M. Sc. CHEMISTRY SYLLABUS

Under Choice Based Credit System

(Effective from Academic Session: 2024-25)

POST GRADUATE DEPARTMENT OF CHEMISTRY
MAHARAJA SRIRAM CHANDRA BHANJA DEO UNIVERSITY
SRIRAM CHANDRA VIHAR
BARIPADA, ODISHA-757 003

MAHARAJA SRIRAM CHANDRA BHANJA DEO UNIVERSITY

COURSE STRUCTURE OF M.Sc. CHEMISTRY

Effective from Academic Session 2024-25

SEMESTER	PAPER CODE	CREDIT	FULL MARK	INTERNAL ASSESSMENT	END SEM EXAM
FIRST	CH-101	5	100	40	60
	CH-102	5	100	40	60
	CH-103	5	100	40	60
	CH-104	5	100	40	60
	CH-105 (Practical)	5	100	30	70
	CH-IKS-106 (Indian Knowledge System)	2	50	20	30
	Life Skill Course	0	50	-	50
	TOTAL	**27**	**600**	**210**	**390**
SECOND	CH-201	5	100	40	60
	CH-202	5	100	40	60
	CH-203	5	100	40	60
	CH-204	5	100	40	60
	CH-205 (Practical)	5	100	30	70
	CH-206 (Open Elective)	5	100	40	60
	TOTAL	**30**	**600**	**230**	**370**
THIRD	CH-301	5	100	40	60
	CH-302	5	100	40	60
	CH-303	5	100	40	60
	CH-304 (Practical)	5	100	30	70
	CH-305 (SWAYAM MOOCS)	3 (Minimun)	100	40	60
	TOTAL	**23**	**500**	**190**	**310**
FOURTH	CH-401	5	100	40	60
	CH-402	5	100	40	60
	CH-403 (Practical)	5	100	30	70
	CH-404 (Project)	5	100	-	100
	TOTAL	**20**	**400**	**110**	**290**
	GRAND TOTAL	**100**	**2100**	**820**	**1280**

DISTRIBUTION OF INTERNAL ASSESSMENT MARKS

Maximum marks	Quiz	Mid Term	Assignment
40	**10**	**20**	**10**

INSTUCTIONS FOR CONDUCTING INTERNAL AND END TERM EXAMINATIONS

(a) 1) 1st quiz- End of Unit-I
2) 2nd quiz- End of Unit-II
3) Midterm- End of Unit-III (Covering all three units), having 6 questions compulsory with 2 marks each from all three units and three questions of 4 marks each from which 2 to be answered covering all 3 units
4) Assignment- End of Unit-IV
5) End Term- After full course covered (Covering all five units) end term will have: 5 questions of 2 marks each which is compulsory, 4 questions to be answered out of 5 with 5 marks each and 3 questions to be answered out of 5 with 10 marks each. Each group to have one question from each unit. Questions are to be easy, little difficult and difficult type. The time duration for end term theory examination is of 03 hrs for each paper.

A: A teacher cam conducts three quizzes to consider the average of best two and also two assignments to consider the best one from among those.
B: Quizzes/Assignments can be conducted without prior notice. But a notice in general can be served to students to make them aware of quizzes without notice.

(b) 1. The questions in quizzes may be MCP but sets may be prepared for the class to avoid cheating in the class/team answering.
or The question may be with expected one-line answer
2. There shall be at least 10 questions and time should not exceed 10 minutes.

(c) The assignment should be done through class room presentation with one/two days prior information.

(d) For mid-term open book system may be adopted, provided questions encourage critical thinking or interpretation.

- The course will be attached with a lesson plan with hours of teaching for each unit and it must be provided to students at the beginning of the course preferably in the first class
- A student must know about the course and its outcome in advance

(e) 75% attendance is a must and there is no medical certificate provision. This is to be ensured as it is the statutory provision.

- A teacher needs to take the attendance within 15 minutes of the beginning of each class
- This is to ensure discipline and punctuality among students.

(f) The Marks distribution for End-Term examination of Indian Knowledge System (LKS) will be as follows-

1. 1×5 = 5 marks (All questions are compulsory)
2. 2 × 5 = 10 (02 Questions will be answered out of Five questions i.e one from each Unit)
3. 3×5 = 15 (03 Questions will be answered out of Five questions i.e one from each Unit)

PROGRAMME OUTCOMES (POs):

On completion of the programme (M.Sc. Chemistry) the students will be able to:

- Acquire conceptual knowledge and comprehensive understanding of the fundamental principles in respective discipline.
- Apply knowledge, understand and critically evaluate the concepts and scientific developments to take up any challenge towards teaching and research.
- Visualize and gain practical knowledge on multidisciplinary aspects related to current research in the fields of Chemical sciences.
- **A**cquire various skills so as to get motivated to innovate, design methods and techniques to carry out research.
- **C**ommunicate effectively, present and publish scientific ideas in Native and English language.
- Employ innovative and greener methods inculcating novel ideas to solve complex and challenging societal and environmental issues.

PROGRAMME SPECIFIC OUTCOMES (PSOS):

On completion of the specific programme, the student will be able to:

- Acquire confidence to face competitive examinations of national level like NET, GATE and capable of doing research independently. Utilize skills in problem solving, critical thinking, and analytical reasoning in chemistry.
- Enhance Skill in planning and conducting advanced level chemical experiments, elucidating the structure of compounds / complexes using chemical characterization techniques.
- Develop a creative scientific mind to communicate effectively in public forum-scientific ideas and their impact on socio-economic issues and also provide value based ethical leadership and sensitize the need for a green environment.
- Apply the knowledge of chemistry to effectively function as an individual / team leader / entrepreneur in academic field, chemical or related industries.
- Opt for two specializations namely Inorganic Chemistry and Organic Chemistry to specialize in their favorite subject.
- Opt for two supportive courses in Sem-II and Sem-III of 10 credits.

SEMESTER-I

CH – 101 (5 Credits, 60 Hrs) **Total Marks- 100 (40+60)**

***Internal Assessment Examination (40 Marks) = 20 (Written) + 10 (Quiz) + 10 (Assignment/Seminar Presentation)**

PHYSICAL CHEMISTRY-I
Marks- 60 (Theory Examination)

COURSE OUTCOMES:-

On completion of the course the student will be able to.

- Realize and appreciate the wave-particle duality at microscopic level and the need of quantum theory, the significance of wave functions, eigenfunctions, eigenvalues and uncertainties
- Learn about the qualitative results from rigid rotor, harmonic oscillator and hydrogen atom problems.
- Learn about theories to approximately calculate eigenvalues and eigenfunctions through the variational and perturbation methods and apply these methods to the helium atom.
- Learn about different types of angular momentums – orbital, spin and total angular momentum of a single particle, rules for vector addition of these angular momentums for multiparticle systems like an atom.
- Learn and apply the semiempirical method of Huckel theory to conjugated molecular systems like ethylene, butadiene, etc and calculate their bond order and charge density.
- Acquire in depth knowledge about theories of chemical kinetics and to calculate specific rate, activation energy and frequency factor
- Acquire knowledge on unimolecular reactions, kinetics of enzyme reactions and study of fast reactions by different methods.
- Study of models on electrified interfaces such as Guay Chapman model and Stern model.
- Acquire knowledge on exchange current density, able to derive Butler Volmer equation and Tafel plot.
- Acquire knowledge on corrosion, Batteries and fuel cells

UNIT–I **(12 Hrs)**

Quantum Chemistry-I: Foundations of quantum mechanics

Postulates of quantum mechanics: wave function and operators, commutation relations, construction of operators, eigen value equation, Hermitian operators, expectation value, the Schrodinger equation. Discussion of solutions of the Schrodinger equation for some model systems viz., particle in a box and the harmonic oscillator

UNIT- II **(12 Hrs)**

Quantum chemistry-II: Angular Momentum

Generalized (orbital, spin, total, rotational) angular momentum, addition of angular momentum in multi-electron systems (total L, S, spin-orbit), commutation relationships,

eigenvalues and eigenfunctions of angular momentum operators; the rigid rotor, the hydrogen atom, electron spin and the hydrogen atom, the spin-statistics theorem and antisymmetry of electronic wavefunctions, the helium atom

UNIT- III **(12 Hrs)**

Quantum chemistry-III: Approximate Methods

The variation theorem, Linear variation principle. Perturbation theory (first order and non-degenerate). Applications of variation method and perturbation theory to the Helium atom ground state.

Molecular Orbital Theory: Huckel Theory of conjugated systems, bond order and charge density calculations, Applications to ethylene, butadiene, cyclopropenyl radical.

UNIT - IV **(12 Hrs)**

Chemical Dynamics

Theories of reaction rates, collision theory of reaction, 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. homogeneous catalysis, kinetics of enzymes reactions, general features of fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis and the nuclear magnetic resonance method.

UNIT – V **(12 Hrs)**

Electrochemistry

Electrochemistry of solutions Debye -Huckel - Onsager treatment and its extension, ion solvent interactions. Deby-Huckel-Jerum mode Thermodynamics of electrified interface equations. Derivation of electro-capillarity, Lippmann equations (surface excess), methods of determination, Structure of electrified interfaces. Guay - Chapman, Stern, model. Over potentials, exchange current density, derivation of Butler Volmer equation, Tafel plot. Introduction to corrosion, Homegenous theory, forms of corrosion, corrosion monitoring and prevention methods.Batteries,primary and secondary fuel cells.

Book Recommended

1. Quantum Chemistry, Ira N.Levine, Prentice Hall
2. Molecular Quantum Mechanics, P.W. Atkins, R. Friedman, Oxford University Press
3. Introducation to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill.
4. Chemical Kinetics, K.J. Laidler, Mcgraw-Hill.
5. Kinetics and Mechanism of Chemical Transformations, J.Rajaraman & J.Kuriacose, McMillan.\.
6. Modern Electrochemistry Vol. I and Vol.ll J.O.M. Bockris and A.K.N.Reddy, Plenum.

CH – 102 (5 Credits, 60 Hrs) **Total Marks- 100 (40+60)**

***Internal Assessment Examination (40 Marks) = 20 (Written) + 10 (Quiz) + 10 (Assignment/Seminar Presentation)**

INORGANIC CHEMISTRY-I
Marks- 60 (Theory Examination)

COURSE OUTCOMES:

On completion of the course the student will be able to

- Discuss the kinetic applications of CFT and valence bond theory; describe the stability of metal complexes in terms of formation constant.
- Able to determine the binary formation constant by pH metry, spectrophotometry and Job;s method of continuous variation.
- Demonstrate detailed functional knowledge about the symmetry, bonding in octahedral and tetrahedral systems, spin orbit coupling and derive term symbols of free ions.
- Understand electronic transitions in metal complexes. interpret the spectra of coordination complexes and learn charge transfer spectra.
- Understand the angular overlap model to estimate amount of interaction takes place between metal d orbitals and ligand orbitals.
- Gain knowledge about the bonding of metal carbonyls, nitrosyls, dinitrogens and metal dioxygen complexes.

UNIT – I **(12 Hrs)**

Reactivity of metal complexes

Energy of a reaction, theromodaynamic and kinetic stability of metal complexes, kinetic applications of valence bond and crystal field theories.

Metal-Ligand Equilibria in Solution

Stepwise and overall formation constants and their interrelation, trends in stepwise constants, factors affecting the stability of metal complexes with reference to nature of metal ion and ligand, chelate effect and its thermodynamic origin, determination of binary formation constants by pH-metry, spectrophotometry, Job's method of continuous variation.

UNIT – II **(12 Hrs)**

Symmetry and Group Theory in Chemistry

Symmetry elements and symmetry operation, definitions of group, subgroup, relation between orders of a finite group and its subgroup. Conjugacy relation and classes. Point symmetry group. Schonflies symbols, representations of groups by matrices (representation for the C_n, C_{nv}, C_{nh}, D_{nh}, etc.groups to be worked out explicitly). Character of a representation. The great orthogonality theorem (without proof) and its importance. Character tables and their use:

UNIT – III **(12 Hrs)**

Electronic Spectra and Magnetic Properties of Transition Metal Complexes

Spectroscopic ground states, correlation, Orgel and Tanabe-Sugano diagrams for transition metals complexes (d^1 to d^9 states), calculations of Dq, B and β parametres, charge transfer spectra, spectroscopic method of assignment of absolute configuration in optically active, metal chelates and their sterochemical information, anomalous magnetic moments, magnetic exchange coupling and spin crossover.

UNIT – IV **(12 Hrs)**

Metal - Ligand Bonding

Limitations of crystal field theory, molecular orbital theory: sigma bonding and energy level diagram in octahedral, tetrahedral and square planar complexes; p-bonding and energy level diagram in octahedral complexes, angular overlap model.

UNIT – V **(12 Hrs)**

Metal π- Complexes

Metal carbonyls, structure and bonding, vibrational, spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls; preparation, bonding, structure and important reactions of transition metal nitrosyl, dinitrogen and dioxygen complexes; tertiary phosphine as ligand.

Books Recommended:

1. Advanced Inorganic Chemistry, Cotton and Wilkinson, John Wiley
2. Inorganic Chemistry, J.E. Huheey, Ellel A. Keiter, Richard L. Keiter & Okhil K.Medhi
3. Inorganic Chemistry, Gary L. Miessler and Donald A. Tarr
4. Symmetry and Spectroscopy of Molecules, K.V, Reddy
5. Chemical Application of Group Theory, F.A. Cotton

CH – 103 (5 Credits, 60 Hrs) **Total Marks- 100 (40+60)**

***Internal Assessment Examination (40 Marks) = 20 (Written) + 10 (Quiz) + 10 (Assignment/Seminar Presentation)**

ORGANIC CHEMISTRY-I

Marks- 60 (Theory Examination)

COURSE OUTCOMES:

On completion of the course the student will be able to.

- Ensures the students to understand and acquire knowledge on topicity and asymmetric synthesis.
- Demonstrate chirality in organic molecules using units such as center, axial, planar and helicity.

- Illustrate the reaction mechanism aspects in the context of addition, elimination and substitution reaction.
- Assess the structural effects of organic molecules and functional groups on the tendency to participate in various types of organic reactions.
- Describe the methods of asymmetric synthesis which involve chiral substrate, chiral reagents, chiral auxiliary and chiral catalyst.
- Understand the mechanism of enzyme catalyzed reactions

UNIT – I **(12 Hrs)**

Stereochemistry, Structure and reactivity

Conformational analysis of decalins, effect of conformation on reactivity. Elements of symmetry, chirality, molecules with more than one chiral center, threo and erythro isomers, optical purity, enantioptic and diasterotopic atoms, groups and faces, stereospecific and steroselective synthesis. Asymmetric synthesis. Optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape. thermodynamic and kinetic requirements, kinetic and thermodynamic control, Curtin-Hammett principle, methods of determining mechanisms, isotope effects.

UNIT – II **(12 Hrs)**

Nucleophilic Substitution Reactions

The S_N2, S_N1, mixed S_N1 and S_N2 mechanisms. The neighbouring group mechanism, neighbouring group participation by Pi and sigma bonds, anchimeric assistance. Classical and non-classical carbocations, phenonium ions, norbornyl system, common carbocations rearrangements.

Substitution at an allylic, aliphatic trigonal ,vinylic carbon.

Substitution on aromatic substrates. Mechanism, reactivity, effects of substrate structure, attacking nucleophile, leaving group and reaction medium, The von Richter, Sommelet-hauser, and smiles rearrangements.

UNIT – III **(12 Hrs)**

Electrophilic Substitution Reaction

Bimolecular mechanisms on aliphatic substrates - The S_E1, S_E2 and S_Ei. Mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity.

Substitution on aromatic substrates-the arenium ion mechanism, orientation and reactivity, Quantitative treatment on reactivity in substrates and electrophiles. Diazonium coupling, Vilsmer reaction, Gattermann-Koch reaction.

UNIT - IV **(12 Hrs)**

Addition and Elimination Reaction

Addition to cyclopropane ring. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydrocarbonylation. Michael reaction. Sharpless asymmetric epoxidation.

Mechanism of metal Hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents, organo zinic and organolithium reagents to carbonyl and unsaturated carbonyl compounds. Witting reaction.

The E_2, E_1 and E_1CB mechanisms and their spectrum, Orientation of the double bond. Reactivity - effect of substrate structures, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination.

UNIT - V **(12 Hrs)**

Free Radical Reactions

Types of free radicals, 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, effect of solvent on reactivity

Allylic halogenations (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts, Sandmayer reaction, free radical rearrangement, Hunsdicker reaction.

Books Recommended:

1. Smith, M. B., March J., (Latest Ed.). March's Advanced Organic Chemistry, John Wiley and Sons, 6th edition, New York.
2. Carey B. F. A., Sundberg R.J., (2007). Advanced Organic Chemistry Part A and Part B, Springer, 5th edition.
3. Kalsi, P.S., (2010). Stereochemistry: Conformation and Mechanism, New Age International (p) Ltd. New Delhi.
4. Morrison, R.T., Boyd, R.N. (2011). Organic Chemistry, Prentice- Hall of India, 6th edition, New Delhi.
5. Sykes, P., (1997). A Guide Book to Mechanism in Organic Chemistry, Prentice Hall, 6th edition.
6. Nasipuri, D. (Latest edition). Stereochemistry of Organic Compounds: Principles & Applications, New Age International Publishers.
7. Structure and Mechanism in Organic Chemistry, C. K. Ingold, Cornell University Press.
8. McMurry J., Organic Chemistry, Asian Book Pvt. Ltd, 8th edition, New Delhi.
9. Bruice Paula, Y., (2015). Organic Chemistry, 7th Edition, Pearson Edition.

10. Lowry, T. H. & Richardson, K. S. Mechanism and Theory in Organic Chemistry Addison-Wesley Educational Publishers, Inc. (1981).
11. Principles of Organic Synthesis, R.O.C., Norman and J.M. Coxon, Blackie Academic & Professional.
12. P.S.Kalsi, Sterochemistry, conformation and mechanism, 7thWiley Eastern Ltd., Chennai
13. Clayden, J.; Greeves, N.; Warren, S., (2012). Organic Chemistry, Oxford University press, 2nd edition.

CH – 104 (5 Credits, 60 Hrs) **Total Marks- 100 (40+60)**

***Internal Assessment Examination (40 Marks) = 20 (Written) + 10 (Quiz) + 10 (Assignment/Seminar Presentation)**

POLYMER CHEMISTRY

Marks- 60 (Theory Examination)

COURSE OUTCOMES:-

On completion of the course the student will be able to

- Acquire knowledge on basics of polymers and various polymerization processes.
- Characterize the polymers with respect to their molecular weight, viscosity and disparity.
- Measure molecular weight by different methods.
- Acquire knowledge on crystalline structure and various properties like melting point,chain flexibility of the polymers.
- Acquire knowledge on various applications of commercial polymers, electrically conducting polymers and biomedical polymers.

UNIT – I (12 Hrs)

Basics

Importance of Polymers. Basic concepts. Monomers, repeat units, degree of polymerization, Linear, branched and network polymers. Classification of Polymers. Polymers. Polymerization : condensation, addition, radical chain-ionic and co-ordination and Co-polymerization. Polymerization conditions and polymer reactions. Polymerization in homogeneous and heterogeneous systems.

UNIT - II (12 Hrs)

Polymer Characterization

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

UNIT – III **(12 Hrs)**

Structure and Properties.

Morphology and order in crystalline polymers-configurations of polymer chains. Crystal structures of polymers. Morphology of polymers. Morphology of crystalline polymers, strain-induced morphology, crystallization and melting. Polymer structure and Physical properties-crystalline melting point, Tm-melting points of homogeneous series, effect of chain flexibility and other steric factors, entropy and heat of fusion. The glass transition temperature, Tg-Relationship between Tm and Tg, effects of molecular weight, diluents, chemical structure, branching and cross linking.

UNIT – IV **(12 Hrs)**

Polumer Processing

Compounding and processing techniques: Calendaring, rotational casting, film casting, injection moulding, blow moulding, extrusion moulding, thermoforming, foaming

UNIT – V **(12 Hrs)**

Properties of Commercial Polymers

Polythylene, polyvinyl chloride, polyamides, polyesters, phenolic resins, epoxy resins , electrically conducting polymers. Biomedical polymers - contact lens, dental polymers, artificial heart kidney, skin and blood cells.

Books Recommended:

1. Text book of Polymer Science, F.W. Billmeyer Jr. Wiley.
2. Polymer Science, V.R. Gowariker, N.V. Viswanathan and J.Sreedhar. Wiley-Eastern.
3. Functional Monomers and Polymers, K.Takemoto.Y.Inaki and R. M. Ottanbrite.
4. Contemporary Polymer Chemistry, H.R.Alcock and F.W.Lambe, Prentice Hall.

CH-105 (5 Credits, 60 Hrs) **Marks-100 (30+70)**

INORGANIC GENERAL PRACTICAL

COURES OUTCOMES:

On completion of the course the student will be able to

- Prepare coordination complexes.
- Estimate amount of Fe and Cu in a mixture solutions of both.
- Estimate amount of Zn and Cu in a mixture solutions of both.
- Identify the unknown radicals present in a inorganic mixture.

1. Qualitative analysis

Analysis of Inorganic salt mixtures containing not more than six radicals (organic acid radicals should be excluded). One of the following rare metal ions like Mo, W, Ti, V and insoluble like TiO_2, $BaSO_4$ etc. may be included.

2. Quantitative Analysis

Separation and determination of two metal ions like Cu-Fe, Zn-Cu, Ni-Zn, Cu-Ni etc. involving volumetric and gravimetric methods.

3. Preparations

Preparation of some selected inorganic compounds and handing of air and moisture sensitive compounds.

(i) $Mn(acac)_3$
(ii) $[Ni(NH_3)_6]Cl_2$
(iii) $K_3[Fe(C_2O4)_3]$
(iv) $Ni(dmg)_2$
(v) *Cis* - $K[Cr(C_2O_4)_2(H_2O)_2]$

Books recommended:

1. A Text book of Qualitative Analysis, A. I. Vogel
2. A Text book of Quantitative Analysis, A. I. Vogel
3. Inorganic synthesis, Vol. 1-20

CH-IKS-106 (2 Credits, 24 Hrs) Total Marks- 50 (20+30)

***Internal Assessment Examination (20 Marks)**

INDIAN KNOWLEDGE SYSTEM

COURSE OUTCOMES:

On completion of the course the student will be able to

- Chemical science of ancient India
- Use of Chemical entity in ancient India

UNIT-I **(5 Hrs)**

Chemistry in Ancient Indian Science

Vatsyana (4^{th} to 6^{th} Century CE), Nagarjuna (7^{th} to 8^{th} Century CE), AI-Biruni's India (11^{th} Century), Rasannavakalpa (11^{th} Century), Vagbhata (13^{th} Century), Qualities of a teacher of Rasasastra, Location and building of rasasala, working arrangement of rasasala according to direction, material and equipment.

UNIT-II **(4 Hrs)**

Vaisesika and Chemistry

Classification of matter by Vaisesika, Padaartha, Dravya:Guna, Karma, Samanya, Visesa and Samavaya, Muni Kanada: Abhava, Anu, Kanada, Dharma.

UNIT-III **(5 Hrs)**

Theory of Atomic Combinations

Chemical combinations, Mono and hetero bhautika compounds, Theory of dynamic contact (Viśtambha), Chemical action and heat, Three axes of Vācaspati (graphical representation of constitution of a bibhautika compound), Conception of molecular motion (parispanda).

UNIT-IV **(5 Hrs)**

Ancient Indian Chemist and Chemical Entity

Kanad, Nagarjuna, Susruta, Kautilya, Chakrapani, Varahamihira, Acharya Prafulla Chandra Ray, Ancient Chemical Compounds (Dyes, Pigment, Cosmetics, Soap, Perfumes, Ink, Alcohols, Liquor) Use of Chemical compounds by Ancient Indian People (Iron, Dyes and Colour, Symmetry, Traditional medicines).

UNIT-V **(5 Hrs)**

Metals and Metallurgical Heritage

Arthaśāstra as the earliest text describing gold, silver and other metals. Processing of gold, silver, copper, iron tin, mercury, lead and Zinc as mentioned in Rasārnava and Rasaratnasamukāyā, Use of Au, Hg, Ag, Cu, and Fe as therapy in ancient India

LIFE SKILL COURSE

Total Marks- 50

Common Course for Semester-I Students

SEMESTER - II

CH – 201 (5 Credits, 60 Hrs) **Total Marks- 100 (40+60)**

***Internal Assessment Examination (40 Marks) = 20 (Written) + 10 (Quiz) + 10 (Assignment/Seminar Presentation)**

FUNDAMENTALS OF ANALYTICAL CHEMISTRY

Marks- 60 (Theory Examination)

COURSE OUTCOMES:

On completion of the course the student will be able to

- Know about classification and selection of analytical methods, errors, accuracy, precision, mean, deviation and sampling.
- Know about Thermo gravimetric analysis (TGA), Differential Thermal analysis(DTA), Ion Chromatography and High performance liquid chromatography(HPLC).
- Know about voltametry, polarography, amperometry, coulometry, conductometry and ion selective electrode.
- Acquire knowledge about Atomic absorption spectroscopy (AAS), Flame photometry and Nephelometric methods.

UNIT-I **(12 Hrs)**

Introduction

Role of analytical chemistry, classification of analytical methods: classical and instrumental, types of instrumental analysis, selection of analytical methods. Errors in analytical chemistry, classification of errors, source and minimization of errors, absolute and relative error, accuracy and precision, significant figures, mean value and deviation, average and standard deviation, median value, range, confidence intervals. Sampling in analysis: Definition, theory of sampling, technique of sampling, statistical criteria of good sampling, stratified sampling, transmission and storage of samples.

UNIT-II **(12 Hrs)**

Solvent Extraction and ion exchange

Solvent Extraction: Principles, classification of extraction, mechanism of extraction, extraction equilibria, techniques of extraction, application in analytical chemistry.

Basic principles and applications of ion chromatograph and high performance liquid chromatography.

UNIT-III **(12 Hrs)**

Thermal analysis

Thermogravimetric analysis (TGA): Instrumentation, derivative thermo gravimetric analysis (DTG), application of theromogravimetry. Differential Thermal Analysis (DTA): Instrumentation and application of differential thermal analysis simultaneous TG-DTA curves. Thermogravimetric titration: Principle and applications.

UNIT-IV **(12 Hrs)**

Electroanalytical methods

Classification of electroanalytical methods, principles and applications of voltammetry, cyclic voltammetry, anodic stripping voltammetry, polarography, amperometry, coulometry, conductometry and ion selective electrodes. (Extensive instrumentations are to be excluded).

UNIT-V **(12 Hrs)**

Spectroscopic methods

Atomic adsorption spectroscopy: Principle and instrumentation, flame atomization, hollow cathode lamps, application of AAS in qualitative and quantitative analysis.

Flame photometric methods: Basic principle and instrumentation, interference in flame photometry, applications in quantitative analysis

Books recommended:

1. Analytical Chemistry, Gary D. Christian, 6th Edition, Wiley publication
2. Basic concepts of Analytical Chemistry, S. M. Khoopkar, New Age publication

3. Instrumental Methods of Chemical Analysis, H Kaur, Prati Prakashan
4. Analytical Chemistry, An Indian Adaptation, Gary D. Christian, Purnendu K. Dasgupta, Kevin A. Schug, Wiley India
5. Essentials of Analytical Chemistry, Ramakrishnan Shobha, Mukhopadhyay Banani, Pearson
6. Analytical Chemistry, C. Krupadanam, G.L.D. Vijaya Prasad, D. Varaprasad Rao, K. Reddy, K.L.N. Sudhakar, University Press

CH – 202 (5 Credits, 60 Hrs) **Total Marks- 100 (40+60)**

***Internal Assessment Examination (40 Marks) = 20 (Written) + 10 (Quiz) + 10 (Assignment/Seminar Presentation)**

ORGANIC CHEMISTRY-II

Marks- 60 (Theory Examination)

COURSE OUTCOMES:

On completion of the course the student will be able to

- Predict and formulate the outcomes of pericyclic reactions in terms of orbital interactions and/or the Woodward-Hoffmann Rules & FMO approach of concerted reactions: Electrocyclic reactions, cycloadditions and sigmatropic rearrangements.
- Gain advanced knowledge on interaction of radiation with matter, principles of photochemistry and its applications.
- Understand the basic principles of light-matter interactions and principles of photochemistry.
- Demonstrate the difference between radiative and non-radiative transitions with the help of Jablonski diagram.
- Identify the mechanism of various photochemical reactions of alkenes, carbonyl compounds and aromatic compounds, and able to compare direct photolysis and sensitized photolysis reactions.
- Understand the mechanism of selected photochemical process.
- Understand the principles of molecular recognition and topological aspects of molecular receptors.
- Understand the principles of biomimetic chemistry involving crown ethers, cyclodextrin and calixarenes merged with catalysis.

UNIT – I **(12 Hrs)**

Pericyclic Reactions

Molecular orbital symmetry, frontier orbitals of ethylene, 1,3- butadiene, 1,3,5 - hexatriene. Classification of pericyclic reactions. Woodward - Hoffmann correlation diagrams. FMO approach. Electrocyclic reactions- conrotatory - antrafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3 dipolar cycloadditions. Sigmatropic rearrangements - suprafacial and antrafacial shifts of H,

Sigmatropic shifts involving carbon moieties, 3,3 - and 5,5 - Sigmatropic rearrangements, Claisen, Cope and aza- Cope and Ene reaction.

UNIT-II **(12 Hrs)**

(a) Photochemical Reactions

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

(b) Photochemistry of Alkenes

Intramolecular reactions of the olefinic bond - geometrical isomerism, cyclisation reactions, rearrangement of 1,4- and 1.5 - dienes.

(c) Photochemistry of Carbonyl Compounds

Intramolecular reactions of carbonyl compounds - saturated, cyclic and acyclic, β,γ- unsaturated and α, β, - unsaturated compounds. cyclohexadienones.

UNIT – III **(12 Hrs)**

Photochemistry of Aromatic Compounds

Isomerisations, additions and substitutions.

Miscellaneous Photochemical Reactions

Photo-Fries reactions of anilides. Photo-Fries rearrangement. Barton reaction. Singlet molecular oxygen reactions. Photochemical formation of smog. Photodegradation of polymers. Photochemistry of vision

UNIT - IV **(12 Hrs)**

Co-Enzyme Chemistry

Cofactors as derived from coenzymes, prosthetic groups, apoenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD^+, $NADP^+$, FMN, FAD, Mechanisms of reactions catalyzed by the above cofactors.

UNIT – V **(12 Hrs)**

Enzyme Models

Host-guest chemistry, chiral recognition and catalysis, molecular recognition, molecular asymmetry and prochirality. Biomimetic chemistry, crownethers, cryptates. Cyclodextrins, cyclodextrin based enzymes models, calixarenes

Book Recommended:

1. Carey B. F. A., Sundberg R.J., (2007). Advanced Organic Chemistry Part A and Part B, Springer, 5th edition.
2. Sankaraman, S. (2005). Pericyclic reactions: Reactions, Applications and Theory, Wiley-VCH.

3. Halton, B.; Coxon J. M. (2011), Organic Photochemistry, Cambridge University Press.
4. Photochemistry & Pericyclic Reactions, Jagdamba Singh & Jaya Singh, New Age International Publishers, Third edition 2012.
5. Dr. Satyajit Dey Dr. Nirmal Kr. Hazra, Through Solved Problems, Techno World Publishers, 2019
6. Fleming, I., Pericyclic Reactions, Oxford Science Publications (1998).
7. Horspool, W. M. Aspects of Organic Photochemistry Academic Press (1976).
8. Fundamentals of Photochemistry, K.K. Rohtagi-Mukherji, Wiley-Eastern limited
9. Essentials of Molecular Photochemistry, A.Gilberi and J.Baggorr, Blackwell Scientific Publication.
10. Molecular Photochemistry, N. J. Turro, W. A. Benjamin..
11. Introductory Photochemistry, A Cox and T.Camp McGraw-Hill.

CH – 203 (5 Credits, 60 Hrs) **Total Marks- 100 (40+60)**

***Internal Assessment Examination (40 Marks) = 20 (Written) + 10 (Quiz) + 10 (Assignment/Seminar Presentation)**

INORGANIC CHEMISTRY-II

Marks- 60 (Theory Examination)

COURSE OUTCOMES:

On completion of the course the student will be able to

- Learn structure, bonding, stablility and reactivity of simple boranes, carboranes and metallo carboranes.
- Explain structural aspects of metallic clusters and polyanions of important compounds
- Explain different types of electron transfer reactions and factors governing them.
- Evaluate and gain knowledge on various mechanism of substitution reactions in coordination complexes.
- Know about ionophores,metal ion transport and storage protein like ferritine,transferrin and siderophores.
- Aquire knowledge on various metalloenzymes, metalcomplexes in transmission of energy, metalloproteins in electron transport processes and on biological nitrogen fixation.

UNIT - I **(12 Hrs)**

Reaction Mechanism of Transition Complexes

Substitution reactions of octahedral complexes: acid hydrolysis, factors affecting acid hydrolysis; base hydrolysis, conjugate base mechanism, direct and indirect evidences in favour of conjugate mechanism; anation reactions, reactions without metal ligand bond cleavage. Substitution reactions in square planar complexes: the trans effect and its

application to synthesis of complexes, theories of trans effect, mechanism of substitution reaction and the factors affecting the substitution reactions.
Redox reactions: Outer-sphere reactions, Marcus theory for outer-sphere reaction, inner sphere reactions.

UNIT – II **(12 Hrs)**

Inorganic ring, cage and cluster compounds

Higher boranes, carboranes, metalloboranes and metallocarboranes, Metal carbonyl and halide clusters, compounds with metal-metal multiple bonds.

UNIT – III **(12 Hrs)**

Metal ions in Biological Systems

Essential and trace metals, role of alkali and alkaline earth metals, Inophores, Na^+-K^+ Pump, Transport of ions and its mechanism, Calcium in living cells and its transport & regulation
Metal ion transport and storage: Ferritin, Transferrin, Siderophores.

UNIT-IV **(12 Hrs)**

Bioenergetics and ATP Cycle

Metal complexes in transmission of energy; chlorophylls, photosystem-I and photosystem-II in cleavage of water. ATP as a energy currency in biological system .

(c) Metalloenzymes

Carbonic anhydrase, carboxypeptidase and vitamin B_{12}.

UNIT – V **(12 Hrs)**

Electron Transfer in Biology

Structure and function of metalloproteins in electron transport processes- cytochromes and ferrodoxin

Nitrogenase

Biological nitrogen fixation, molybdenum nitrogenase, spectroscopic and other evidences.

Books Recommended:

1. Principles of Bioinorganic Chemistry, S. J. Lippard and J. M. Berg, University Science Books.
2. Bioinorganic Chemistry, I Bertini, H.B.Gray, S.J.Lippard and J.S Valentine, University Science Books.
3. Inorganic Chemistry, J.E. Huheey, Ellel A. Keiter, Richard L. Keiter & Okhil K.Medhi.
4. Inorganic Chemistry, Gary L. Miessler and Donald A. Tarr
5. Bioinorganic Chemistry. Asim K. Das
6. Hughes, M. N. The Inorganic Chemistry of Biological Processes, 2nd Ed., Wiley

(1981).
7. Lippard, S. J. & Berg, J. M. Principles of Bioinorganic Chemistry Univ. Science Books (1994).
8. Lippard, S. J. Progress in Inorganic Chemistry Vols. 18 and 38, Wiley-Interscience (1991).

CH – 204 (5 Credits, 60 Hrs) **Total Marks- 100 (40+60)**

***Internal Assessment Examination (40 Marks) = 20 (Written) + 10 (Quiz) + 10 (Assignment/Seminar Presentation)**

SPECTROSCOPY-I

Marks- 60 (Theory Examination)

COURSE OUTCOMES:

On completion of the course the student will be able to

- Familiarize themselves about the basic elements of practical spectroscopy such as components of a spectrometer, resolving power and signal to noise ratio.
- Learn about microwave activity of different types of molecules. Gain in-depth knowledge on rotational spectra of diatomic molecules using both rigid rotor and non-rigid rotor models. Apply these concepts to calculate different molecular properties.
- Get detailed insight into the infrared spectra of diatomic molecules by treating them using both harmonic and anharmonic oscillator model. Apply these concepts to calculate different molecular properties.
- Learn about Raman activity of molecules using the polarizability ellipsoids, analyze the rotational and vibrational bands in Raman spectra.
- Learn about the coarse spectra of hydrogen-like species, learn about their spectral fine structure. Learn about the term symbols in multi-electron atoms, and about the spectra of helium and alkaline earth metals.
- Understand the molecular spectra at dissociation and predissociation limits. Apply these concepts to understand the spectrum of the simplest molecule, H_2.
- Learn about the basic principles of photoelectron spectroscopy and apply to study spectra of simple molecules.
- Learn about the basic principles of spin resonance spectroscopy of NMR and ESR. Learn to explain NMR spectra through chemical shift and coupling of nuclear spins. Learn about the g-factor, electron-nucleus coupling and hyperfine structure.

UNIT – I (12 Hrs)

Introduction: Characterization of electromagnetic radiation, quantization of energy, regions of the spectrum, mechanism of light and mater interaction, representation of the spectra,

components of a spectrometer, signal-to-noise ratio and resolving power, width and intensity of spectral transitions, Fourier transform spectroscopy

Microwave Spectroscopy: Classification of molecules, rotational energy levels of rigid diatomic molecule, intensities of spectral lines, effect of isotopic substitution, the non-rigid rotator

UNIT – II **(12 Hrs)**

Infrared Spectroscopy: Vibrational energies of diatomic molecules: simple harmonic oscillator, force constant and bond strengths, anharmonicity and Morse potential energy function, Vibration-rotation spectroscopy, selection rules, P, Q, R branches, breakdown of Born-Oppenheimer approximation, vibration of polyatomic molecules, normal modes of vibration, group frequencies, overtone and combination frequencies, influence of nuclear spin

UNIT– III **(12 Hrs)**

Raman Spectroscopy: Classical and quantum theories of Raman effect, polarizability and Raman activity of vibrations, mutual exclusion principle, pure rotational and vibrational Raman spectra, selection rules, rotational fine structure

Atomic Spectroscopy: Brief discussion of atomic structure, Hydrogen atom spectrum, spin-orbit coupling and fine structure of Hydrogen atom spectrum, spectra of Hydrogen-like species and alkali metals, many electron atoms, Term symbols, spectrum of Helium and alkaline earths.

UNIT – IV **(12 Hrs)**

Molecular Spectroscopy: Born-Oppenheimer approximation, Intensities of vibronic transitions, Frank-Condon principle, dissociation and predissociation of molecules, molecular orbitals, molecular term symbols, selection rules, spectrum of Hydrogen molecule, re-emission of energy by excited molecule: radiative and non-radiative decay

Photoelectron Spectroscopy: Basic principles, photoelectric effect, ionization process of atoms and molecules, Koopman's theorem, Auger electron spectroscopy- basic idea.

UNIT – V **(12 Hrs)**

Introduction to Spin Resonance Spectroscopy

Nuclear and electronic spin, interaction between spin and magnetic field, Larmor precession and nuclear magnetic resonance (NMR) and electron spin resonance (ESR), population of energy levels, relaxation time and width of signal, NMR spectroscopy: the chemical shift and coupling constant, coupling between several nuclei and the multiplet structure; ESR

spectroscopy: the g factor, electron-nucleus coupling and hyperfine structure of ESR, McConnel equation and electron density distribution, application to methyl and benzene radical

Books Recommended

1. Fundamentals of molecular spectroscopy, C.N Banwell and E. M. McCash
2. Modern Spectroscopy, J.M. Hollas, John Wiley
3. Introduction to molecular spectroscopy, G .M Barrow
4. Introduction to photoelectron spectroscopy, P.K Ghosh
5. Atomic structure and chemical Bonding including molecular spectroscopy, Manas Chandra
6. Applied Electron Spectroscopy for Chemical Analysis Ed. H. Windawi and F.L. Ho, Wiley interscience

CH – 205 (5 Credits, 60 Hrs) **Marks-100 (30+70)**

PHYSICAL GENERAL PRACTICAL

COURSE OUTCOMES:-

On completion of the course the student will be able to

- Determine the rate constant of acid catalysed hydrolysis of ethyl acetate by volumetric titration method.
- Determine the rate constant of base-catalysed hydrolysis of ethyl acetate - by volumetric titration method.
- Conductometric titration of a mixture of HCL + CH_3COOH against NaOH.
- Potentiometric titration of a strong acid vs strong base.
- Determine the rate constant of Inversion of cane sugar by polarimetry method and concentration of unknown sugar.
- Verification of Beer-Lambert's law and determination of extinction coefficient

CHEMICAL KINETICS

1. To determine the rate constant of acid catalysed hydrolysis of ethyl acetate by volumetric titration method.
2. To determine the rate constant of base-catalysed hydrolysis of ethyl acetate - by volumetric titration method.
3. To determine the bimolecular rate constant of the oxidation of iodide ions by hydrogen peroxide in aqueous medium.

HETEROGENEOUS EQUILIBRIA

1. To determine the partition coefficient of iodide between carbon tetrachloride and water.

2. To determine the equilibrium constant of the tri-iodide formation $I_2 + I^- \rightleftharpoons I_3^-$ in aqueous solution.

CONDUCTOMETRY:

1. Conductometric titration of a mixture of HCL + CH_3COOH against NaOH.
2. To detrmine the rate constant of saponification of ethyl acetate - conductometrically
3. To determine the ionizatiion constant of weak acid.

POTENTIOMETRY

1. Potentiometric titration of a strong acid vs strong base.
2. Solubility product of a sparingly soluble salt.

POLARIMETER

1. To determine the rate constant of Inversion of cane sugar in acid medium.
2. To determine the concentration of unknown sugar.

SPECTROPHOTOMETER

1. Verification of Beer-Lambert's law.

Book Recommended:

1. Experimental Physical Chemistry by R.C. Das and B. Behera, Tata, Mc Graw Hill.

CH – 206 (5 Credits, 60 Hrs) **Total Marks- 100 (40+60)**

***Internal Assessment Examination (40 Marks) = 20 (Written) + 10 (Quiz) + 10 (Assignment/Seminar Presentation)**

GENERAL ENVIRONMENTAL CHEMISTRY

Marks- 60 (Theory Examination)

COURSE OUTCOMES:

On completion of the course the student will be able to

- Understand the scope of environmental chemistry and its basic terminology.
- Understand ozone destruction, green-house effect, global warming and El-Nino effects.
- Understand sources, classification and monitoring of air pollution.
- Able to identify water pollutants and understand water quality parameters.
- Understand phenomenon like acid rain, photochemical smog.
- Understand air quality standards.

- Identify effect of metals and other toxic pollutants and their biochemical effects.
- Understand the phenomenon of Bioaccumulation and biomagnifications.
- Outline the principles of green chemistry and its industrial applications.
- Understand application of green chemistry in sustainable development.

UNIT - I **(12 Hrs)**

Introduction to Environmental Chemistry

Concept and scope of environmental chemistry, Environmental terminology and nomenclatures, Environmental segments

Atmosphere

Regions of atmosphere, Earth's radiation balance, chemistry of ozone layer, role of chemicals in ozone destruction, ozone hole, green-house gases and its effect, Global warming, measures to check global warming, El-Nino phenomenon.

UNIT - II **(12 Hrs)**

Air Pollution

Air Pollutants: sources, classification, sampling and monitoring. Aerosols, Acid Rain, Photochemical smog, Auto exhausts, Air-quality standards.

UNIT – III **(12 Hrs)**

Water Pollution

Water pollutants (sources, sampling and monitoring), Water-quality parameters and standards: physical and chemical parameters (colour, odour, taste and turbidity). Effects of fluoride in drinking water. Fresh water conservation in India.

UNIT – IV **(12 Hrs)**

Chemical Toxicology

Toxic chemicals in the environment, impacts of toxic chemicals on enzymes, biochemical effects of arsenic, cadmium, lead, mercury, carbon monoxide, pesticides, insecticides and carcinogens. Bioaccumulation and biomagnifications.

UNIT – V **(12 Hrs)**

Radioactive Pollution

Introduction, Radioactive Pollution, Sources of Radioactive Pollution, Effects of Radioactive Pollution, Disposal of Radioactive Waste.

Books Recommended:

1. Environmental Chemistry , S.E. Manahan, Lewis Publishers
2. Environmental Chemistry, Shariha & Krishna Publishers

3. Environmental Chemistry, A.K. De, Wiley Eastern.
4. Environmental Pollution Analysis, S.M. Khopkar, Wiley Eastern
5. Standard Method of Chemical Anal., F.J. Welcher Vil. - III, Van Nostrand Reinhold Co.
6. Environmental Toxicology, Ed. J. Rose, Gordon and Breach Science Publication.
7. Elemental Analysis of Airborne Particles, Ed. S. Landsberger and M. Creatchman, Gordon and Breach Science Publication.
8. Environmental Chemistry, C. Baird, W.H. Freeman
9. Hand Book of Environmental Analysis, Pradyot Patnaik, Lewis Publishers (1997)
10. Standard Methods for the Examination of Water and Wastewater, APHA, AWWA, WPCF, Washington D.C. 20005, USA, 17th Edition (1998)

SEMESTER - III

CH – 301 (5 Credits, 60 Hrs) **Total Marks- 100 (40+60)**

***Internal Assessment Examination (40 Marks) = 20 (Written) + 10 (Quiz) + 10 (Assignment/Seminar Presentation)**

ADVANCED ENVIRONMENTAL CHEMISTRY

Marks- 60 (Theory Examination)

COURSE OUTCOMES:

On completion of the course the student will be able to

- Understand types of environment and human interference with the environment
- Understand various photochemical reactions in the atmosphere.
- Describe soil profile and harmful effects of soil pollution.
- Describe source and effects of radioactive pollution, and disposal of radioactive waste.
- Identify effect of metals and other toxic pollutants in the environment and their effect on human health.

UNIT – I **(12 Hrs)**

Environment

Introduction, Earth, Environment, Types of Environment, Environmental Segments, Vertical Temperature of Atmosphere, Heat Budget of Earth's Atmospheric System, Human Interference with Environment, biogeochemical cycles in environment: water, carbon, oxygen and nitrogen.

UNIT – II **(12 Hrs)**

Atmosphere

Chemical Composition of Atmosphere**:** Introduction, Particulates, Ions, Radicals, Smog

Chemical and Photochemical Reactions in the Atmosphere**:** Introduction, Oxygen, Ozone, Nitrogen, Oxides of Nitrogen, Oxides of Sulphur, Oxides of carbon.

UNIT - III **(12 Hrs)**

Soil Pollution

Introduction, Formation of Soil and its Characteristics, Soil Profile, Types of Soil, Alkaline, Acidic, and Neutral Soil, Plant Nutrients, Environmental Concerns of Soil Pollution, Harmful Effects of Soil Pollution.

UNIT – IV **(12 Hrs)**

Water Pollution

Types of Water Pollutants, Water, Pollution in Various Water bodies, Harmful Effects of Water Pollution, Sewage and Domestic Wastes, Industrial Effluents, Agricultural Discharge, Detergents, Toxic Metals.

UNIT – V **(12 Hrs)**

Green Chemistry

Basic concept, History, rules of green chemistry, Environmental impact, pollution control, industrial applications of green chemistry. Application of Green Chemistry in Sustainable development.

Books Recommended:

1. Advanced Environmental Chemistry, V K Ahluwalia, Teri (The Energy and Resource Institute), 2017
2. Environmental Chemistry , S.E. Manahan, Lewis Publishers

2. Environmental Chemistry, Shariha & Krishna Publishers
3. Environmental Chemistry, A.K. De, Wiley Eastern.
4. Environmental Pollution Analysis, S.M. Khopkar, Wiley Eastern
6. Environmental Toxicology, Ed. J. Rose, Gordon and Breach Science Publication.
8. Environmental Chemistry, C. Baird, W.H. Freeman

CH – 302 (5 Credits, 60 Hrs) **Total Marks- 100 (40+60)**

***Internal Assessment Examination (40 Marks) = 20 (Written) + 10 (Quiz) + 10 (Assignment/Seminar Presentation)**

PHYSICAL CHEMISTRY-II

Marks- 60 (Theory Examination)

COURSE OUTCOMES:

On completion of the course the student will be able to

- Differentiate between thermodynamics of closed and open systems. Learn about free energy in closed system as opposed to partial molar properties and chemical potential in open

systems. Learn about the concept of fugacity and its determination for a real gas by graphical method.

- Learn about the concepts in statistical thermodynamic such as, distribution of molecular states, microstates and macrostates of a system, equilibrium state and entropy, most probable distribution. Derive the statistical distribution formula for Maxwell-Boltzman statistics, Fermi-Dirac statistics and Bose-Einstein statistics.
- Derive expressions for atomic and (diatomic) molecular partition functions for different degrees of motion: electronic, translational, rotational and vibrational partition functions. Derive and express thermodynamic properties in terms of ensemble partition function.
- Apply of the concept of partition function to evaluate thermodynamic properties of some realistic systems. Study of heat capacity behavior of monoatomic crystals using Einstein and Debye theory. Learn about the thermodynamics of systems that are not in equilibrium and about spontaneous processes. Derive expression for entropy production in spontaneous processes both due to flow of heat and matter.

UNIT – I **(12 Hrs)**

Classical thermodynamics

Brief resume of law of thermodynamics, free energy in closed system, thermodynamics of open systems: partial molar properties, chemical potential, Gibbs-Duhem equation, chemical potential and its relations to other partial molar properties and phase equlibrium, chemical potential of a system of ideal gas, determination of partial molar volume: slope and intercept method, concept of fugacity and determination of fugacity of a gas. Activity, activity coefficient, ionic strength

UNIT-II **(12 Hrs)**

Equilibrium statistical thermodynamics

Concepts: distribution of molecular states, microstates and macrostates of a system, equilibrium state and entropy, most probable distribution, canonical ensemble, grand canonical and microcanonical ensemble, time average and ensemble average of thermodynamic property

Statistical distribution formula: Bose-Einstein statistics, Fermi-Dirac statistics, Maxwell-Boltzman statistics

UNIT – III **(12 Hrs)**

Partition functions

Boltzman factor and partition function, atomic and molecular partition functions: electronic, translational, rotational and vibrational partition functions; canonical partition function for a system of non-interacting particles (distinguishable and identical particles), thermodynamic properties (internal energy, pressure, entropy, enthalpy, free energy, etc) in terms of canonical ensemble partition function

UNIT-IV **(12 Hrs)**

Application of partition function

Application to a system of monoatomic and diatomic ideal gas, heat capacity behavior of monoatomic crystals: Einsten and Debye theory, equilibrium constant of ideal gas reactions in terms of partition functions.

UNIT-V **(12 Hrs)**

Non-equilibrium thermodynamics

Fluxes and forces in irreversible processes, Phenomenological laws and Onsager's reciprocal relations, entropy production in spontaneous processes - due to flow of heat and matter, Prigogines principle of minimum entropy production

Books Recommended

1. Molecular Thermodynamic by D. A. McQuarrie and J. D. Simon
2. Physical Chemistry by Ira N Levine
3. Physical Chemistry by P. Atkins and J. de Paula
4. Statistical Thermodynamics by M.C. Gupta
5. Fundamentals of Statistical Mechanics by B. B. Laud
6. Introduction to Modern Statistical Mechanics, by D. Chandler, Oxford University Press (NY)
7. An introduction to Statistical Thermodynamics by T. L. Hill Dover (NY).

CH – 303 (5 Credits, 60 Hrs) **Total Marks- 100 (40+60)**
(Elective-I, Group-A)

***Internal Assessment Examination (40 Marks) = 20 (Written) + 10 (Quiz) + 10 (Assignment/Seminar Presentation)**

ORGANIC SYNTHESIS - I

Marks- 60 (Theory Examination)

COURSE OUTCOMES:

On completion of the course the student will be able to

- Assess the mechanism and synthetic uses of selected organometalic reagent in organic synthesis.
- Predict the structure, mechanism and stereochemistry of reactions involving selected oxidizing and reducing agents on organic molecules.
- Understand the principles of constructing small ring (three and four membered) heterocycles involving cyclization and cycloaddition reactions.

UNIT – I **(12 Hrs)**

Organometallic reagent

Application of organometallic reagent in organic synthesis: Group - I and Group - II metal : Li, Mg, and Zn. Transition metals : Cu, Pd, Ni, Rh and Other elements Si and B. Metal catalyzed coupling reactions (Heck coupling, Suzuki coupling, Negeshi Coupling, Stille coupling, Hiyama coupling, Kumada Coupling, Tsuji-Trost Coupling and Sonagashira coupling), Grubb's catalyst, Metathesis reactions .

UNIT - II **(12 Hrs)**

Oxidation

Use of modern Methods, reactivity, selectivity and representative examples in oxidation of hydrocarbons, alcohols, activated and unactivated C-H bond, carbon-carbon double bond, ketones, palladium-catalyzed oxidation of alkenes, oxidation with ruthenium and thallium (III) nitrate.

UNIT - III **(12 Hrs)**

Reduction

Use of modern methods, reactivity, selectivty and representative examples in reductions: catalytic hydrogenation, reductions with metals in solutions, hydride transfer reagents, borane, dialkyl-boranes and trialkyltin hydrides and trialkyl-silanes.

UNIT – IV **(12 Hrs)**

Molecular Rearrangement

General mechanistic consideration, nature of migration, migratory aptitude, A detail study of Arndt-Eistert Synthesis, Beckmann, Bayer-Villiger, Curtius, Favorski, Wagner-Meerwein, Schmidt, Shapiro reaction, and Wittig.

UNIT – V **(12 Hrs)**

Heterocycle synthesis

Principles of heterocyclic synthesis involving cyclization reactions and cycloaddition reactions involving small ring heterocycles Three-membered and four-membered heterocycles-synthesis and reaction of aziridines, oxiranes, thiiranes, azetidines, oxetanes and thietanes.

Books Recommended:

1 Warren, S. Organic Synthesis: The Disconnection Approach John Wiley & Sons (1984).
2. Organic Synthesis - Concept, Methods and Starting Materials, J. Furhrop and G. Penzillin, Verlage VCH.
3. Modern Methods of Organic Synthesis, Cambridge University Press; 4th edition. 2015
4. Principles of Organic Synthesis, R. Norman and J. M. Coxon, Blackie Academic &

Professional.
5. Advanced Organic Chemistry Part B, F.A. Carey and R.J. Sundberg, Plenum Press.
6. Organic Chemistry, Jonathan Clayden , Nick Greeves, Stuart Warren, Oxford University Press; 2nd edition 2014.
7. Organic Synthesis, Jagdamba Singh & L D S Yadav, Pragati Prakashan, Meerut, 2015
7. Wiley's Problems in Organic Chemistry, K. Singh, Wiley, 2015.
8. Heterocyclic Chemistry, Raj K Bansal, New Age International Publishers, 6 thEdition, 2019
9. Heterocycle, Joules, Mills & Smith

CH – 303 (5 Credits, 60 Hrs) **Total Marks- 100 (40+60)**
(Elective-I, Group-B)

***Internal Assessment Examination (40 Marks) = 20 (Written) + 10 (Quiz) + 10 (Assignment/Seminar Presentation)**

PHOTOINORGANIC AND SUPRAMOLECULAR CHEMISTRY

Marks- 60 (Theory Examination)

COURSE OUTCOMES:

On completion of the course the student will be able to

- Learn on excited state of metal complexes and their comparison with organic compounds, Charge transfer spectra , Charge transfer excitation and metal complex sensitizers.
- Know about Electron relay, metal colloid systems, semiconductor supported metal oxide systems, water-photolysis, nitrogen fixation and CO_2 reduction.
- Know about Redox reactions of metal complexes in excited states and life-times of excited states in these complexes along with introductory idea of Photo Chemistry of transition metal carbonyls.
- Aquire knowledge on Concept of Supramolecular Chemistry, Supramolecular Structure through non covalent interactions, Molecular receptors for neutral, cationic and anionic substrates, design and synthesis of co-receptors and multiple recognition, molecular self assembly in Supra Molecular Chemistry with Examples
- Aquire knowledge on Supramolecules in transport processes and carrier design, Supramolecular reactivity and catalysis, Supramolecular photochemistry, Supramolecular electronic, ionic switching devices.

UNIT – I **(12 Hrs)**

Excited state of Metal complexes

Excited state of Metal complexes, comparison with organic compounds, electronically excited states of metal complexes, CT spectra, CT excitations.

Metal complex sensitizers:

Metal complex sensitizers**,** Electron relay, metal colloid systems, semiconductor supported metal oxide systems, water-photolysis, nitrogen fixation and CO_2 reduction.

UNIT – II **(12 Hrs)**

Redox Reactions in Metal Complexes

Redox reactions of metal complexes in excited states, excited electron transfer, examples using $[Ru(bpy)_3]^{2+}$ complex and $[Fe(bpy)_3]^{3+}$ complex. Role of spin-orbit coupling, life-times of excited states in these complexes.

Introductory idea of Photo Chemistry of transition metal carbonyls with examples.

UNIT – III **(12 Hrs)**

Ligand Field Photochemistry

Photo substitution, Photo oxidation and Photo reduction of Cr (III) and Co (III) Complexes, lability and selectivity, Zero vibrational levels of ground state and excited state , energy content of excited state, zero-zero spectroscopic energy, development of the equations for redox potentials of the excited states.

UNIT – IV **(12 Hrs)**

Fundamentals of Supra molecular Chemistry

Concept of Supramolecular Chemistry, Supramolecular Structure through non covalent interactions

Molecular recognition: Molecular receptors for neutral, cationic and anionic substrates, design and synthesis of co-receptors and multiple recognition,

UNIT – V **(12 Hrs)**

Applications of Supra molecular Chemistry

Self assembly in Supra Molecular Chemistry with Examples, Supramolecules in transport processes and carrier design, Supramolecular reactivity and catalysis, Supramolecular devices, Supra molecular photochemistry, Supra molecular electronic, ionic and switching devices.

Books recommended:

1. An Introduction to Supramolecular Chemistry, Asim K. Das & Mahua Das
2. Progress in Inorganic Chemistry, Vols. 18 and 38 ed.
3. Supramolecular Chemistry - J.M. Lehn, VCH
4. Inorganic photochemistry, J. Chem Education, Vol. 60, No. 10, 1983.
5. Photochemistry of Coordination compounds, V. Balzari and V. Carassti, Acdemic Press

CH – 303 (5 Credits, 60 Hrs) **Total Marks- 100 (40+60)**
(Elective-I, Group-C)

***Internal Assessment Examination (40 Marks) = 20 (Written) + 10 (Quiz) + 10 (Assignment/Seminar Presentation)**

BIOPHYSICAL CHEMISTRY

Marks- 60 (Theory Examination)

COURSE OUTCOMES:

On completion of the course the student will be able to

- Learn on structure and functions of proteins, enzymes, DNA and RNA in living systems, Standard free energy change in biochemical reactions
- Learn on statistical distribution end to end dimensions calculation of average dimensions for various chain structures.
- Acquire knowledge on various bioploymer interactions Thermodynamics of bioploymer solutions.
- Cell membrane and transport of ions Bioploymers and their molecular weight

UNIT – I (12 Hrs)

Biological cell and its constituents

Biological cell, Structure and functions of proteins, enzymes, DNA and RNA in living systems, Helix coil transition.

Bioenergetics

Standard free energy change in biochemical reactions, exergonic, endergonic, Hydrolysis of ATP from ADP.

UNIT-II (12 Hrs)

Statistical mechanics in bioplolymers

Chain configuration of macromolecules, Statistical distribution end to end dimensions, calculation of average dimensions for various chain structures, Polypeptides and protein structures, Introduction to protein folding problem.

UNIT - III (12 Hrs)

Bioploymer interactions

Forces involved in biopolymer interactions, Electrostatic changes and molecular expansion, hydrophobic forces, dispersion force interactions, Multiple equilibria and various types of binding processes in biological systems, Hydrogen ion titration curves.

Thermodynamics of bioploymer solutions

Thermodynamics of biopolymer solutions, Osmotic pressure, Membrane equilibrium, Muscular contraction and energy generation in mechanochemical system.

UNIT – IV (12 Hrs)

Cell membrane and transport of ions :

Structure and functions of cell membrabe, Ion transport through cell membrane, Irreversible thermodynamic treatment of membrane transport, Nerve conduction.

UNIT – V **(12 Hrs)**

Bioploymers and their molecular weight

Evaluation of size, shape, molecular weight and extent of hydration of biopolymers by various experimental techniques, Sedimentation equilibrium, hydrodynamic methods diffusion, sedimentation velocity, Viscocity, Electrophoresis and rotational motions.

Books Recommended:

1. Principles of Biochemistry by Lehninger, D.L. Nelson and M. Cox.
2. Bio-chemistry by Voet and Voet
3. Biothermodynamics by T.T. Edsall and H. Gutfreund, Wiley (NY)
4. BioPhysical Chemistry by J. Edsall and J. Wyman, Academic (NY)
5. Bioenergetics, A.L. Lehinger, Benjamin (NY)

CH – 303 (5 Credits, 60 Hrs) **Total Marks- 100 (40+60)**
(Elective-I, Group-D)

***Internal Assessment Examination (40 Marks) = 20 (Written) + 10 (Quiz) + 10 (Assignment/Seminar Presentation)**

MACROMOLECULAR SYNTHESIS AND CHARACTERIZATIONS

Marks- 60 (Theory Examination)

COURSE OUTCOMES:

On completion of the course the student will be able to

- Learn on Ionic and Coordination Polymerization.
- Learn on different synthetic methods to prepare different types of Polymer.
- Acquire knowledge on Ring - opening Polymerization of different polymers
- Learn on spectral characterization of polymers.

UNIT - I **(12 Hrs)**

Ionic and Coordination Polymerization

Chemistry of Non-radical chain polymerization, Cationic polymerization, Mechanism & Kinetic with examples, Anionic polymerization, mechanism and Kinetics with example. Coordination polymerization (Zingler - Natta Catalyst), Steroregular polymerization, mechanism and kinetics of ring opeing polymerizatiion.

UNIT – II **(12 Hrs)**

Synthesis of Polymer

Bulk, Solution, Suspension, Emulsion, Precipitatiion Gas Phase, Solid State and interfacial methods of polymerization.

Polymerization and hydrogen transfer polymerization : Preparation Nylon 6.6 Poly (1.1. - undecanoamide). Poly (Decamethylene oxamide) Poly (Ethylene Terepthalate). Poly sulphone from Bio-Phenol - A & dichlorophenyl sulphone.

Thermal polymerization of styrene in Bulk, Emulsion polymerization of styrene with persulfate, suspension polymerization of styrene solution and emulsion polymerization of vinyl acetate, solution polymerization of Acrylamide.

UNIT – III **(12 Hrs)**

Ring - opening Polymerization

Fast polymerization of caporolactam to Nylon-6 with anion catalysts, low temperature polymerization of L-Piperidine to Nylon-5, polymerization of Ethylene oxide and Tetrahydrofuran and Preparation of linear polysilcons.

UNIT – IV **(12 Hrs)**

Non-classical routes to polymers-polymerization of Anhydrous formaldehyde to polyoxymethylene, solid state polymerization of Troioxane. Preparation of n-butylisolyanate, Diazomethan and Norbornlene.

Preparation of Pehnol-formaldehyde resin, Urea-formadehyde resin, Epoxy resin, Allyl resins.

UNIT – V **(12 Hrs)**

Characterisation of Polymers

UV-VIS Spectroscopy of Polymers, characterisation of polymer and copolymer by IR. NMR & EPR of polymers. X-ray difraction and electron diffraction of polymers, composites. Thermal analysis of polymers by TG, DTG, DTA, DSC chromatograCH - Pyrolysis Gas chromatograCH and other chromatographic characterisation.

Books recommended:

1. Polymer Science, Gowariker, Viswanathan & Sreedhar
2. Polymer Scince, Premamaya Ghosh
3. Organic Polymer Chemistry, K.J. Saunders
4. Organic Chemistry of Macromolecules, A. Rayve
5. Polymer Chemistry, A.B. Seymour & C.E. Carraher
6. Experiments in Polymer Science, Edw and A. Collin & F.W. Billmeyer
7. Principle of Polymerization, Flory
8. Characterization of POlymer, N.M. Bikales

9. NMR of Polymers, I.Y. Slorium & A.N. Lyubimor
10. FT-IR Characterization of Polymer, H. Ishida

CH – 304 (5 Credits, 60 Hrs) **Marks – 100 (30+70)**

ORGANIC GENERAL PRACTICAL

COURSE OUTCOMES

On completion of the course the student will be able to

- Acquire skills in different laboratory techniques such as melting point, distillation, TLC, column chromatography, crystallization and preparation of dry solvents.
- Separation and qualitative analysis of two component mixtures of organic compounds: characterization of derivatives and identification of the components.
- Design single stage synthesis of simple organic compounds and execute them in the laboratory.
- Single stage preparation of organic compounds using some classical organic reactions.
- Extraction of caffeine from tea leaves, piperine from pepper, lachanoric acid from lichens and casein from milk.

1. **Analysis of Organic Compound**

   Separation and identification of components of a mixture of two organic compounds (solid-solid, solid-liquid, liquid-liquid).

2. **Organic Synthesis (Single Step)**

   a) Preparatiion of p-bromoacetanilide.
   b) Preparation of 3, 5 -dibromobenzoic acid.
   c) p-bromo aniline preparation from aromatic electrophilic substitution reaction.
   d) Preparation of p-chlorotolune.
   e) Preparation of Methyl orange.
   f) Preparation of Asprin
   g) Preparation of Anthranilic acid.

3. **Estimation**

   a) Estimation of Keto Group (>C=O)
   b) Estimation of Acetyl group (-CO - CH_3)

4. **Separation**

Acetylation of Cholesterol and separation of cholesteryl acetate by column chromatograCH.

Books Recommended:

1. Vogel's Text Book of Practical Organic Chemistry, Furniss, S. B.; Hannaford, A. J.; Smith, P. W. G.; Tatchell, A. R. 5Th Ed.; Longman Scientific & technical, England, 1989.
2. Laboratory Manual of Organic Chemistry, Dey and Sitaraman, Allied Publishers, 1992.
3. Laboratory Manual of Organic Chemistry, Raj K Bansal, New Age International Publishers, 2008

CH – 305 (3 Credits) **Total Marks- 100 (40+60)**

SWAYAM MOOCS

(Offered by NPTEL)

CH-AIT (03 Credit, 36 Hrs) **Marks- 50**

CERTIFICATE COURSE

ANALYTICAL INSTRUMENTATION TECHNIQUES

Course Outcome

- To provide concepts on the several instrumentation techniques at the structural and chemical level which has become essential tools for chemical research.
- Understand and describe the fundamental principles behind the methods of characterization which are included in the course.
- To acquire skills in the use and selection of instrumental techniques for characterization of molecules, materials and application of these techniques to solving problems.
- To develop tools for analysis and methodologies that promotes multidisciplinary research for better understanding of composition-structure-properties correlation.
- To provide a general understanding of instrumental techniques & will prepare students for advanced research or development in industry.

UNIT-I **(12 Hrs)**

General Introduction

Instrumentation methods of analysis, classification, advantage of instrumental methods, limitations, sensitivity and detection limit, precision and accuracy.

UNIT-1I **(12 Hrs)**

Fluorescence Spectroscopy

Basic principles, general instrumentation and applications of Fluorescence Spectrophotometer: relationship between excitation spectra and fluorescence spectra, factors affecting fluorescence emission.

UNIT-III **(12 Hrs)**

Atomic Absorption Spectroscopy

Basic principles, instrumentation and applications of Atomic Absorption Spectroscopy (AAS).

UNIT-IV **(12 Hrs)**

Thermal Methods of Analysis **[**

Basic principles, general instrumentation and applications: TGA (Thermo Gravimetric Analysis), DTA (Differential Thermal Analysis), DSC (Differential Scanning Calorimetry).

UNIT-V **(12 Hrs)**

Methods for Composition Analysis

Basic principles, general instrumentation and applications: Powder X-ray Diffraction (XRD), Particle size Analyzer (DLS) and Surface area Analyzer.

Books Recommended:

1. Principles of Instrumental Analysis – Douglas A. Skoog, Saunders College Publ. III Edition, 1985.
2. Text Book of Quantitative Inorganic Analysis – A.I. Vogel, ELBS, III Edition, 1976, and IV Edition, 1985.
3. Vogel's Text Book of Quantitative Chemical Analysis – A.I. Vogel, Pearson Education Ltd, VI Edition, 2001.
4. Principles of Instrumental Analysis – Skoog and Leary, Saunders College Publ. IV Edition, 1992
5. Instrumental Analysis – Gary D. Christian & James, E. O'Reilly, Allyn & Bacon Inc, II Edition, 1986.
6. Principles and Practice of Analytical Chemistry, F.A. Fifield & Dacid Kealy, Blackwell Publishing, 5thEdn, 2000.

SEMESTER – IV

CH – 401 (5 Credit, 60 hour) **Total Marks- 100 (40+60)**

***Internal Assessment Examination (40 Marks) = 20 (Written) + 10 (Quiz) + 10 (Assignment/Seminar Presentation)**

SPECTROSCOPY-II

Marks- 60 (Theory Examination)

COURSE OUTCOMES:

On completion of the course the student will be able to

- Learn the principles of Infrared and Raman spectroscopy, correlate with the molecular modes of vibration and apply the rules to interpret the spectra of organic molecules.
- Understand the basic principles of Mossbauer spectroscopy and apply to elucidate the structure of inorganic molecules.

- Learn the concept and rules of electronic transitions in organic molecules and their correlation with UV absorption spectroscopy.
- Describe the applications of UV-Visible spectroscopy in the identification of conjugation in organic compounds.
- Understand the basic principles of NMR and able to analyze the ^{1}H NMR data of simple organic compounds.
- Analyze and apply the rules of Mass spectroscopy for the fragmentation pattern in different types of organic functional groups.
- Analyze and identify simple organic molecules by using UV, IR, Mass and ^{1}H NMR data.

UNIT – I **(12 Hrs)**

(a) Vibrational Rotational Spectroscopy.

Group vibration concept and its limitations, Use of symmetry arguments to determine the number of active infrared and Raman lines. Applications of infrared and Raman spectroscopy for determination of inorganic structures.

(b) **Mossbauer Spectroscopy.**

Basic principles, interpretation of isomeric shift, electronic quadrupole intractions, spectrum display. magnetic interaction, mossbaur emmission spectroscopy, application of Mossbauer Spectroscopy 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 inequivalent MB atoms.

UNIT - II **(12 Hrs)**

Ultraviolet and Visible Spectroscopy

Various electronic transitions (185- 800 mm.) 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 compunds, ultraviolet spectra of aromatic compounds.

UNIT-III **(12 Hrs)**

Infrared Spectroscopy

Instrument and sample handling. Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols aryl amines. Detailed study of vibrational frequencies of carbonyl compounds (Ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance.

UNIT – IV **(12 Hrs)**

Nuclear Magnetic Resonance Spectroscopy

General introduction and definition, chemical shift, spin-spin interaction, shielding mechanism, mechanism of measurement, chemical shift values and correlation for protons bonded to carbon (Aliphatic, olefinic, enols, carboxylic acids, amines, amides & mercapto), chemical exchange, effect of deuteration, complex spin-spin interaction between two, three, four and five nuclei (first order spectra), virtual coupling. Stereochemistry, hindred rotation, Karplus curve-variation of coupling constant with dihedral angle. Simplification of complex spectra nuclear magnetic double resonance, contact shift reagents, solvent effects. Fourier transform technique, nuclear Overhauser effect (NOE), Resonance of other nuclei-F, P

UNIT – V **(12 Hrs)**

Mass Spectrometry

Introduction ion production - EI, CI, FD and FAB, factors affecting fragmentation, ion analysis,ion abundance. Mass spectral fragmentation of organic compounds,common functional groups, molecular ion peak, metastable peak, Mc Lafferty rearrangement. Nitrogen rule. High resolution mass spectrometry. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

Books Recommended:

1. Structural Methods in Inorganic Chemistry, E.A.V. Wbsworth, D.W.H. Rankin and S. Cradock, ELBS.
2. Infrared and Raman Spectra: Inorganic and Coordination Compounds, K. Nakamoto, Wiley.
3. Symmetry in bonding and spectra: An Introduction by B.E Douglas, Academic Press.
4. Fundamental of Molecular Spectroscopy, C.N.Banwell & Elaine M. McCASH, Fourth edition (2017)
5. Spectrometric Identification of Compounds, R. M. Silverstein, G.C. Bassler and T.C. Morrill, John Wiley.
6. Speectroscopy of Organic Compounds, P. S. Kalsi, New Age International Publishers, 2020, 8 th Ed
7. Spectroscopy, H Kaur, Pragati Prakashan, 2017
8. Introduction to Spectroscopy, Donald J Pavia, Gary M. Lampman & George S. Kriz Cengage Learning India Private Limited; 5th edition (2015)
9. Organic spectroscopy by William Kemp 3rd edn W.H.Freeman & Co, 1991
10. Spectroscopy Methods in Organic Chemistry, D. H. Williams, I. Fleming, Tata McGraw.

CH – 402 (5 Credits, 60 Hrs) **Total Marks- 100 (40+60)**
(Elective-II, Group-A)

***Internal Assessment Examination (40 Marks) = 20 (Written) + 10 (Quiz) + 10 (Assignment/Seminar Presentation)**

ORGANIC SYNTHESIS - II

Marks- 60 (Theory Examination)

COURSE OUTCOMES:

On completion of the course the student will be able to

- Acquire knowledge on disconnection approach as well as role of modern synthetic reagents in organic transformations.
- Compile and demonstrate knowledge on retrosynthesis and various terminologies, retro synthesis of simple molecules-alcohols, alkenes and dicarbonyl compounds, formation of C-C bond using different coupling reactions.
- Analyze and formulate the chemistry of protection and de-protection strategies involved in hydroxyl group by ether and ester, carbonyl group, and amino groups and functional group interconversion by substitution reactions.
- Describe the important concepts of the organic chemistry for the synthesis of new molecule, introduction of different functional group.
- Understand the principles of ring synthesis involving saturated and aromatic heterocycles.
- Retrosynthetic analysis and synthesis of some complex molecules.

UNIT – I **(12 Hrs)**

Disconnection approach

An introduction to synthons and synthetic equivalents, disconnection approach, functional group inter-conversion, 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 andamine synthesis.

UNIT – II **(12 Hrs)**

Protecting groups

Principle of protection and deprotection of alcohol, amine, carbonyl and carboxyl groups.

UNIT – III **(12 Hrs)**

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

UNIT – IV **(12 Hrs)**

Ring synthesis

Balwdin's rules for ring closure, Saturated heterocycles, Synthesis of 3-, 4-, 5- and 6-membered rings, aromatic heterocycles in organic synthesis.

UNIT – V **(12 Hrs)**

Synthesis of some complex molecules

Application of the above in the synthesis of following compounds: Camphor, Longifoline, Reserpine, Vitamin D, Aphidicolin and Fredericamycin A.

Books Recommended:

1. Warren, S. Organic Synthesis: The Disconnection Approach John Wiley & Sons (1984).
2. Organic Synthesis - Concept, Methods and Starting Materials, J. Furhrop and G. Penzillin, Verlage VCH,
3. Modern Methods of Organic Synthesis, Cambridge University Press; 4th edition. 2015
4. Principles of Organic Synthesis, R. Norman and J. M. Coxon, Blackie Academic & Professional.
5. Advanced Organic Chemistry Part B, F.A. Carey and R.J. Sundberg, Plenum Press.
6. Organic Chemistry, Jonathan Clayden , Nick Greeves, Stuart Warren, Oxford University Press; 2nd edition 2014.
7. Organic Synthesis, Jagdamba Singh & L D S Yadav, Pragati Prakashan, Meerut, 2015.
Wiley's Problems in Organic Chemistry, K. Singh, Wiley, 2015.
8. Heterocyclic Chemistry, J A Joule & K. Mills, Wiley, 5 th Edition.
9. Organic Chemistry, Volume 2: Stereochemistry and the Chemistry Natural Products, I. L. Finar, Pearson, 5th Edition

CH – 402 (5 Credits, 60 Hrs) **Total Marks- 100 (40+60)**

(Elective-II, Group-B)

***Internal Assessment Examination (40 Marks) = 20 (Written) + 10 (Quiz) + 10 (Assignment/Seminar Presentation)**

ORGANO-TRANSITION METAL CHEMISTRY

Marks- 60 (Theory Examination)

COURSE OUTCOMES:

On completion of the course the student will be able to

- Learn about synthesis, stability and decomposition pathways of transition metal alkyl and aryl complexes, role of organo-copper in organic synthesis.
- Learn about Transition metal compounds with bonds to hydrogen, synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions on the ligands of carbene and carbyne complexes.

- Learn about preparation, properties, nature of bonding , structural features and important reactions relating to nucleophilic and electrophilic attack on ligands of alkenes, alkynes, allyl, diene, dienyl, arene and trienyl complexe
- Acquire knowledge on fluxionality and dynamic equilibria in compounds such as η^2 - olefin, η^3 - allyl and dienyl complexes. Synthesis, structure of organometallic reagents of transition metals such as Pd, Rh, Ni, and Fe and their applications in organic synthesis.
- Acquire knowledge on fundamental reactions like insertion (CO and SO_2) , elimination reactions, oxidative and reductive eliminations
- Learn about Stoichiometric reactions for catalysis, homogeneous catalytic isomerisation, hydrogenation of olefines, Zeigler-Natta polymerization of olefins, hydrocarbonylation of olefins (oxo reaction).

UNIT – I **(12 Hrs)**

Alkyls and Aryls of Transition Metals

Types, routes of synthesis, stability and decomposition pathways, organo-copper in organic synthesis.

Transition Metal Compounds with Bonds to Hydrogen

Transition metal compounds with bonds to hydrogen

UNIT-II **(12 Hrs)**

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 – III **(12 Hrs)**

Transition Metal π -Complexes

Transition Metal -complexes with usaturated 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 – IV **(12 Hrs)**

Fluxional Organometallic Compounds

Fluxionality and dynamic equilibria in compounds such as η^2 - olefin, η^3 - allyl and dienyl complexes.

Organometallic Reagents - Synthesis, structure of organometallic reagents of transition metals such as Pd, Rh, Ni, and Fe and their applications in organic synthesis.

UNIT – V **(12 Hrs)**

Organometallic reactions and catalysis

Fundamental reactions: Insertion (CO and SO_2) and elimination reactions, oxidative and reductive eliminations, activation of C-H bond.

Stoichiometric reactions for catalysis, homogeneous catalytic hydrogenation, Zeigler-Natta polymerization of olefins, hydro carbonylation of olefins (oxo reaction).

Books Recommended:

1.Principles and Application of Organo transition 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.

5. Concepts and Models of Inorganic Chemistry by B.E. Douglas, D.H.McDaniel and J.J Alxendar, John Wiley, 1993 3rd Ed.

6. Reaction mechanism in Inorganic Chemistry by R.R.Jordan Oxford Univ. Press, 1998 2nd ED.

7. Advanced Inorganic Chemistry by F.A. cotton and G.W. Wilkison.John-Wiley & Sons, 1988, 5th Ed.

CH – 402 (5 Credits, 60 Hrs) **Total Marks- 100 (40+60)**

(Elective-II, Group-C)

***Internal Assessment Examination (40 Marks) = 20 (Written) + 10 (Quiz) + 10 (Assignment/Seminar Presentation)**

SURFACE CHEMISTRY

Marks- 60 (Theory Examination)

UNIT – I **(12 Hrs)**

Adsorption

Surface tension, capillary action, pressure difference across curved surface, vapour pressure of droplets, Gibbs adsorption isotherm, estimation of surface area (BET) equations, catalytic activity at surfaces.

UNIT – II **(12 Hrs)**

Micelles

Surface active agents, classification of surface active agents, micellization, hydrophobic interactions, critical micellar concentration (CMC) factors affection CMC, Solubilization, micromulsion and reverse micelles.

UNIT-III **(12 Hrs)**

Macromolecules

Macromolecules: Polymer-definition, types of polymer, electrically conducting, fire resistant, liquid crystal polymer. Molecular mass, number and mass average molecular mass, molecular mass determination (osmometry, viscometry, diffusion and light scattering), sedimentation, chain configuration of macromolecules, calculation of average dimension of various chain structures.

UNIT-IV **(12 Hrs)**

Surface reactions: General aspects, co-adsorption, poisoning and promotion effects, model reactions, Examples of surface reactions, detection of adsorbates on surfaces. High pressure catalytic reactions on single crystal surfaces: examples - CO oxidation and methanation, ammonia synthesis, epoxidation reactions.

UNIT-V **(12 Hrs)**

Techniques of Surface Investigation. Electron diffraction, scanning tunneling microscopy (STM), High resolution electron energy loss spectroscopy (HREELS), X-ray and Ultravoilet photoelectron Spectroscopy (XPS and UPS). Inverse photo emission, ion scattering (LEIS, SIMS), Auger electron spectroscopy (AES), Thermal desorption and work function measurements-Basic principles and applications.

.Books Recommended:

1. Adsorption and Catalysis, by D.K. Chakraborty
2. Solid state chemistry and its application, by A.R. West
3. Physical chemistry, by G.M. Barrow.
4. Solid state chemistry, by H.V. Keer

CH – 402 (5 Credits, 60 Hrs) **Total Marks- 100 (40+60)**
(Elective-II, Group-D)

***Internal Assessment Examination (40 Marks) = 20 (Written) + 10 (Quiz) + 10 (Assignment/Seminar Presentation)**

PHYSICAL CHEMISTRY OF POLYMERS

Marks- 60 (Theory Examination)

UNIT – I **(12 Hrs)**

Thermodynamic of Polymer Mixture

Partial molar function, ideal and non-ideal solution, enthalpy and entropy of mixing & florykingbaurn theory. Free energy of mixing of a polymer with a solvent - Thermodynamics of swelling of cross-linked polymers.

UNIT – II **(12 Hrs)**

Morphology and Crystallinity

Cofiguraion of Polymer chain, Crystal structure of polymers, Morphology of Polymer single crystals structure of polymers crystallised from melt. Crystalizatiion. Orientation and drawing. Amorphous Polymers.

UNIT – III **(12 Hrs)**

Rheology and Mechanical Properties of Polymers

Viscous flow, viscoelasticity, the glassy state and the glass transition. Mechanical properties of crystalline polymers. Statistical behavious of polymer moleculars. Random fight - chain model freely rotating chain model, Hindered rotation model. Rotationl Isomeric state model.

UNIT - IV **(12 Hrs)**

Technology of Polymers

Additives of Polymers: Filleers and Rainforcement Plasticisers, Antioxidants, Stabilsers, Crosslinking agents, Activators, accelerations, Lubricating agents, antistatic agents colourants.

UNIT – V **(12 Hrs)**

Fabrication Film casting, casting of casting of articles in models, compression and transfer molding. Thermoforming and welding, calendering, multipolymer systems & composites. Laminates, Foam, Coatings, Adhesives, Pressure sensitive Adhesive.

Books Recommended:

1. Introduction to Polymer Science and Technology, H.S. Kaufman & J.J. Falcetta.
2. Viscoelastic properties of the Polymers, J.D. Ferry
3. Physical Chemistry of Polymer, A. Tagor
4. Statistical Mechanis of Polymers, P.J. Flory
5. Text Book of Polymer Science and Engineering, Anil Kumar Gupta.
6. Plastic Materials, J.A. Brydson.
7. Essential Fiber Chemistry, M.E. Cartel
8. Textile Fibers, J. Peters.

CH - 403 (5 Credits, 60 Hrs) **Marks-100 (30+70)**

PRACTICAL (Elective, Group -A)

COURSE OUTCOMES:

On completion of the course the student will be able to

- Reduction of camphor to borneol with Sodium Borohydride
- Isolation of Caffeine from tea bags.
- Isolation of lactose from milk.
- Preparation of phenylazo-2-napthol from aniline.

- Separation and qualitative analysis of three component mixtures of organic compounds: characterization of derivatives and identification of the components.

1. Qualitative analysis

Separation and identification of Organic Compound of binary mixture (one liquid and one solid)

2. Organic synthesis (single step)

a) Preparation of Salicylaldehyde.
b) Preparation of quinoline
c) Cannizzaro reaction : 4 - chlorobenzaldehyde as substrate.
d) Aldol condensation : Dibenzal acetone from benzaldehyde.

3. Organic synthesis (multi step)

Benzene Nitrobenzene Aniline Phenol

4. Quantitative analysis

Determination of the percentage or number of hydroxyl groups in an organic compunds by acetylation method.

5. Spectrophotometric estimation

Amino Acids.

Books Recommended:

1. Vogel's Text Book of Practical Organic Chemistry, Furniss, S. B.; Hannaford, A. J.; Smith, P. W. G.; Tatchell, A. R. 5Th Ed.; Longman Scientific & technical, England, 1989.
2. Laboratory Manual of Organic Chemistry, Dey and Sitaraman, Allied Publishers, 1992.
3. Laboratory Manual of Organic Chemistry, Raj K Bansal, New Age International Publishers, 2008

CH-403 (5 Credit, 60 Hrs) **Marks-100 (30+70)**

PRACTICAL (Elective, Group-B)

After completion of this course student will be able to

- Prepare complexes of Cr (III)/Co(III)and estimate the amount of constituents.
- Determine the free acid and metal content in $FeCl_3$ /$CuSO_4$solution by ion exchange methods

- Determine the composition of a complex compound in solution by job's continuous variation method.

1. Preparation and Characterization

Preparation of simple complex compounds of Cr(III)/Co(III). Estimation of the metal content and other components of the complexes such as:

Cis - $K[Cr(C_2O_4)_2(H_2O)_2]$

Tranns- $[Co(en)_2Cl_2]Cl$

2. Ion exchange methods of separation and estimation

(i) Separation of mixtures of cations (Co-Ni, Fe-Zn, Zn-Mg, Cd-Zn) by ion exchange method and estimation of the components after separation.

(ii) Determination of metal content and free acid in $FeCl_3/CuCl_2$ solution.

3. Spectrophotometry

(i) Determination of composition of a complex compound in solution by Job's continuous variation method.

(ii) Determination of acid dissociation constant of pentaammine(salicylato)-cobalt(III) complex.

4. Quantitative analysis

Analysis of solder and brass.

5. Potentiometry

Determination of acid dissociation constants of simple coordinated ligands by pH metry

Books Recommended:

1. A Text book of Qualitative Analysis, A. I. Vogel
2. A Text book of Quantitative Analysis, A. I. Vogel
3. Inorganic synthesis, Vol. 1 -20

CH – 403 (5 Credits, 60 Hrs) **Marks-100 (30+70)**

PRACTICAL (Elective, Group -C)

1. Spectrophotometry

Verification of additivity law.

Characterization of complexes by spectroscopic data.

Estimation of metal ions by spectrophotometric titration.

To determine of pH of an indicator

2. Potentiometery

To determine first and second ionization constant of multi basic acid.

To determine the standard electrode potential of Ferrous-Ferric system.

3. **Conductometry**

To determine hydrolysis constant of aniline hydrochloride.
To determine solubility and solubility product of a sparingly soluble salt.
Verification of Debye-Huckel and Onsager's limiting law.

4. **Surface / phase**

To study the adsorption of acetic acid on activated charcoal.
To determine the demerization constant of benzoic acid in benzene medium by partition method.

5. **Solid state**

XRD of simple solids (NaCl, CsCl, Graphite etc. Spectral data analysis only)

6. **Viscometery**

Determination of molecular weight by Ubbelhood Viscometer.

CH - 403(5 Credits, 60 hrs) **Marks-100 (30+70)**

PRACTICAL (Elective, Group -D)

1. Determination of Molecualar weight of given Polymer by Ubblehode Viscometer.
2. Determination of molecular weight of a given polymer by end group analysis.
3. Chemical Testing of polymers.
4. Determination of Tg of a given polymer by Thermogravimetric analysis.
5. Polymerisation of vinyl monomer by free radical method and characterization.
6. Polymerization of PMMA by emulsion polymerisation method.

CH-404 (5 Credit, 60 Hrs) **Marks-100**

PROJECT WORK

The project work will consist of experimental / review work under direct supervision of faculty members.

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