age International Publishers New Age International Publishers.
2. Medicinal chemistry and drug discovery, M.E. Wolf, John Wiley and Sons, NY.
3. Burgers Med. chemistry and drug discovery 6th Edition, John Wiley, New York.
4. Qualitative Structure Activity Relationship in Drug Design Vol I,C. Hanch, Academic Press,
5. Molecular Connectivity in Chemistry and Drug Research, L.B. Kier, L.H. Hall, Academic Press. London.
6. Quantitative Aspects of Chemical Pharmacology, R.B. Barlow, Vroom Helm, London.
7. Principles of Organic Medicinal Chemistry , Ramarao, Bande ndls, New Age International P Ltd,
8. Graph Theory and Topology in Chemistry, Ed. R. B. King and D.H. Roury, Elsevier Sc. Publishers. AMSTERDAM.
9. Topological indices and Related Descriptors in QSAR and QSPR, James Defilers, CTC Press, 2000.
10. Sadhana Index in Nanotechnology, Khadi kar, Agrawal, Aziz, Lambert, Amazon.

COURSE OUTCOMES

After studying the course, the students will be able to

- Calculate various indices (Physicochemical Topological) for obtaining models for predicting the biological activities of new molecules.
- Learn the statistical methods and tools.
- Perform 3Q QSAR and docking which will help in selecting new functional groups for belle activity.
- Work in pharmacy industries for developing new drugs by way of QSAR.

SEMESTER –IV

PRACTICAL

(Duration: 6 hrs in each branch)

Inorganic Chemistry

COURSE OBJECTIVES

The students will learn

- Quantitative determination of different metal ions.
- Synthesis and characterization of metal complexes.

Experiment - 1	15
Experiment -2	15
Viva Voce	10
Record	10
Total	**50**

1. **Quantitative determinations of metal ions from three component mixture**
   One volumetrically and two gravimetrically
   (a) Cu^{+2}, Ni^{+2}, Zn^{+2}
   (b) Cu^{+2}, Ni^{+2}, Ag^{+2}
   (c) Cu^{+2}, Ni^{+2}, Ba^{+2}

2. **Synthesis and characterization of following metal complexes**
   (a) Sodium tetrathionate $Na_2S_4O_6$
   (b) Metal complex of dimethyl sulfoxide: $CuCl_2.2DMSO$
   (c) Synthesis of metal acetylacetonate
   (d) Synthesis of copper and nickel Schiff base complexes
   (e) Synthesis of copper and nickel dithiocarbamates

Books Suggested

1. Synthesis and characterization of Inorganic Compounds, W. L. Jolly, Prentice Hall.
2. A Handbook of Analytical Inorganic Chemistry, D. Sharma, International Scientific Publishing Academy, India, 2005.
3. A collection of Interesting General Chemistry Experiments, A. J. Elias, Universities Press, Sangam Books Ltd., 2002.
4. Vogel's Textbook of Quantitative Analysis, revised, J. Bassett, R. C. Denney, G. H. Jeffery and J. Mendham, ELBS.

COURSE OUTCOMES

The students will be able to

- Determine the metal ions from a three component mixture.
- Synthesis and characterize the metal complexes.

Physical Chemistry

COURSE OBJECTIVES

The students will learn

- Identification and determination of $E_{1/2}$ of compounds.
- Determination of pK value of indicators and stability of Iron complex.

Experiment - 1	15
Experiment -2	15
Viva Voce	10
Record	10
Total	**50**

1. **Electrochemistry**
   (a) Identification and estimation of metal ions such as Cd^{2+}, Pb^{2+}, Zn^{2+} and I^{2+} etc. polarographically.
   (b) Study of a metal ligand complex polarographically (using Lingane's method).

2. **Spectroscopy**
   (a) Determination of pK_a of an indicator (e.g. methyl red) in (a) aqueous and (b) micellar Media.
   (b) Determination of stoichiometry and stability constant of Ferric isothiocyanate ion complex in solution.

Books Suggested

1. Experimental Physical Chemistry, R. C. Das and B. Behera, Tata McGraw Hill.
2. Practical Physical Chemistry, A. M. James and F. E. Prichard, Longman.
3. Experimental Physical Chemistry: A Laboratory Prescribed Book, A. M. Halpern, G. C. McBane and W. H. Freeman, 3rd ed., 2006.
4. Experimental Physical Chemistry, V. D. Athawale, New Age International, 2007.

COURSE OUTCOMES

The students will be able to

- Identify and estimate the polarograms.
- Determine pK value of indicator and stability of Iron complex.

Organic Chemistry

COURSE OBJECTIVES

Students will learn

- Multistep synthesis of organic compounds.
- Isolation of compounds from natural products.

Experiment - 1	15
Experiment -2	15
Viva Voce	10
Record	10
Total	**50**

1. **Multi-step Synthesis of Organic Compounds**
   The exercise should illustrate the use of organic reagents and may involve purification of the products by chromatographic techniques. Prepreparation in steps: Benzophenone →Benzpinacol→Benzpinacolone Beckmann rearrangement : Benzanilide from benzene, Benzene →Benzophenone →Benzphenone oxime→ Benzanilide, Benzilic acid rearrangement : Benzilic acid from benzoin, Benzoin→Benzil→Benzilic acid Synthesis of heterocyclic compounds Skraup synthesis : Preparation of quinoline from aniline, Fisher Indole synthesis : Preparation of 2-phenylindole from phenylhydrazine, Enzymatic synthesis Enzymatic synthesis Enzymatic reduction : reduction of ethyl acetoacetate using Baker's yeast to yield enantiomeric excess of S (+) ehtyl-3-hydroxybutanoate and determine its optical purity. Biosynthesis of ethanol from sucrose. Synthesis using microwave Alkylation of diethyl malonate with benzyl chloride. Synthesis using phase transfer catalyst. Alkylation of diethyl malonate or ethyl acetoacetate with an alkylhalide.

2. **Isolation**
   (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 LC and PC and Rf values reported).
   (d) Isolation of nicotine dipicrate from tobacco.
   (e) Isolation of piperine from black pepper.
   (f) Isolation of lycopene from tomatoes.
   (g) Isolation of b-carotene from carrots.
   (h) Isolation of eugenol from clove.
   (i) Isolation of (+) limonine from citrus rind

Books Suggested

1. The systematic Identification of Organic Compounds, R.L. Shriner and D.Y. curlin.
2. A Practical text book by Singh and Yadav, Pragati prakashan.
3. Vogel's Textbook of Practical Organic Chemistry, ELBS.
4. Macroscale and Microscale Organic Experiments, K. L. Williamson and D. C. Heath.

COURSE OUTCOMES

Students will gain knowledge of

- Multistep organic synthesis.
- Isolation of compound from natural products.