Department of Chemistry

Scheme and Syllabus
for
M. Sc. (Chemistry)

SLIET

(Deemed-to-be-University)

(Session 2021 onwards)

ANNEXURE-I
M.Sc (CHEMISTRY)

SEMESTER – I

S. No.	Code No.	Subject	L	T	P	Credits
1.	AC 8101	Physical Chemistry- I	4	0	0	4
2.	AC 8102	Inorganic Chemistry-I	4	0	0	4
3.	AC 8103	Organic Chemistry-I	4	0	0	4
4.	AC 8104	Computer for Chemists	2	0	0	2
5.	AC 8105 A/B	Mathematics for Chemists/Biology for Chemists*	2	0	0	2
6.	AC 8151	Organic Chemistry Lab	0	0	6	3
7.	AC 8152	Inorganic Chemistry Lab	0	0	6	3
8.	AC 8153	Computer Lab	0	0	2	1
Total			16	0	14	**23**

* Mathematics for chemists for students of B.Sc. (medical) and Biology for chemists for students of B.Sc. (Non-medical)

SEMESTER – II

S.No.	Code No.	Subject	L	T	P	Credits
1.	AC 8201	Physical Chemistry- II	4	0	0	4
2.	AC 8202	Inorganic Chemistry-II	4	0	0	4
3.	AC 8203	Organic Chemistry-II	4	0	0	4
4.	AC 8204	Group theory and spectroscopy	3	0	0	3
5	AC 8205	Analytical Chemistry	3	0	0	3
6	AC 8251	Physical Chemistry Lab.	0	0	6	3
7	AC 8252	Analytical Chemistry Lab.	0	0	6	3
Total			18	0	12	**24**

SEMESTER – III

S.No.	Code No.	Subject	L	T	P	Credits
1.	AC 9101	Spectroscopic Techniques	5	0	0	5
2.	AC 9102	Environmental Chemistry-I	4	0	0	4
3.	AC 91*	Elective – I*	4	0	0	4
4.	AC 91*	Elective – II*	4	0	0	4
5	AC 91*	Elective – III*	4	0	0	4
6	AC 9151	Advanced Lab. Techniques – I*	0	0	6	3
Total			21	0	06	**24**

* The student shall be required to select elective subjects from the list of subjects offered (depending upon the availability of the concerned faculty) during this semester under his/her specialization.

SEMESTER – IV

S.No.	Code No.	Subject	L	T	P	Credits
1.	AC 92*	Elective – IV	3	0	0	3
2.	AC 92*	Elective –V	3	0	0	3
3.	AC 92*	Elective – VI	3	0	0	3
4.	AC 9251	Dissertation*	0	0	22	11
Total			9	0	22	**20**

* The dissertation work shall be undertaken on daily basis. Each student has to give SEMINAR to defend his/her dissertation in the department.

In addition, Students are encouraged to undergo:

- **(i) Summer training of 4-6 weeks after 2nd Semester in summer vacations [in Industry or IIT's or IISER's or National research laboratories or National/State universities of Repute]**
- **(ii) Industrial/Educational tour**
- **(iii) Students may opt Elective Courses from MOOCs/Swayam (Max *Two*)**

LIST OF ELECTIVE SUBJECTS AS PER SPECIALIZATION

Students are required to select any **six (I-VI)** of the following elective papers as per the specialization allotted during the start of 2nd year.

1. ORGANIC CHEMISTRY

Elective -I

AC- 9103 Bio-organic Chemistry

Elective -II

AC-9104 Chemistry of Natural Products

Elective –III (Common)

AC-9109A Chemistry of Materials
AC-9109B Organometallic Chemistry
AC-9109C Instrumental Methods of Analysis

Elective – IV-VI

AC-9201A Organic Synthesis-I
AC-9201B Organic Synthesis-II
AC-9201C Organic synthesis - III
AC-9201D Heterocyclic Chemistry
AC-9201E Green Chemistry
AC-9201F Polymer Chemistry
AC-9201G Organic Photochemistry
AC-9201H Medicinal Chemistry
AC-9201 I Molecular Modeling in Chemistry

2. INORGANIC CHEMISTRY

Elective -I

AC-9105 Advanced Coordination Chemistry

Elective –II

AC-9106 Bio-inorganic Chemistry

Elective –III (Common)

AC-9109A Chemistry of Materials
AC-9109B Organometallic Chemistry
AC-9109C Instrumental Methods of Analysis

Elective – IV-VI

AC-9202A Inorganic Photochemistry
AC-9202 B Supramolecular Chemistry
AC-9202C Physical Methods in Inorganic Chemistry
AC-9202D Special Topics in Inorganic Chemistry
AC-9202E Inorganic Polymers
AC-9202F Inorganic Photochemistry
AC-9201 I Molecular Modeling in Chemistry

3. PHYSICAL CHEMISTRY

Elective -I

AC-9107 Statistical Mechanics

Elective -II

AC-9108 Quantum Mechanics

Elective –III (Common)

AC-9109A Chemistry of Materials
AC-9109B Organometallic Chemistry
AC-9109C Instrumental Methods of Analysis

Elective – IV-VI

AC-9203A Macromolecules and Surface Chemistry
AC-9203B Advanced Statistical Thermodynamics
AC-9203C Physical Methods in Chemistry
AC-9203D Electrochemistry and Chemical Kinetics
AC-9203E Photo-physical Chemistry
AC-9203F Molecular Reaction Dynamics
AC-9203G Biophysical Chemistry

DETAILED SYLLABUS

M. Sc. (Chemistry)

AC 8101 PHYSICAL CHEMISTRY -I

L	T	P	Cr
4	0	0	4

Course Objective: To develop a fundamental understanding of classical and statistical thermodynamics, chemical equilibrium, reaction kinetics phase rule and solutions.

UNIT-I

Electrochemistry: Oxidation numbers. Redox potential. Electrochemical series. Redox indicators. Electrochemical cell reactions, Nernst equation, Electrode Kinetics, electrical double layer, electode/electrolyte interface, Batteries, primary & secondary Fuel Cells, corrosion and corrosion prevention. **(7 hr)**

Thermodynamics: First law of thermodynamics, relation between C_p and C_v; enthalpies of physical and chemical changes; temperature dependence of enthalpies. Second law of thermodynamics, entropy, Gibbs-Helmoholtz equation. Third law of thermodynamics and calculation of entropy. **(7 hr)**

Statistical Thermodynamics: Thermodynamic probability and entropy; Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics. Partition function: rotational translational, vibrational and electronic partition functions for diatomic molecules; calculations of thermodynamic functions and equilibrium constants. Theories of specific heat for solids. **(9 hr)**

Chemical Equilibrium: Free energy and entropy of mixing, partial molar quantities, Gibbs-Duhem equation. Equilibrium constant, temperature-dependence of equilibrium constant. **(5 hr)**

Non-equilibrium Thermodynamics: Postulates and methodologies, linear laws, Gibbs equation, Onsager reciprocal theory. **(4 hr)**

UNIT -II

Reaction Kinetics: Review of basic concepts in kinetics, Experimental techniques, Rates of chemical reactions, methods of determining rate laws, Mechanisms of chemical reactions and steady state approximation, Law of absorption of light, laws of photochemistry, kinetics of photochemical and composite reactions, chain and oscillatory reactions, collision and transition state theories, steric factor, treatment of unimolecular reactions, Ionic reactions: salt effect. Homogeneous catalysis and Michaelis-Menten kinetics; heterogeneous catalysis, Reaction dynamics. **(11 hr)**

Phase rule: Phase diagram of one- and two-component systems, phase rule. Thermodynamic description of phase transitions, mixtures and chemical equilibrium. **(6 hr)**

Ideal and Non-ideal solutions: Colligative properties of solutions, excess functions, activities, concept of hydration number: activities in electrolytic solutions; mean ionic activity coefficient; Debye-Huckel treatment of dilute electrolyte solutions. **(7 hr)**

Learning Outcome Upon successful completion of this course the students will be able to understand

1. The chemistry of oxidation and reduction processes, working of electrochemical and electrolytic cells and operations of batteries.
2. The significance and quantitative analysis of chemical thermodynamics.
3. The quantum concepts and how they are applied to basic to understanding of molecular structure
4. The significance of chemical kinetics including reaction rate expressions, properties of gases and solutions

References:

1. P.W. Atkins, Physical Chemistry: International Eleventh Edition, Oxford university Press, 2018
2. C. Kalidas, Chemical Kinetic Methods : Principles of Fast Reaction Techniques And Applications New Age International (P) Ltd. 2018.
3. Raza Tahir-Kheli, General and Statistical Thermodynamics, 2011.
4. R.P. Rashtogi, An Introduction to Chemical Thermodynamics, Vikas Publication, 2018.
5. K. J. Laidler, Chemical Kinetics, McGraw-Hill, 2003.
6. J. Rajaraman and J. Kuriacose, Kinetics and Mechanism of Chemical Transformations, McMillan, 2000.
7. K.L. Kapoor, A text book of Physical Chemistry, McGraw-Hill, 2018.

AC 8102 INORGANIC CHEMISTRY - I

L	T	P	Cr
4	0	0	4

Course Objective: To introduce the concept, theories of chemical bonding, reaction mechanism and reactivity patterns of main group elements, the coordination complexes and how these theories are used to address the electronic and magnetic properties of the coordination complexes; detailed HSAB principle. To give concept of lanthanide and actinides, their properties.

UNIT -I

Main Group Elements: General Characteristics of main group elements and their compounds, allotropy, synthesis, bonding and structures. **(10 hr)**

Stereochemistry and Bonding in Main Group Compounds: Valence Shell Electron Pair Repulsion Theory-stereochemical rules and explanation of the shapes of molecules and ions of non-transition elements with 2-7 valence shell electron pairs. MO theory, Walsh diagrams (tri- and penta- atomic molecules), d_{π}-p_{π} bonds, Bent rule and energetics of hybridization. **(10 hr)**

HSAB Theory: Classification of acids and bases as hard and soft; HSAB principle, theoretical basis of hardness and softness; Lewis-acid base reactivity approximation; donor and acceptor numbers, E and C equation; applications of HSAB concept. **(6 hr)**

UNIT -II

Metal-Ligand Bonding in Transition Metal Complexes: Magnetic criterion and bond type for TM metal complexes. Crystal field splitting diagrams in complexes of low symmetry; Spectrochemical and Nephelauxetic series; thermodynamic and structural effects; site selection in spinels, Jahn-Teller distortions; experimental evidence for metal-ligand orbital overlap; ligand field theory, molecular orbital theory of octahedral complexes, brief introduction to Angular Overlap Model. Bonding of carbonyls and nitrosyls. **(14 hr)**

Chemistry of f-block elements: Lanthanoid and actinoid chemistry; periodic properties, spectral and magnetic properties; analytical applications. **(16 hr)**

Learning Outcome Upon successful completion of this course the students will be able to

1. understand general chemical bonding including stereochemistry, concept of acid and base.
2. understand the nature of bonding and stability of coordination compounds.
3. calculate the spin-only magnetic moment of metal complexes.
4. explain the stability of complexes in terms of hard and soft interactions between the metal ions and ligands.
5. understand about the lanthanide elements and compounds.

References:

1. F.A. Cotton, G. Wilkinson, C.A. Murillo and M. Bochmann, Advanced Inorganic Chemistry, Wiley, 2021.
2. A.G. Massy, Main Group Chemistry, Wiley, 2000.
3. J.E. Huhey, Harpes & Row, Inorganic Chemistry, Pearson, 2006
4. N.N. Greenwood and A. Earnshow, Chemistry of the Elements, Pergamon, 1984
5. A.B.P. Lever, Inorganic Electronic Spectroscopy, Elsevier, 1968.
6. Ivano Bertini, Metal-Ligand Interactions in Chemistry, Physics and Biology, Springer, 2000.

AC 8103 ORGANIC CHEMISTRY - I

L	T	P	Cr
4	0	0	4

Course Objective: To develop an understanding and recognition of both structure and chemical transformations of organic molecules.

UNIT - I

General Aspects of Reaction Mechanism: Thermodynamic and kinetic requirements, kinetic and thermodynamic control, Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects; Effect of structure on reactivity - resonance and field effects, steric effect, quantitative treatment, Delocalized chemical bonding-conjugation, cross conjugation, resonance, hyperconjugation, tautomerism. Aromaticity in benzenoid and non-benzenoid compounds, alternant and non-alternant hydrocarbons, Huckel's rule.

(8 hr)

Organic Reaction Intermediates: Carbanions: Generation, structure and stability of carbanions, Ambient ions and their general reactions; **Carbocation:** Structure and stability of carbocations, Classical and non-classical carbocations, phenonium ions, norbornyl system, Neighbouring group mechanism, neighbouring group participation by π and σ bonds, anchimeric assistance, and rearrangements including Wagner-Meerwein, Pinacol-pinacolone, semi-pinacol rearrangement, C-C bond formation involving carbocations; **Carbenes and Nitrenes**: Structure of carbenes, generation of carbenes, addition and insertion reactions, rearrangement reactions of carbenes, and N-heterocyclic carbene (NHCs), Structure of nitrenes, generation and reactions of nitrenes and related electron deficient nitrogen intermediates, Curtius, Hoffmann, Schmidt, Beckmann rearrangement reactions; **Free Radicals**: Generation of radical intermediates and its (a) addition to alkenes, alkynes (inter & intra-molecular) for C-C bond formation and Baldwin's rules (b) fragmentation and rearrangements. Name reactions involving radical intermediates such as Barton deoxygenation and decarboxylation, McMurry coupling etc

(14 hr)

Aliphatic Nucleophilic Substitution: The S_N2, S_N1, mixed S_N1 and S_N2 and SET mechanisms. The S_Ni 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

(6 hr)

UNIT - II

Aliphatic Electrophilic Substitution: Bimolecular mechanisms- S_E2 and S_Ei. The S_E1 mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity

(5 hr)

Aromatic Electrophilic Substitution: 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 reaction, Gattermann-Koch reaction.

(6 hr)

Aromatic Nucleophilic Substitution: The S_NAr, S_N1, benzyne and $S_{RN}1$ mechanisms. Reactivity - effect of substrate structure, leaving group and attacking nucleophile. The von Richter, Sommelet-Hauser and Smiles rearrangements.

(5 hr)

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. Reactvity in the attacking radicals. The effect of solvents on reactivity. Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction. Free radical rearrangement. Hunsdiecker reaction.

(6 hr)

Elimination Reactions: The E_2, E_1 and E_1cB mechanisms and their spectrum. Orientation of the double bond. Reactivity - effects of substrate structures, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination

(6 hr)

Learning Outcome Upon successful completion of this course the students will be able to

1. predict outcomes and draw mechanisms for substitution and elimination reactions.
2. understand aromaticity, nonaromaticity and antiaromaticity in organic compounds.

3. explain the effect of solvent polarity and temperature on the reaction mechanism.
4. utilize their knowledge for multi-step synthetic planning.

References:

1. F. A. Carey and R. J. Sundberg, Advanced Organic Chemistry, Springer, 2008.
2. Peter Sykes, A Guide Book to Mechanism in Organic Chemistry, Pearson, 2013
3. R. Bruckner, Advanced Organic Chemistry: Reaction Mechanisms, Academic press (Elsevier), 2001.
4. R. T. Morrison and R. N. Boyd, Organic Chemistry 7th Edition, Pearson, 2010.
5. S. M. Mukherji and S. P. Singh, Reaction Mechanism in Organic Chemistry, Macmillan, 2007.
6. Jerry March, Advanced Organic Chemistry-Reactions, Mechanism and Structure, John Wiley, 2015.

AC 8104 COMPUTERS FOR CHEMISTS

L	T	P	Cr
2	0	2	2

Course Objective: To divulge the knowledge of computer and use of modern computing resources in chemistry; to learn C programming language and apply in chemical problems; to prepare materials for publishing in papers in chemical drawings and models.

UNIT-I

Introduction to Computers and Computing: Basic structure and functioning of computers, Memory, Input/Output devices, Computer languages, Operating systems, Introduction to UNIX and WINDOWS. **(6 hr)**

Computer Programming using C language: Elements of the computer language. Constants and variables, Operations and symbols, Expressions, Arithmetic statement, Input and Output statements, Branching statements, functions, arrays and structures, files and pointers. LOGICAL variables. Double precision variables. Subscripted variables and DIMENSION. DO statement. FUNCTION and SUBROUTINE. COMMON and DATA statements. **(8 hr)**

UNIT-II

Applications of C language in chemistry: Development of small computer codes involving simple formulae in chemistry, such as van der Waals equation, pH titration, kinetics, radioactive decay. Evaluation of lattice energy and ionic radii from experimental data. Linear simultaneous equations to solve secular equations within the Huckel theory. **(6 hr)**

Use of Computer in Chemistry: Use of excel in chemistry, chemistry drawing and molecular modeling packages. (Accelrys Draw, MarvinSketch, Chemsketch, Avogadro, Chemoffice, ADF, Scigress or Spartan), modeling of organic and inorganic molecules using molecular mechanics method. Elementary structural features such as bond lengths, bond angles, dihedral angles etc. of molecules extracted from a database such as Cambridge data base. Plotting of graphs (Gnuplot, Origin or any other graphing package) **(8 hr)**

Learning Outcome Upon successful completion of this course the students will be able to

1. use computer in chemical applications
2. write a C program for problem solving
3. design computer-based programs for chemistry.
4. evaluate and verify data.
5. prepare matters for chemistry publications.

References:

1. R. Hunt and J. Shelley, Computers and Common Sense, Prentice Hall, 1983.
2 A.C. Norris, Computational Chemistry, Wiley–Blackwell, 1981
3 J.P. Killngbeck, Microcomputer Quantum Mechanics, Adam Hilger, 1983.

4 Y. Kantkar, Let us C, BPB Publications, 2004.
5 V. Rajaraman and T. Radhakrishnan, An Introduction to Digital Computer Design, Prentice Hall, 2004
6. M. Sipser, Introduction to theory of computation, Course Technology, 2012.
7. P. Norton, Introduction to computer, McGraw Hills, 2017.

AC- 8105A MATHEMATICS FOR CHEMISTS

L	T	P	Cr
2	0	0	2

Course Objective: To provide a foundation of basic mathematics for chemists at an introductory level.

UNIT-I

Real number system; Linear and quadratic equations; Permutations and combinations; Binomial theorem, Complex numbers; Limit. Continuity and differentiability, Cartesian graphing with first and second derivatives, Asymptotes and Dominant terms, Taylor series. Integration by parts, Substitution, Partial fraction, Definite Integrals and applications to length of curves, Area of Regions. **(13 hr)**

UNIT-II

Differential equations of first order, second order differential equations with constant coefficients.
Determinants and matrices: Elementary operations. Solution of Linear systems, Matrix Inversion.
Systems of Co-ordinates in Two-Dimension, distance formula, area of triangle, locus, slope of line, various forms of equations of a line, equation of circle (Standard and general form) **(15 hr)**

Learning Outcome Upon successful completion of this course the students will be able to

1. estimate the numerical accuracy of results
2. plot and interpret graphs

References:

1. H.S. Hall and S.R. Knight, Higher Algebra, Laxmi Publications, 2016.
2. G.B. Thomas and R.L. Finney, Calculus and Analytical Geometry, Pearson Education, 2010.
3. G.F Simmons Differential Equations (with historical notes), McGraw Hill, 2017.
4. G. Zill, Advanced Engineering Mathematics, Jones & Bartlett, 2017.
5. R. Bronson, Differential Equations, McGraw Hills, 2014.

AC- 8105B BIOLOGY FOR CHEMISTS

L	T	P	Cr
2	0	0	2

Course Objective: To introduce structure function and mechanistic action of the major classes of biomolecules.

UNIT-I

Cell Structure and Functions: Structure of prokaryotic and eukaryotic cells, intracellular organelles and their functions, comparison of plant and animal cells. **(2 hr)**

Carbohydrates: Conformation of monosaccharides, structure and functions of important derivatives of monosaccharides 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 functions of glucosaminoglycans or mucopolysaccharides; Role of sugars in biological recognition; Blood group substances. **(5 hr)**

Lipids: Fatty acids, essential fatty acids, structure and function of triacylglycerols, glycerophospholipids, sphingolipids, cholesterol, bile acids, prostaglandins. Lipoproteins composition 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. **(5 hr)**

UNIT-II

Amino-acids, Peptides and Proteins: Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing. Secondary structure of proteins forces responsible for holding of secondary structures. α-helix, β-sheets, super secondary structure, triple helix structure of collagen. Tertiary structure of protein- folding and domain structure; Quaternary structure. **(8 hr)**

Nucleic Acids: Purine and pyrimidine bases of nucleic acids, base pairing via H-bonding. Structure of ribonucleic acids (RNA) and deoxyribonucleic acids (DNA), double helix model of DNA and forces responsible for holding it; The chemical basis for heredity, an overview of replication of DNA, transcription, translation and genetic code. **(8 hr)**

Learning Outcome Upon successful completion of this course the students will be able to

1. understand working principles of living cell.
2. know the molecular structures, function and energetic of bio-molecules.
3. understand the significance of bio-molecules.

References:

1. A. L. Lehninger, Principles of Biochemistry, Worth Publishers, 2017.
2. L. Stryer, Biochemistry, W.H. Freeman, 2017.
3. J. David Rawn, Neil Patterson, Biochemistry, Pentice Hall, 2006.
4. Voet and Voet, Biochemistry, John Wiley, 2018.
5. E. E.Conn and P. K. Stumpf, Outlines of Biochemistry, John Wiley, 1972.
6. P. Kuchel, Enzymes, MGraw Hill, 2009.
7. R. Horton, Principle of Biochemistry, Pearson, 2011.

AC 8201 PHYSICAL CHEMISTRY II

L	T	P	Cr
4	0	0	4

Course Objective: To introduce the fundamental principles of quantum chemistry, the quantum chemical description of chemical bonding, reactivity and their applications in molecular spectroscopy and inorganic chemistry, surface chemistry, macromolecules.

UNIT-I

Quantum Chemistry

Quantum mechanics: Introduction, Schrodinger equation and the postulates of quantum mechanics. Discussion of solutions of the Schrodinger equation to some model systems viz., particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom. **(6 hr)**

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. **(3 hr)**

Angular Momentum: Ordinary angular momentum, generalized angular momentum, eigen functions for angular momentum, eigen values of angular momentum, operator using ladder operators, addition of angular momenta, spin, anti symmetry and Pauli exclusion principle. **(6 hr)**

Electronic Structure of Atoms: Electronic configuration, Russell-Saunders terms and coupling schemes, Slater-Condon parameters, term separation energies of the p^n configuration, term separation energies for the d^n configurations, magnetic effects: spin-orbit coupling and Zeeman splitting, introduction to the methods of self - consistent field, the virial theorem. **(9 hr)**

Molecular orbital theory: Hydrogen molecule ion. LCAO-MO and VB treatments of the hydrogen molecule; electron density, forces and their role in chemical binding. Hybridization and valence MOs of H_2O, NH_3 and CH_4. Huckel theory of conjugated systems, bond order and charge density calculations. Applications to ethylene, butadiene, cyclopropenyl radical and cyclobutadiene. **(12 hr)**

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), and catalytic activity at surfaces. **(5 hr)**

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, solubilization, micro emulsion, reverse micelles. **(5 hr)**

Macromolecules: Polymer - definition, types of polymers, electrically conducting, fire resistant, liquid crystal polymers, kinetics of polymerization, and 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 dimensions of various chain structures. **(10 hr)**

Learning Outcome Upon successful completion of this course the students will be able to

1. understand quantum chemical description Schrodinger equation for a particle in a box.
2. explain electronic and Hamiltonian operators for molecules.
3. demonstrate knowledge and understanding of basic concepts in quantum mechanics, atomic and molecular structure.
4. understand significance of adsorption isotherms and catalytic activity at the solid surfaces
5. demonstrate knowledge and understanding of polymerization process.

References:

1. P.W. Atkins, Physical Chemistry, Oxford Press University, 2018.
2. A. K. Chandra, Introduction to Quantum Chemistry, Tata McGraw Hill, 2017.
3. I. N. Levine, Quantum Chemistry, Pearsons, 2013.
4. A. McWeeny, Coulson's Valence, Oxford Press University, 1979.

5. V. Moroi, Micelles, Theoretical and Applied Aspects, Springer, 1992.
6. A. McQuarrie, Quantum Chmistry, Viva Books, 2016.
7. G. Elias, Macromolecules: Applications of Polymer, Wiley, 2009.

AC 8202 INORGANIC CHEMISTRY - II

L	T	P	Cr
4	0	0	4

Course Objective: To introduce theories, reaction mechanism and stability of the coordination complexes, metal carbonyls, metal clusters, organometallics and nuclear chemistry.

UNIT-I

Thermodynamics and Kinetics of Transition Metal Complexes: Energy profile of a reaction, reactivity of metal complexes, 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, anation reactions, reactions without metal ligand bond cleavage. Substitution reactions in square planar complexes, the trans effect, mechanism of the substitution reaction. Redox reactions, electron transfer reactions, mechanism of one electron transfer reactions, electron transfer reaction in biological systems. Inorganic photochemistry, photochemistry of dn complexes, Photochemistry of carbonyl compounds. **(14 hr)**

Metal-Ligand Equilibria in Solution: Stepwise and overall formation constants and their interaction, trends in stepwise constants, 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 pH-metry and spectrophotometry. **(14 hr)**

UNIT-II

Organometallic Chemistry: Hapto-nomenclature, classification of ligands (no. of electron donors), 18-electron rule, synthesis, structure and bonding aspects of complexes of two electron donor (olefin and acetylenic complexes of transition metals); three electron donor (π-allyl complexes of transition metals); four electron donor (butadiene and cyclobutadiene complexes of transition metals); five electron donor (cyclopentadienyl complexes of transition metals – metallocenes with special emphasis to ferrocenes); and six electron donor [Benzene (arene) complex].Important reactions (hydroformylation, Insertion reactions) **(12 hr)**

Cages and Metal Clusters: Higher boranes, carboranes, metalloboranes, metallocarboranes, compounds with metal-metal multiple bonds, Metal carbonyls. **(10 hr)**
Nuclear Chemistry: Nuclear reactions, fission and fusion, radio-analytical techniques and activation analysis. **(6 hr)**

Learning Outcome Upon successful completion of this course the students will be able to

1. understand reaction mechanism and stability of the coordination complexes.
2. demonstrate knowledge and understanding of organomattlics and the formation of metal clusters.

References:

1. F.A. Cotton, G. Wilkinson, C.A. Murillo and M. Bochmann, Advanced Inorganic Chemistry, Wiley, 2021.
2. J.E. Huheey, Inorganic Chemistry, Pearsons, 2006.
3. N.N. Greenwood and A. Earnshow, Chemistry of the Elements., Pergamon, 2012.
4. A.B.P. Lever, Inorganic Electronic Spectroscopy, Elsevier, 1968.
5. A.L. Carlin, Magneto-chemistry, Springer, 1986.
6. G. Wilkinson, A.D. Gillars and J.A. McCleverty, Comprehensive Coordination Chemistry, Elsevier, 2003.
7. P. J. Dyson and J.S. McIndoe, Transition metal carbonyls cluster chemistry, CRC press. 2019.

AC 8203 ORGANIC CHEMISTRY-II

L	T	P	Cr
4	0	0	4

Course Objective: To divulge advanced knowledge of aromaticity, stereoisomerism in organic compounds and photochemical and pericyclic reactions in organic chemistry.

UNIT - I

Stereochemistry: Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity, conformation of sugars, steric strain due to unavoidable crowding. Elements of symmetry, chirality, R-S nomenclature, diastereoisomerism in acyclic and cyclic systems; E-Z isomerisms. Interconversion of Fischer, Newman and Sawhorse projections, molecules with more than one chiral center, threo and erythro isomers, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis. Optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape. Stereochemistry of the compounds containing nitrogen, sulphur and phosphorus.

(18 hr)

Photochemical Reactions: Cis-trans isomeriation, Paterno-Buchi reaction, Norrish Type I and II reactions, photoreduction of ketones, di-pimethane rearrangement, photochemistry of arenes

(10 hr)

UNIT - II

Pericyclic Reactions: Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3- butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams. FMO and PMO approach.

(10 hr)

Electrocyclic reactions: Conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems. Cycloadddithions - antarafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3 dipolar cycloadditions and cheleotropic reactions.

(8 hr)

Sigmatropic rearrangements: - Suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 3,3- and 5,5- sigmatropic rearrangements. Claisen, Cope and aza-Cope rearrangements; Fluxional tautomerism. Ene reaction.

(10 hr)

Learning Outcome Upon successful completion of this course the students will be able to

1. explain conformational changes of cycloalkanes, reactivity, chirality, interconversion, resolution and asymmetric synthesis.
2. understand basics concepts of organic photochemistry.
3. demonstrate the knowledge and understanding of thermally and photochemically pericyclic reactions.

References:

1. P. S. Kalsi, Stereochemistry: conformation and mechanism, New Age Publisher, 2009.
2. D. Nasipuri, Stereochemistry of Organic Compounds, New Age Publisher, 2020.
3. E. I. Eliel, Stereochemistry of Organic Compounds, Tata McGraw-Hill, 2008.
4. S. M. Mukherji, Pericyclic Reactions: A Mechanistic Study, Macmillan, 1979.
5. I. Fleming, Pericyclic Reactions, OUP Oxford, 2015.
6. B. Dinda, Essential of Pericylic and Photochemistry, Springer, 2017

AC 8204 GROUP THEORY AND SPECTROSCOPY

L	T	P	Cr
3	0	0	3

Course Objective: To introduce the basic concepts of group theory in chemistry, electronic, molecular, rotation, vibration, Raman spectroscopy and their applications.

UNIT-I

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}). Character of a representation. The great orthogonality theorem and its importance. Character tables and their uses. **(10 hr)**

Unifying Principles: Electromagnetic radiation, interaction of electromagnetic radiation with matter - absorption, emission, transmission, reflection, refraction, dispersion, polarisation and scattering. Uncertainty relation and natural line width and natural line broadening, transition probability, results of the time dependent perturbation theory, transition moment, selection rules, intensity of spectral lines, Born-Oppenheimer approximation, rotational, vibrational and electronic energy levels. **(15 hr)**

UNIT-II

Microwave Spectroscopy: Classification of molecules, rigid rotor model, effect of isotopic substitution on the transition frequencies, intensities, non-rigid rotor. Stark effect, nuclear and electron spin interaction and effect of external field. Applications. **(5 hr)**

Vibrational Spectroscopy: *Infrared Spectroscopy* – Simple harmonic oscillator, vibrational energies of diatomic molecules, zero-point energy, force constant and bond strengths; anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy, P, Q, R branches. Breakdown of Oppenheimer approximation; vibrations of polyatomic molecules. Selection rules, normal modes of vibration, group frequencies, overtones, hot bands, factors affecting the band positions and intensities, metal-ligand vibrations, normal co-ordinate analysis. **(6 hr)**

Raman Spectroscopy - Classical and quantum theories of Raman effect. Pure rotational, vibrational and vibrational-rotational Raman spectra, selection rules, mutual exclusion principle. Resonance Raman spectroscopy, coherent anti Stokes Raman spectroscopy (CARS). **(6 hr)**

Electronic Spectroscopy: *Atomic Spectroscopy* - Energies of atomic orbitals, vector representation of momenta and vector coupling, spectra of hydrogen atom and alkali metal atoms. **(6 hr)**

Molecular Spectroscopy - Energy levels, molecular orbitals, vibronic transitions, vibrational progressions and geometry of the excited states, Franck-Condon principle, electronic spectra of polyatomic molecules. Emission spectra; radiative and non-radiative decay, internal conversion, spectra of transition metal complexes, charge-transfer spectra. **(10 hr)**

Learning Outcome Upon successful completion of this course the students will be able to

1. categorize molecules on the basis of their symmetry properties, which allow the prediction of many molecular properties explain conformational changes of cycloalkanes, reactivity, chirality, interconversion, resolution and asymmetric synthesis.
2. use microwave, infrared-vibration-rotation and Raman spectroscopy techniques for chemical analysis.
3. demonstrate the knowledge and understanding Electronic and molecular spectroscopy of different elements and molecules.

References:

1. J.M. Hollas, Modern Spectroscopy, John Wiley, 2004.
2. Ed. H. Windawi and F.L. Ho, Applied Electron Spectroscopy for Chemical Analysis, Wiley Interscience, 1982.
3. R.V. Parish, NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, Ellis Harwood, 1990.
4. R.S. Drago, Physical Methods in Chemistry, Saunders College, 1992.
5. F. A. Cotton, Chemical Applications of Group Theory, Wiley, 2020.
6. G.M. Barrow, Introduction to Molecular Spectroscopy, McGraw Hill, 2018.
7. R. Chang, Basic Principles of Spectroscopy, McGraw Hill, 1971.
8. H.H. Jaffe and M. Orchin, Theory and Applications of UV Spectroscopy, IBH- Oxford, 1962.

AC 8205 ANALYTICAL CHEMISTRY

L	T	P	Cr
3	0	0	3

Course Objective: To introduce the concepts of various analytical techniques, to evaluate data and statistical evaluation. To gain fundamental concept for instrumentation and non-instrumentation analysis and applications.

UNIT-I

Errors in Quantitative Analysis: Accuracy, precision, sensitivity, specificity, standard deviation, classification of errors and their minimization, significant figures, criteria for rejection of data, Q-test, t-test and F-test, control chart, sampling methods, sampling error, Standard Reference, Materials, Statistical data treatment. **(10 hr)**

Theories of non-instrumental methods of Analysis: Nucleation, co-precipitation, post-precipitation, precipitation from homogeneous solutions; Organic reagents, Precipitation titration (Volhards and Mohrs methods) redox titrations, complexometric titrations, metal ion indicators, masking. **(8 hr)**

UNIT-II

Spectral methods: Principle, instrumentation, advantages, applications and limitations of – Spectrophotometery, Beer-Lambert Law, Analysis of mixtures, Atomic absorption spectrometery (AAS), Flame photometry (AES), single and double beam spectrophotometers, fluorimetry, nepheleometry and turbimetry. **(8 hr)**

Electroanalytical methods: Voltammetry, cyclic voltammetry, amperometry, coulometry and conductometry, ion-selective electrodes. Anodic stripping voltammetry; Potentiometry. **(6 hr)**

Modern Techniques: XRD, SEM, TEM, TGA, DTA, DSC - Instrumentation, methodology, applications. **(6 hr)**

Chromatographic Techniques: Basic principles and applications high performance liquid chromatography (HPLC), gas chromatography (GC), ion chromatography (IC). **(3 hr)**

Learning Outcome Upon successful completion of this course the students will be able to

1. calculate error, precision and accuracy
2. get through knowledge on instrumental and non-instrumental method analysis

References:

1. L.G. Hargis, Analytical Chemistry Principles and Techniques, Prentice Hall, USA, 1987.
2. H.H. Willard, L.L. Merritt, Jr., J.A. Dean and F.A. Settle, Instrumental methods of analysis, CBS Publishers, 2004.
3. D.A. Skoog, F.J. Holler and S.R. Crouch, Principles of instrumental analysis, Cengage Learning, 2020.
4. G.H. Jeffery, J. Bassett, J. Mendham and R.C. Denney, Vogel's Text book of Quantitative Chemical Analysis, Longman Scientific and Technical, 1989.
5. A. R. Tatchell Vogel's Textbook of Practical Organic Chemistry, Wiley, 1989.
6. J. Shen, Spectral Methods, Springer, 2011.
7. F. Scholz, Electroanalytical methods, Springer, 2010.

AC 9101 SPECTROSCOPIC TECHNIQUES

L	T	P	Cr
5	0	0	5

Course objective; Introduce the theory of the various instruments and the signals produced when analysing compound. Equip the student with enough information to be able to interpret signals from spectroscopic instruments

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 and heterocyclic compounds. Steric effect in biphenyls. **(12 hr)**

Infrared Spectroscopy: Instrumentation and sample handling. Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and 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. FT IR. IR of gaseous, solids and polymeric materials. **(10 hr)**

UNIT-II

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, aldehydic and aromatic) and other nuclei (alcohols, phenols, 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, hindered rotation, Karplus curvevariation of coupling constant with dihedral angle. Simplification of complex spectranuclear magnetic double resonance, contact shift reagents, solvent effects. Fourier transform technique, nuclear Overhauser effect (NOE).

Resonance of other nuclei-F & P. **^{13}C-NMR Spectroscopy:** General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants; Two-dimensional NMR spectroscopy - COSY, NOESY, DEPT, INEPT, APT and INADEQUATE techniques. **(22 hr)**

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, McLafferty rearrangement. Nitrogen rule. High resolution mass spectrometery. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination. **(12 hr)**

Learning Outcomes

1. Study the spectra of compounds and propose structures for compounds. (Skills)
2. Study spectra of compounds, determination of functional groups and skill to write structures

References:

1. R.S. Drago, Physical Methods for Chemistry (2nd Ed.), East West Press Pvt. Ltd. 2016.
2. E.A.V. Ebsworth, D.W.H. Rankin and S. Cradock Structural Methods in Inorganic Chemistry (2nd Ed) Blackwell 1991.
3. K. Nakamoto, Infrared and Raman Spectra: Inorganic and Coordination Compounds (6th Ed.), Wiley, 2008.
4. A.P.B. Lever, M.F. Leppert, Inorganic Electronic Spectroscopy, Elsevier Science Ltd. 1968.
5. R.V. Parish, NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, Ellis Horwood Ltd. 1990.
6. M.L. Martin, J.J. Delpeuch and G.J. Martin, Practical NMR Spectroscopy, Heyden, 1980.
7. R. M. Silverstein, F.X. Webster, D.J. Kiemle, and D.L. Bryce, Spectrometric Identification of Organic Compounds (8th Ed.), Wiley, 2014.
8. R. J. Abraham, J. Fisher and P. Loftus, Introduction to NMR Spectroscopy, Wiley, 1988.
9. J. R. Dyer, Application of Spectroscopy of Organic Compounds, Prentice Hall, 1988.
10. D. H. Williams, I. Fleming, Spectroscopic Methods in Organic Chemistry, Tata McGraw-Hill Education 2011.

AC 9102 ENVIRONMENTAL CHEMISTRY

L	T	P	Cr
4	0	0	4

Course Objective: To introduce the fundamental principles of Biogeochemical cycles, Hydrological cycle, Water quality parameters, Chemical composition of atmosphere, Industrial Pollution

UNIT-I

Environment: Introduction. Composition of atmosphere, vertical temperature, heat budget of the earth atmospheric system, vertical stability atmosphere. Biogeochemical cycles of C, N, P, S and O. Bio-distribution of elements. **(8 hr)**
Hydrosphere: Chemical composition of water bodies - lakes, streams, rivers and wet lands etc. Hydrological cycle, Aquatic pollution - inorganic, organic, pesticide, agricultural, industrial and sewage, detergents, oil spills and oil pollutants. Water quality parameters - dissolved oxygen, biochemical oxygen demand, solids, metals, content of chloride, sulphate, phosphate, nitrate and micro-organisms. Water quality standards, Analytical methods for measuring BOD, DO, COD, F, Oils, residual chloride and chlorine demand, Purification and treatment of water. **(10 hr)**
Soils: Composition, micro and macro nutrients, Pollution-fertilizers, pesticides, plastics and metals. Waste treatment. **(10 hr)**

UNIT-II

Atmosphere: Chemical composition of atmosphere - particles, ions and radicals and their formation. Chemical and photochemical reactions in atmosphere, smog formation, oxides of N, C, S, O and their effect, pollution by chemicals, petroleum, minerals, chlorofluorohydrocarbons. Green house effect, acid rain, air pollution controls and their chemistry. Analytical methods for measuring air pollutants. Continuous monitoring instruments **(10 hr)**
Industrial Pollution: Disposal of wastes and their management **(8 hr)**
Environmental Toxicology: Chemical solutions to environmental problems, biodegradability, principles of decomposition, better industrial processes. **(10 hr)**

Learning outcomes: Upon successfully completion of this course the students will be able to

1. Knowledge of hydrosphere and various processes.
2. Understanding of biogeochemical cycles of C, N, O.
3. Knowledge of atmosphere and its components.
4. Knowledge of industrial waste and its management.

References:

1. S. E. Manahan, Environmental Chemistry, CRC Press, 2009.
2. B.K. Sharma, Environmental Chemistry, Krishna Publishers, 2019.
3. A. K. De, Environmental Chemistry (8th Ed.), New Age International Publishers, 2016.
4. S.M. Khopkar, Environmental Pollution Analysis, New Age International Publisher, 2020.
5. F.J. Welcher, Standard Method of Chemical Analysis, Vol. III, Van Nostrand Reinhold Co. 1966.
6. J. Rose (Ed.), Environmental Toxicology, Gordon and Breach Science Publication, 1998.
7. C. Baird and M. Cann, Environmental Chemistry, W. H. Freeman, 2008.

AC 9103 BIO-ORGANIC CHEMISTRY

L	T	P	Cr
4	0	0	4

Course Objective: To introduce the fundamental principles of Biosynthetic reactions, Mechanism of Enzyme Catalysis, Examples of some typical enzyme mechanisms, Enzyme catalyzed reactions.

UNIT-I

Basic concepts: Introduction, Background, Proximity and Orientation Effects, Molecular Adaptation **(5 hr)**
Biosynthetic reactions: Introduction, Catalytic Reactions, Phosphate in Biosynthesis, Hydride Transfer Reactions, Oxidation Reactions, Elimination Reaction, Acylation Reactions, Alkylation Reactions, Reduction, Condensation Reactions, Keto-enol Tautomerism **(6 hr)**
Enzymes: Introduction, History, General Characteristics of Enzymes, Chemical and Biological Catalysis, Specificity of Enzymes, Enzyme Regulation, Sources of Enzyme, Enzyme Units, Nomenclature and Classification, Extraction and

Purification, The Mechanism of Enzyme Catalysis, Factors Affecting Rate of Enzymic Reactions, Enzyme Kinetics **(6 hr)**

Mechanism of enzyme action: Introduction, Transition-State Theory, Examples of some typical enzyme mechanisms like mechanism for Chymotrypsin, Ribonuclease, Lysozyme and Carboxypeptidase A **(6 hr)**

Enzyme catalyzed reactions: Introduction, Nucleophilic Displacement on Phosphorus Atom (Formation of ATP from ADP; Formation of ADP from ATP; Nucleophilic Displacements at Phosphorous in ATP; Multiple Nucleophilic Displacements in ATP), Enzyme Catalyzed Hydrolysis of RNA, Transfer of Sulphate, Addition and Elimination Reactions, Enolic Intermediates in Isomerization Reactions, Elimination (β-Cleavage) Reactions, Condensation Reactions, Isomerization Reactions, Rearrangement Reactions (Claisen Rearrangement , [2,3]-Sigmatropic Rearrangement, Cyclo-addition Rearrangements, Carbonium ion Rearrangements), Enzyme Catalyzed Carboxylation and Decarboxylation. **(10 hr)**

UNIT-II

Co-enzyme chemistry: Introduction, Reactions and functions of - Coenzyme A, Thiamine Pyrophosphate, Pyridoxal Phosphate, Nicotinamide Adenine Dinucleotide (NAD) and Nicotinamide Adenine Dinucleotide Phosphate (NADP), .Flavin Mononuleotide (FMN) and Flavin Adenine Dinucleotide (FAD), Lipoic Acid, Cyanocobalamin (Vitamin B_{12}) **(10 hr)**

Enzyme models: Introduction, Molecular Recognition, Chiral Recognition, Supra-molecular Chemistry (Host-guest chemistry), Biomimetic Chemistry and Artificial Enzymes, Crown Ethers, Cryptates or Cryptands, Cyclodextrins, Calixarenes, Ionophores, Synthetic (Artificial) Enzymes (Synzymes) **(8 hr)**

Biotechnological Applications of Enzymes: Introduction, Immobilized Enzymes, Applications of Enzymes in Food Processing, Fruit Juices & Beverages, Dairy Industry, Oil and Fat Industry, Cereal Industry, Enzymes as Target for Drug Design, Clinical Uses of Enzymes. **(5 hr)**

Learning outcomes: Upon successfully completion of this course the students will be able to

1. Knowledge of Oxidation Reactions, Elimination Reaction in biosynthesis reactions.
2. Understanding of concepts of The Mechanism of Enzyme Catalysis, Factors Affecting Rate of Enzymic Reactions, Enzyme Kinetics
3. Understanding of Enzyme catalyzed reactions.

References:

1. S.J. Lippard and J.M. Berg, Principles of Bioinorganic Chemistry, University Science Books, 1994.
2. H. Dugas and C. Penny, Bioorganic Chemistry: A Chemical Approach to Enzyme Action, Springer Verlag, 1981.
3. T. Palmer, Understanding Enzymes, Ellis Horwood Ltd. 1995.
4. M. D. Trevan, Immobilized Enzymes: An Introduction and Applications in Biotechnology, Wiley-Blackwell, 1980.
5. H. K. Chopra, A. Parmar, and P. S. Panesar, P. S. Bio-organic Chemistry: Alpha Science Int. UK, 2013.
6. A. L. Lehninger and M.M. Cox, Principles of Biochemistry (8^{th} Ed.), Macmillan Learning, 2021.

AC 9104 CHEMISTRY OF NATURAL PRODUCTS

L	T	P	Cr
4	0	0	4

Course objective; make the students aware of the many pharmaceutically active products of natural origin, give students an awareness of the richness and diversity of plants and animal around them.

UNIT-I

Terpenoids and Carotenoids: Classification, 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, Zingiberene, Santonin, Phytol, Abietic acid and β-Carotene. **(8 hr)**

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 Ephedrine, (+)- Coniine, Nicotine, Atropine, Quinine and Morphine.

(8 hr)

Steroids: Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of Cholesterol, Bile acids, Androsterone, Testosterone, Estrone, Progestrone, Aldosterone. Biosynthesis of steroids **(10 hr)**

UNIT-II

Plant Pigments: Occurrence, nomenclature and general methods of structure determination. Isolation and synthesis of Apigenin, Luteolin, Quercetin, Myrcetin, Quercetin-3-glucoside, Vitexin, Diadzein, Butein, Aureusin, Cyanidin-7-arabinoside, Cyanidin, Hirsutidin. Biosynthesis of flavonoids: Acetate pathway and Shikimic acid pathway. **(6 hr)**

Porphyrins: Structure and synthesis of Haemoglobin and Chlorophyll. **(4 hr)**

Prostaglandins: Occurrence, nomenclature, classification, biogenesis and physiological effects. Synthesis of PGE_2 and $PGF_{2\alpha}$. **(4 hr)**

Pyrethroids and Rotenones: Synthesis and reactions of Pyrethroids and Rotenones **(2 hr)**

Learning outcomes

1. identify and characterize various classes of natural products by their structures;
2. appreciate the biogenesis of many natural products of importance;
3. have some knowledge of some of the plants around them and their pharmaceutical importance.
4. have some knowledge of bacteria, fungi and other life forms from which useful pharmaceuticals are derived;
5. have acquired the skills to isolate and purify simple products that are derived from plants and some animals;

References:

1. J. Mann, R.S.Davidson, J.B. Hobbs,. D.V. Banthrope and J. B. Harborne, Natural Products: Chemistry and Biological Significance, Longman,Essex, 1994.
2. I.L. Finar, Organic Chemistry, Vol. 2, Pearson Education India, 2013.
3. M. Nogradi Stereoselective Synthesis: A Practical Approach, VCH, 1994.
4. Ed. S. Coffey Rodd's Chemistry of Carbon Compounds, Elsevier, 1965.
5. K. Hostettmann, M.P. Gupta and A. Marston (Eds.), Chemistry, Biological and Pharmacological Properties of Medicinal Plants from the Americas, Routledge, 2018.
6. B.A. Bohm, Introduction to Flavonoids, CRC Press, 1999.
7. Atta-ur-Rahman and M.I. Choudhary New Trends in Natural Product Chemistry, CRC Press, 1998.
8. S. Dev and O. Kaul, Insecticides of Natural Origin, Routledge, 2017.
9. P.S. Kalsi, S. Jagtap, Pharmaceutical, Medicinal and Natural Product Chemistry, Alpha Science International Ltd. 2013.

AC- 9105 ADVANCED CO-ORDINATION CHEMISTRY

L	T	P	Cr
4	0	0	4

Course Objective: To give theoretical background of electronic spectra and magnetic properties of the transition metal and coordination complexes; Electron Paramagnetic Resonance Spectroscopy, Nuclear Quadruple Resonance (NQR) and Reactions of coordinated ligands.

UNIT-I

Electronic Spectra of Transition Metal Complexes: Determination of state functions of R-S terms of d^2 and p^2, transition metal ions, Spectroscopic ground states; Orgel energy level and Tanabe-Sugano diagrams for transition metal complexes; Charge transfer spectra; electronic spectra of octahedral and tetrahedral Co(II) and Ni(II) complexes and calculation of ligand-field parameters. **(11 hr)**

Magnetism in Coordination Complexes: Derivation of Van Vleck's expression and spin-only formula, orbital contribution for d-metal ions and quenching in cubic crystal field. Magnetic moments based on crystal field ground term, Perturbation Theory and its application, Spin orbit coupling operator for magnetic susceptibility and magnetic moment of T terms and A, E terms. Anomalous magnetic moments in magnetically dilute and concentrated system in various symmetrical environments of coordination complexes. **(10 hr)**

UNIT-II

Electron Paramagnetic Resonance Spectroscopy (EPR): Theory and Instrumentation of EPR, Spin Hamiltonian, Isotropic and anisotropic EPR spectra, Magic Pentagon rule. Applications of EPR spectroscopy in structur determination of inorganic complexes and metalloproteins (Fe, Cu). **(9 hr)**

Nuclear Quadruple Resonance (NQR) Principle selection rule for NQR. Factors for splitting of quadruple energy levels in NQR, Effect of Magnetic Field. Application of NQR: Structural information from NQR. **(6 hr)** **6 hr)**

Reactions of coordinated ligands: Non-chelate forming reactions: Reaction of donor atoms (Halogenation of coordinated N atoms, Alkylation of coordinated S and N atoms, Solvolysis of coordinated phosphorus atoms). Reactions of non-donor atoms (nucleophilic behaviour of the ligand, electrophilic bahaviour of the ligand). Chelate ring forming reactions: (reactions predominantly involving thermodynamic template effects, reactions predominantly involving kinetic affects). Chelate modifying reactions. **(10 hr)**

Learning Outcome Upon successful completion of this course the students will be able to

1. explain the and interpret electronic spectra and magnetic properties of the coordination complexes.
2. interpret the EPR and NQR spectra of simple and complex molecules.
3. to identify, write and give the mechanism of the reaction of coordinated ligands in metal complexes.

References:.

1. Magnetism and Transition Metal Complexes", F. E. Mabbs and D. J. Machin (Chapman and Hall) London (1973).
2. Introduction to Magnetochemistry, A. Earnshaw, Academic Press, (1968).
3. Elements of Magnetochemistry, R. L. Dutta and A. Syamal, Affiliated East/West Press Pvt. Ltd. 2007.
4. Inorganic Chemistry, D.F.Shriver, P.W.Atkins and C.H.Langford, Oxford, 2nd. edn. 1994.
5. An Introduction to Inorganic Chemistry by K.F.Purcell and J.C.Kotz, Saunders 1990, Chapter 14.
6. Comprehensive Coordination Chemistry, Vol.1. G Wilkinson (Ed) Wiley, New York, 1967.

AC- 9106 BIO-INORGANIC CHEMISTRY

L	T	P	Cr
4	0	0	4

Course Objective: To understands the concepts of Bio-inorganic chemistry in biological process, and to utilize this knowledge to analyze the influence of such process on the reactivity of a metal centre.

UNIT-I

Metalloporphyrins: Porphyrins and their salient features, characteristic absorption spectrum of porphyrins, chlorophyll (structure and its role in photosynthesis). **(8 hr)**

Metalloenzymes: Definitions: Apoenzyme, Coenzyme, Metalloenzyme, structure and functions of carbonic anhydrase A & B, carboxy peptidases. **(7 hr)**

Oxygen Carriers: *Natural oxygen carriers:* Structure of hemoglobin and myoglobin, Bohr effect, Models for cooperative interaction in hemoglobin, oxygen Transport in human body (-perutz machanism), Cyanide poisoning and its remedy. Non-heme protiens (Hemerythrin & Hemocyanin).

Synthetic oxygen carriers: Oxygen molecule and its reduction products, model compounds for oxygen carrier (Vaska's Iridium complex, cobalt complexes with dimethyl glyoxime and Schiff base ligands). **(6 hr)**

UNIT-II

Transport and storage of metals: The transport mechanism, transport of alkali and alkaline earth metals, ionophores, transport by neutral macrocycles and anionic carriers, sodium/potassium pump, transport and storage of

Iron (Transferrin & Ferritin). Transport of Iron in microorganisms (sidrophores), types of sidrophores (catecholate and Hydroxmato siderophores). **(8 hr)**

Inorganic compounds as therapatic Agents: - Introduction chelation therapy, synthetic metal chelates as antimicrobial agents, antiarthritis drugs, antitumor, anticancer drugs (Platinum complexes), Lithium and mental health. **(7 hr)**

Nitrogen Fixation:

I. Nitrogen molecule (M.O.picture) and its transition metal complexes, reactivity of coordinated dinitrogen, In vitro & In vivo nitrogen fixation, Nitrogen cycle, Symbiotic and Asymbiotic nitrogen fixation.

II. ***Nitrogen metabolism:*** Introduction, elementary idea about nitrogen nutrition in various forms (Nitrate and ammonia nitrogen, organic nitrogen and molecular nitrogen).. **(6 hr)**

Learning Outcome Upon successful completion of this course the students will be able to

1. apply the principles of coordination chemistry in the context of medicinal & pharmaceutical chemistry.
2. understand the concepts of coordination chemistry in biological environments, and to utilizes this knowledge to analyze the influence of such an environment on the reactivity of a metal centre.
3. describe the different functions metal ions can have in biological systems.

References :.

1. M. N. Hughes, The Inorganic Chemistry of Biological Processes, Wiley-Blackwell, 1981.
2. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, Wiley, 1999.
3. J. N.Lowe and L. Ingraham, An Introduction to Biochemcial Reaction Mechanism, 1974.
4. M.R. Blatt, Plant Physiology Oxford Academic, 2021.

AC-9107 STATISTICAL MECHANICS

0L	T	P	Cr
4	0	0	4

UNIT-I

Course Objective: To introduce the fundamental principles of Statistical Mechanics, Partition Function, Bose-Einstein Distribution, Fermi-Dirac Distribution and Non-equilibrium States.

Review of Basic Statistical Mechanics: A Review of Thermodynamics and Kinetic theory of gases. Phase space. Ensemble. Liouville theorem. Equal a priori probability. Microcanonical ensemble. Quantization of phase space. Classical limit. Various distributions using micocano-nical ensemble. Entropy. Gibbs paradox. Entropy of a two level system. Canonical and grand canonical ensembles. Equipartition of energy. Ideal gas in canonical and grand canonical ensembles. **(12 hr)**

Partition Function: Review of rotational, vibrational and translational partition functions. Application of partition function to specific heat of solids and chemical equilibrium. Real gases. **(12 hr)**

UNIT-II

Bose-Einstein Distribution: Einstein condensation. Thermodynamic properties of ideal BE gas. **(3 hr)**

Fermi-Dirac Distribution: Degenerate Fermi Gas. Electron in metals. Magnetic susceptibility. **(5 hr)**

Fluctuations : Mean square deviation and fluctuation in ensembles. Concentration fluctuation in quantum statistics. **(5 hr)**

Non-equilibrium States : Boltzmann transport equation.Particle diffusion. Electrical conductivity **(5 hr)**

Learning Outcome Upon successful completion of this course the students will be able to

1. UnderstandEnsemble, Microcanonical ensemble, Ideal gas in canonical and grand canonical ensembles
2. ExplainEntropy. Gibbs paradox, Equipartition of energy.
3. demonstrate knowledge and understanding of basic concepts in rotational, vibrational and translational partition functions.
4. understand significance of partition function to specific heat of solids. Difference in BE and FD distribution.

References:

1. B.K. Agarwal and M. Eisner, Statistical Mechanics, Wiley Eastern, New Delhi, 1988.
2. D.A. McQuarrie, Statistical Mechanics, Harper and Row Publishers, New York, 1976.
3. P. Ehrenfest and T. Ehrenfest, The Conceptual Foundations of Statistical Approach in Mechanics, Dover Publications, 2014.
4. B. Bagchi, Statistical Mechanics for Chemistry and Material Science, CRC Press, 2018.

AC 9108 QUANTUM MECHANICS

L	T	P	Cr
4	0	0	4

Course Objective: To introduce the fundamental principles of Classical and quantum Mechanics, Approximation Methods, group theory, tunneling problem and Ab initio and Semi-empirical Methods for Closed Shell Systems.

UNIT-I

Fundamentals: Review of Classical Mechanics. General formulation of Qunatum Mechanics. Theory of angular momentum. Angular momentum of composite systems. Review of rigid rotor, harmonic oscillator and H- atom problems. **(10 hr)**

Approximation Methods: Stationary perturbation theory for non-degenerate and degenerate systems with examples. Variation method. Ground state of He atom. Time-dependent perturbation theory. Radiative transitions. Einstein coefficients. **(10 hr)**

UNIT-II

Group Theory : Review and applications. **(6 hr)**

Tunneling Problem : Tunneling through a rectangular barrier. Application examples. **(4 hr)**

Ab initio and Semi-empirical Methods for Closed Shell Systems: Roothaan-Hartree-Fock method. Selection of basis sets. Semiempirical methods. Density functional theory. **(12 hr)**

Learning Outcome Upon successful completion of this course the students will be able to

1. Understand the difference between classical and quantum mechanics, harmonic oscillator.
2. Explain H atom related problems.
3. demonstrate knowledge and understanding of basic concepts in approximation methods and group theory.
4. understand significance of group theory.

References :

1. P.W. Atkins and R.S. Friedman, Molecular Quantum Mechanics, Oxford University Press, 1997.
2. I.N. Levine, Quantum Chemistry, Pearson Educ. Inc. 2000.
3. A.K. Chandra, Introductory Quantum Chemistry (4^{th} Ed.), Mc-Graw Hill, 2017.

AC-9109A CHEMISTRY OF MATERIALS

L	T	P	Cr
4	0	0	4

Course Objective: To introduce the fundamental principles of Role of Chemistry in Material design, Synthesis and characterization of materials,; Fe-C phase transformations in ferrous alloys, Organic Materials, High T_c Materials.

UNIT-I

Introduction: Materials and their classification, Role of Chemistry in Material design. **(2 hr)**
Synthesis and characterization of materials: Preparative techniques: Ceramic methods; chemical strategies, chemical vapour deposition; preparation of nanomaterials, Langmuir- Blodgett Films. Fabrication of ordered nanostructures. Composition and purity of materials. **(4 hr)**
Multiphase Materials: Ferrous alloys; Fe-C phase transformations in ferrous alloys; stainless steels, non-ferrous alloys, properties of ferrous and non-ferrous alloys and their applications. **(4 hr)**
Glasses, Ceramics, Composites and Nanomaterials: Glassy state, glass formers and glass modifiers, mechanical properties, clay products. Refractories, applications.
Microscopic composites; dispersion-strengthened and particle-reinforced, fibre-reinforced composites, macroscopic composites. Nanocrystalline phase, preparation procedures, special properties, applications, ceramic structures, characterizations, properties. **(4 hr)**
Organic Materials : Conducting organics - Metals from molecules, charge transfer materials and conducting polymers. Organic superconductors. Fullerenes. Molecular ferromagnets and ferroelectrics. Liquid crystals: mesomorphic behaviour, optical properties of liquid crystals, display devices. **(4 hr)**

UNIT-II

Non-linear materials: Second and third order non-linear effects; molecular rectifiers and frequency doublers; unimolecular electronic devices. Photochromic materials; optical data storage, memory and switches. **(3 hr)**
Polymeric Materials: Molecular shape, structure and configuration, crystallinity, stress-strain behaviour, thermal behaviour, polymer types and their applications, conducting and ferro-electric polymers. **(3 hr)**
Ionic Conductors: Types of ionic conductors, mechanism of ionic conduction, interstitial jumps. (Frenkel); vacancy mechanism, diffusion superionic conductors; phase transitions and mechanism of conduction in superionic conductors, examples and applications of ionic conductors. **(6 hr)**
High T_c Materials: Defect perovskites, high Tc superconductivity in cuprates, preparation and. characterization of 1-2-3 and 2-1-4 materials, normal state properties; anisotropy; temperature dependence of electrical resistance; optical phonon modes, superconducting state; heat capacity; coherence length, elastic constants, position lifetimes, microwave absorption-pairing and multigap structure in high Tc materials, applications of high Tc materials. **(8 hr)**
Materials for Solid State Devices: Rectifiers, transistors, capacitors -IV-V compounds, low-dimensional quantum structures, optical properties. . **(6 hr)**

Learning outcomes: Upon successfully completion of this course the students will be able to
1. Knowledge of Role of Chemistry in Material design
2. Understanging of Ceramic methods; chemical strategies, chemical vapour deposition
3. Knowledge of Microscopic composites and its applications
4. Knowledge of Non-linear materials and Ionic Conductors

References:

1. W.D. Callister, Material Science and Engineering: An Introduction, Wiley, 2013.
2. H.V. Keer, Principles of the Solid State, Wiley Eastern, 2017.
3. J.C. Anderson, K.D. Leaver, J.M. Alexander and A.D. Rawlings, Materials Science, Springer, 1990.
4. G.W. Gray, Thermotropic Liquid Crystals, Wiley, 1988.
5. R. Upadhyay, Ionic Conductors, Random Publication, 2017.

AC 9109B ORGANOMETALLIC CHEMISTRY

L	T	P	Cr
3	0	0	3

Course Objective: To introduce the fundamental principles of organometallic compounds, polyhedral model of metal clusters, Metal carbenes and carbynes.

UNIT-I

Organometallic compounds: Overview of the comparative aspects of synthesis, structure and bonding of different types of organometallic compounds: Ionic covalent-Main group compounds containing M-C σ bonds, metal alkyls and aryls, electron deficient organometallic compounds, compounds of transition metal: metal alkyls and acyl compounds. Organometallic compounds with π-bonding ligands (non-classically bonded organometallics), concept of heptacity, 18 electron rule for π donor complexes, carbenes, alkylidenes, carbynes and alkylidynes; olefin or alkenyl, alkynyl, allyl, butadiene complexes; cyclic π complexes, cyclobutadiene, cyclopentadienyl, arene, cycloheptatrienyl and cyclooctatetraene complexes. **(10 hr)**

Metal-metal bonding in carbonyl and halide clusters:- Polyhedral model of metal clusters, effect of electronic configuration and coordination number, Structures of metal carbonyl clusters of three atoms $M3(CO)_{12}$ (M=Fe, Ru & Os), Four metal atoms (tetrahedra) [$M_4(CO)_{12}$ {M=, Co, Rh &Ir}] and octahedron of type $M_6(CO)_{16}$ [M= Co &Rh], and halide derivatives of Rhenium(III) triangels, Fluxional organometallic compounds (with acyclic alkenes, σ–bonded and π-bonded), metal carbonyls involving bridged-terminal exchange and scrambling of CO group. **(14 hr)**

UNIT-II

Transition Metal-Carbon multiple bonded compounds:-Metal carbenes and carbynes (preparation, reactions, structure and bonding considerations). **(6 hr)**

Applications of Organometallics Homogeneous catalysis by transition metal organometallics, the 16 and 18 electron rule in homogenous catalysis, hydroformylation, hydrogenation of olefins, olefins metathesis, Wacker Process, Polymerization of Alkenes (olefins) using Ziegler Natta catalyst, and Monsanto acetic acid synthesis.

Biological applications and environmental aspects of organometallic compounds, Organometallic compounds in medicine, agriculture and industry. **(12 hr)**

Learning Outcome Upon successful completion of this course the students will be able to

1. Knowledge of organometallic compound and its synthesis
2. Knowledge of Metal-metal bonding in carbonyl and halide clusters
3. Understating of Transition Metal-Carbon multiple bonded compounds and Applications of Organometallics

References:

1. P. Powell, principles of organometallic compounds, Springer, 1998.
2. R.C.Mehrotra, Organometallic Chemistry, New Age Publishers, 2020.
3. R. H. Crabtree Organometallic compounds of Transition Metals, Wiley, 2019.
4. N.N. Greenwood and A. Earnshaw, Chemistry of the Elements, Butterworth-Heinemann, 1997.
5. B. D. Gupta and A. J. Elias, Basic Organometallic Chemistry, Universities Press, 2013.
6. C. Masters, Homogeneous transition metal catalysis, Springer, 1981.
7. A. Nakamura and M. Tsutsui, Principles and Application of Homogeneous Catalysis, Wiley, 1980.

AC 9109C INSTRUMENTAL METHODS OF ANALYSIS

L	T	P	Cr
4	0	0	4

Course objective; Introduce the theory of the various instruments and the signals produced when analyzing compound. Equip the student with enough information to be able to interpret signals from spectroscopic instruments

UNIT-I

General Introduction to spectroscopy: Nature of radiation, energies corresponding to various kind of radiation, energies for atomic and molecular transitions. **(4 hr)**

Infrared Spectroscopy: Theory of IR absorption, types of vibrations, observed number of modes of vibrations, Intensity of absorption bands, theoretical group frequencies, factors affecting group frequencies and band shapes (Physical state, vibrational coupling, electrical effects, resonance, Inductive effects, Ring strain) vibrational-rotational fine-structure. Experimental method, application of IR to the following:

i) Distinction between
   a) Ionic and coordinate anions such as NO_3, SO_4 and SCN   b) Lattice and coordinated water.

ii) Mode of bonding of ligands such as urea, dimethylsulphoxide and hexamethylphosphoramide. **(8 hr)**

UNIT-II

Nuclear Magnetic Resonance Spectroscopy: - Historical introduction to magnetic resonances, chemical shift, mechanism of electron shielding and factors contributing to the magnitude of chemical shift, Nuclear overhausser effect, Double resonance, chemcial exchange, Lanthanide shift reagents and NMR spectra of paramagnetic complexes. Experimental technique. **(10 hr)**

Stereochemical non-rigidity and fluxionality: Introduction, use of NMR in its detection, its presence in trigonal bipyramidal molecules, Systems with coordination number six or more and organometallic molecules (PF_5, $Ti(acac)_2Cl_2$, $Ti(acac)_2Br_2$, $Ta_2(OMe)_{10}$,). **(8 hr)**

Mossbauer Spectroscopy: - Basic concepts (Radiation Source, Mossbauer Nuclei, Recoiless gamma resonance fluorescence. Use of the Doppler effect of vary the γ-ray energy). The effect of Isomeric shift, quadrupole hyperfine interaction and magnetic hyperfine interaction on MB spectra, MB experiment, Application of MB spectroscopy in structural determination of the following:

i) High spin Fe (II) and Fe (III) halides FeF_2, $FeCl_2.2H_2O$, FeF_3, $FeCl_3.6H_2O$. Low spin Fe(II) and Fe(III) Complexes-Ferrocyanides, Ferricyanides, Prussian Blue.
ii) Iron carbonyls. $Fe(CO)_5$, $Fe_2(CO)_9$ and $Fe_3(CO)_{12}$
iii) Inorganic Sn(II) and Sn(IV) halides. **(12 hr)**

Learning Outcomes

1. Study the spectra of compounds and propose structures for compounds.(Skills)
2. Study spectra of compounds, determine functional groups and write structures

References:

1. R.S. Drago, Physical Methods for Chemistry (2nd Ed.), East West Press Pvt. Ltd. 2016.
2. K. Nakamoto, Infrared and Raman Spectra: Inorganic and Coordination Compounds (6th Ed.), Wiley, 2008.
3. F.A. Cotton, Basic Inorganic Chemistry, Wiley, 1995.
4. J.D.Lee, A New Concise Inorganic Chemistry, Oxford University Press, 2008.
5. E. D.Olsen, Modern Optical methods of Analysis, Mc-Graw Hill, 1975.
6. C.N.R. Rao and J.R. Ferraro, Spectroscopy in Inorganic Chemistry, Elsevier, 1971.
7. F.A. Cotton, Progress in Inorganic Chemistry Vol. 8, Wiley, 2009.

AC 9201A ORGANIC SYNTHESIS - I

L	T	P	Cr
3	0	0	3

Course Objective: To introduce the fundamental principles of Organo-metallic reagents, oxidations, reduction and rearrangements

UNIT-I

Organo-metallic reagents: Principle, preparations, properties and applications of the following in organic synthesis with mechanistic details:

(i) Organotitanium Compounds (Titanium tetrachloride, titanium tetraisopropoxide, titanocene dichloride)
(ii) Organolithium Reagents [Metal alkyls: Butyl Lithium, Lithium dialkyl cuprates (Gilman's Reagent)],

(iii) Organopalladium Reagents (Palladium acetate, Palladium chloride; use of palladium reagents in the following reactions: Suzuki-miyaura coupling, Stille coupling, Negishi reaction, Kumada reaction, Hiyama reaction, Sonogashira coupling, Heck reaction, Buchwald-hartwig reaction, Cyanation reaction, Carbonylation reaction)

(i) Organosilicon Reagents: Trialkylhalosilanes

(ii) Organo-rhodium Reagents: Triphenyl phosphinechlororhodium

(iii) Organotin reagents: Tri-n-butyltinhydride

(iv) Other organometallic Reagents: Mercuric acetate, Thallium trifluoroacetate, Diisobutyl aluminium hydride and, Nickel tetracarbonyl

(12 hr)

Oxidations: Introduction, Different oxidative process; Hydrocarbons: alkenes, aromatic rings, saturated C-H groups (activated and unactivated). Alcohols, diols, aldehydes, ketones, ketals and carboxylic acids. Amines, hydrazines and sulphides; Oxidation with ruthenium tetraoxide, iodobenzene diacetate and thallium (III) nitrate. **(10 hr)**

UNIT-II

Reductions: Introduction, Different reductive processes; Hydrocarbons: alkanes, alkenes, alkynes & aromatic rings. Carbonyl compounds: aldehydes, ketones, acids and their derivatives. Epoxides; Nitro, Nitroso, azo and oxime groups; Hydrogenolysis. **(10 hr)**

Rearrangements: General mechanistic considerations-nature of migration, migratory aptitude, memory effect. A detailed study of the following rearrangements: Benzil-Benzilic acid, Favorskii, Arndt-Eistert synthesis, Neber, Backmann, Hofmann, Curtius, Schmidt, Benzidine, Baeyer-Villiger, Shapiro rexn, Fritsch-Buttenberg-Wiechell rearrangement; Metallocenes: Non-benzoid aromatics and polycyclic aromatic compounds. **(10 hr)**

Learning outcomes: Upon successfully completion of this course the students will be able to

1. Knowledge of various organo-metallic reagents and their applications
2. Understanding of oxidation and reduction reactions
3. Understanding of various rearrangement reactions.

References : -

1. S. Warren, Designing Organic Synthesis, Wiley, 1978.
2. J. Fuhrhop and G. Penzillin, Organic Synthesis- Concept, Methods and starting materials, Verlage VCH, 1984.
3. W. Carruthers, Some modern methods of Organic synthesis, Cambridge University Press, 1987.
4. H.O. House, Modern Synthetic Reactions, 1972.
5. J. March, Advanced Organic Chemistry-Reactions Mechanisms and structure, Wiley, 2015.
6. R. Norman and J. M. Coxon, Principles of Organic Synthesis Blakie Academic and Professional, 1993.
7. F.A. Carey and R. J. Sundburg, Advanced organic Chemistry Part-B, Plenum Press, 2008.
8. R. C. Mehrotra, A. Singh, Organometallic Chemistry-A Unified Approach, 2020.

AC 9201B ORGANIC SYNTHESIS - II

L	T	P	Cr
3	0	0	3

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, chemo-selectivity, reversal of polarity cyclisation reactions, amine synthesis. **(10 hr)**

Protecting Groups: Principle of protection of alcohol, amine, carbonyl and carboxyl groups. **(8 hr)**

UNIT-II

a) One Group C-C Disconnection: Alcohols and carbonyl compounds, regioselectivity. Alkene synthesis, use of acetylenes in organic synthesis; **Two Group C-C Disconnection** **(12 hr)**

b) Ring Synthesis

Saturated heterocycles, synthesis of 3-, 4-, 5- and 6-membered rings, aromatic hetero cycles in organic synthesis.

Synthesis of some complex molecules **(12 hr)**

References : -

1. S. Warren, P. Wyatt, Organic Synthesis: The Disconnection Approach, 2nd Edition, Wiley, 2009
2. J. Fuhrhop and G. Penzillin, Organic Synthesis- Concept, Methods and starting materials, Verlage VCH, 1984.
3. W.Carruthers , Some modern methods of Organic synthesis, Cambridge University Press, 1987.
4. H.O.House, Modern Synthetic Reactions, 1972.
5. R. Norman and J. M. Coxon, Principles of Organic Synthesis Blakie Academic and Professional, 1993.
6. J. March, Advanced Organic Chemistry-Reactions Mechanisms and structure, Wiley, 2015.

AC 9201C ORGANIC SYNTHESIS - III

L	T	P	Cr
3	0	0	3

UNIT-I

Addition to Carbon-Carbon Multiple Bonds: 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 bonds, hydrogenation of aromatic rings. Hydroboration. Michael reaction. Sharpless asymmetric epoxidation. **(12 hr)**

Addition to Carbon-Hetero Multiple Bonds: Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents, organozinc reagents to carbonyl and unsaturated carbonyl compounds. Wittig reaction. Mechanism of condensation reactions involving enolates - Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions. Hydrolysis of esters and amides, ammonolysis of esters. **(12 hr)**

UNIT-II

Reagents in Organic Synthesis: Use of the following reagents in organic synthesis and functional group transformations; Complex metal hydrides, Gilman's reagent, lithium disopropylamide (LDA) dicyclohexylcarbodimide. 1,3-Dithiane, trimethylsilyl iodide, Woodward and prevost hydroxylation, osmium tetroxide, DDQ, selenium dioxide, phase transfer catalysts, crown ethers and Merrifield resin, Peterson's synthesis, Wilkinson's catalyst, Baker yeast. Protecting groups, Discussion of synthetic strategies and tactics **(18 hr)**

References:

1. S. Warren, Designing Organic Synthesis, Wiley, 1978.
2. J. Fuhrhop and G. Penzillin, Organic Synthesis- Concept, Methods and starting materials, Verlage VCH, 1984.
3. W. Carruthers , Some modern methods of Organic synthesis, Cambridge University Press, 1987.
4. H.O. House, Modern Synthetic Reactions, 1972.
5. J. March, Advanced Organic Chemistry-Reactions Mechanisms and structure, Wiley, 2015.
6. R. Norman and J. M. Coxon, Principles of Organic Synthesis Blakie Academic and Professional, 1993.
7. F.A. Carey and R. J. Sundburg, Advanced organic Chemistry Part-B, Plenum Press, 2008.

AC 9201D HETEROCYCLIC CHEMISTRY

L	T	P	Cr
3	0	0	3

Course objective; To outline the role of heterocycles in organic, pharmaceutical and biological chemistry and to explain the methods for the chemical synthesis, elaboration and use.

UNIT-I

Nomenclature of Heterocycles: Replacement and systematic nomenclature (Hantzsch-Widman system) for monocyclic, fused and bridged heterocycles. **(4 hr)**
Aromatic Heterocycles: General chemical behaviour of aromatic heterocycles, classification (structural type), criteria of aromaticity (bond lengths, ring current and chemical shifts in ^1H NMR-spectra, empirical resonance energy, delocalization energy and Dewar resonance energy, diamagnetic susceptibility exaltations).Heteroaromatic reactivity and tautomerism in aromatic heterocycles **(6 hr)**
Non-aromatic Heterocycles: Strain - bond angle and torsional strains and their consequences in small ring heterocycles. Conformation of six-membered heterocycles with reference to molecular geometry, barrier to ring inversion, pyramidal inversion and 1,3-diaxial interaction. Stereo-electronic effects - anomeric and related effects. Attractive interactions - hydrogen bonding and intermolecular nucleophilic- electrophilic interactions **(8 hr)**

UNIT-II

Heterocyclic Synthesis: Principles of heterocyclic synthesis involving cyclization reactions and cycloaddition reactions:

i. **Small Ring Heterocycles:** Three-membered and four-membered heterocycles -synthesis and reactions of aziridines, oxiranes, thiiranes, azetidines, oxetanes and thietanes **(4 hr)**
ii. **Benzo-Fused Five-Membered Heterocycles:** Synthesis and reactions including medicinal applications of benzopyrroles, benzofurans and benzothiophenes **(4 hr)**
iii. **Meso-ionic Heterocycles:** General classification, chemistry of some important meso-ionic heterocycles of type-A and B and their applications. **(3 hr)**
iv. **Six-Membered Heterocycles with One Heteroatom:** Synthesis and reactions of pyrylium salts and pyrones and their comparison with pyridinium and thiopyrylium salts and pyridones. Synthesis and reactions of quinolizinium and benzopyrylium salts, coumarins and chromones **(6 hr)**
v. **Six-Membered Heterocycles with Two or More Heteroatoms:** Synthesis and reactions of diazines, triazines, tetrazines and thiazines
vi. Seven- and Large-Membered Heterocycles: Synthesis and reactions of azepines, oxepines, thiepines, diazepines thiazepines, azocines, diazocines, dioxocines and dithiocines. (5 hr)

Learning Outcomes

Students will understand the importance heterocycles in biological systems and in pharmaceuticals. Students will be able to draw mechanisms for reactions involving heterocycles as starting materials, intermediates and products, and be able to propose syntheses of heterocycles from the major classes. Students will be able to relate significant chemical properties to structure.

References:

1. T. Eicher, S. Hauptmann and A. Speicher, The Chemistry of Heterocycles, Wiley, 2012.
2. J. A. Joule, K. Mills and G.F. Smith, Heterocyclic Chemistry, Springer, 1995.
3. T.L Gilchrist, Heterocyclic Chemistry, Prentice Hall, 1995.
4. J.A. Joules and K. Mills, Heterocyclic Chemistry, Wiley-Blackwell, 2010.
5. R.K. Bansal, Heterocyclic Chemistry, New Age International Publishers, 2017.

AC 9201E GREEN CHEMISTRY

L	T	P	Cr
3	0	0	3

Course Objective: To introduce the fundamental principles of Basic Principles of Green Chemistry, Green Chemistry in Day-to-Day Life, Microwave Induced Green Synthesis and Enzymes Catalysed Hydrolytic Processes

UNIT-I

Designing a Green Synthesis: Choice of Starting Materials, Choice of Reagents, Choice of Catalysts, Choice of Solvents. **(2 hr)**

Basic Principles of Green Chemistry: Prevention of Waste/By-Products, Maximum Incorporation of the Reactants into the Final Product, Prevention or Minimization of Hazardous Products, Designing Safer Chemicals, Energy Requirements for Synthesis, Selection of Appropriate Solvent, Selection of Starting Materials, Use of Protecting Groups, Use of Catalyst, Products Designed Should be Biodegradable, Designing of Manufacturing Plants, Strengthening of Analytical Techniques. **(4 hr)**
Green Chemistry in Day-to-Day Life: Dry Cleaning of Clothes, Versatile Bleaching Agent. **(2 hr)**
Green Reagent: Dimethylcarbonate, Polymer Supported Reagents. **(1 hr)**
Green Catalysts: Acid Catalysts, Oxidation Catalysts, Basic Catalysts, Polymer Supported Catalysts. **(2 hr)**
Phase Transfer Catalysis in Green Synthesis: Introduction, Applications of PTC in Organic Synthesis, Oxidation Using Hydrogen Peroxide Under PTC Condition, Crown Ethers. **(3 hr)**
Microwave Induced Green Synthesis: Introduction, Applications - Microwave Assisted Reactions in Water, Microwave Assisted Reactions in Organic Solvents, Microwave Solvent Free Reactions (Solid State Reactions).
Ultrasound Assisted Green Synthesis: Introduction, Applications of Ultrasound. **(6 hr)**
Biocatalysts in Organic Synthesis: Introduction, Biochemical (Microbial) Oxidations, Biochemical (Microbial) Reductions, Enzymes Catalysed Hydrolytic Processes. **(4 hr)**

UNIT-II

Aqueous Phase Reactions: Introduction, Diels-Alder Reaction, Claisen Rearrangement, Wittig-Homer Reaction, Michael Reaction, Aldol Condensation, Knoevenagel Reaction, Pinacol Coupling, Benzoin Condensation, Claisen-Schmidt Condensation, Heck Reaction, Strecker Synthesis, Wurtz Reaction, Oxidations, Reductions, Polymerisation Reactions, Photochemical Reactions, Electrochemical Synthesis, Miscellaneous Reactions in Aqueous Phase. **(4 hr)**
Organic Synthesis in Solid State: Introduction, Solid Phase Organic Synthesis Without Using Any Solvent, Solid Supported Organic Synthesis. **(2 hr)**
Versatile Ionic Liquids as Green Solvents: Green Solvents, Reactions in Acidic Ionic, Liquids, Reactions in Neutral Ionic Liquids. **(2 hr)**
Synthesis Involving Basic Principles of Green Chemistry: Some Examples; Introduction, Synthesis of Styrene, Synthesis of Adipic Acid, Catechol and 3-dehydroshikirnic Acid (a potential replacement for BHT), Synthesis of Methyl Methacrylate, Synthesis of Urethane, An Environmentally Benign Synthesis of Aromatic Amines, Selective Alkylation of Active Methylene Group, Free Radical Brornination, Acetaldehyde, Furfural from Biomass, Synthesis of (S)-metolachlor, an Optically Active Herbicide, Synthesis of Ibuprofen, Synthesis of Paracetamol, Green Synthesis of Epoxystyrene, Synthesis of Citral, Synthesis of Nicotinic Acid, Use of Molting Accelerators to Replace More, Toxic and Harmful Insecticides, An Environmentally Safe Marine Antifoulant. **(10 hr)**

Learning outcomes: Upon successfully completion of this course the students will be able to
1. Knowledge of green chemistry and its day life uses.
2. Understanding of microwave induced green synthesis.
3. Knowledge of enzyme catalysed processes.

References:

1. P. Anastas and H. Williamson (Eds.), Green chemistry frontiers in benign chemical synthesis and processes, Oxford University Press, 1998.
2. T. McKeag, Green Chemistry in Practice: Greener Material and Chemical Innovation through Collaboration, Elsevier, 2021.
3. M.C. Cann and M. E. Connelly, Real world cases in green chemistry, ACS Publications, 2000.
4. T. Clayton, Policies for cleaner Technologies, Earthscan Ltd. 1999.
5. V. K. Ahluwalia and M. Kidwai, New Trends in Green Chemistry, Anamaya Publishers, New Delhi, 2004.

AC 9201F POLYMER CHEMISTRY

L	T	P	Cr
3	0	0	3

Course Objective: To introduce the fundamental principles of Classification of polymers, Measurement of molecular weights, Morphology of crystalline polymers, Polymer Processing

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. **(8 hr)**

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 weights. End-group, viscocity, light scattering, osmotic and ultracentrifugation methods. Analysis and testing of polymerschemical 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. **(10 hr)**

UNIT-II

Structure and Properties of polymers: Morphology and order in crystalline polymers-configurations of polymer chains. Crystal structures 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, chain topology, branching and cross linking. Property requirements and polymer utilization. **(10 hr)**

Polymer Processing: Plastics, elastomers and fibres. Compounding. Processing techniques: Calendering, die casting, rotational casting, film casting, injection moulding, blow moulding, extrusion moulding, thermoforming, foaming, reinforcing and fibre spinning. **(6 hr)**

Properties of Commerical Polymers: Polyethylene, polyvinyl chloride, polyamides, polyesters, phenolic resins, epoxy resins and silicone polymers. Functional polymers - Fire retarding polymers and electrically conducting polymers. Biomedical polymers -contact lens, dental polymers, artificial heart, kidney, skin and blood cells. **(8 hr)**

Learning outcomes: Upon successfully completion of this course the students will be able to

1. Knowledge of Polymer and its classification.
2. Understanding of molecular weight determination methods.
3. Understanding about the morphology of polymer.
4. Knowledge of synthesis ofpolymer and its application.

References:

1. F.W. Billmeyer, Textbook of Polymer Science, Wiley, 1984.
2. V.A. Gowariker, N.V. Viswanathan and J. Sreedhar, Polymer Science, Wiley, 1987.
3. K. Takemoto, Y. Inaki and R.M. Ottanbrite, Functional Monomers and Polymers, CRC Press, 1997.
4. S.V. Canevarolo, Polymer Science: A Textbook for Engineer and Technologists, Carl Hanser Verlag, 2019.

AC 9201G ORGANIC PHOTOCHEMISTRY

L	T	P	Cr
3	0	0	3

Course Objective: To introduce the fundamental principles of Basic Principles of Photochemistry, Photochemistry of aromatic compounds, Photochemistry of carbonyl compounds.

UNIT-I

Introduction and Basic Principles of Photochemistry: Absorption of light by organic molecules, properties of excited states, mechanism of excited state processes and methods of preparative photochemistry. **(6 hr)**

Photochemistry of alkenes and related compounds: Isomerization, Di-p-methane rearrangement and cycloadditions. **(10 hr)**

UNIT-II

Photochemistry of aromatic compounds: Ring isomerization and cyclization reactions. **(6 hr)**
Photochemistry of carbonyl compounds: Norrish type-I cleavage of acyclic, cyclic and unsaturated carbonyl compounds, Norrish type-II cleavage. Hydrogen abstraction: Intramolecular and intermolecular hydrogen abstraction, photoenolization. Photocyclo-addition of ketones with unsaturated compounds: Paterno-Buchi reaction, photodimerisation of unsaturated ketones, rearrangement of enones and dienones, Photo-Fries rearrangement. **(20 hr)**

Learning outcomes: Upon successfully completion of this course the students will be able to
1. Knowledge of principle of photochemistry.
2. Understanding of photochemistry of hydrocarbons and aromatic compounds
3. Understanding of photochemistry of aldehydes and ketones.

References

1. J. D. Coyle, Introduction to Organic Photochemistry, Wiley, 1986.
2. A. Padwa, Organic Photochemistry, CRC Press, 2020.
3. F.A. Carey and R.J. Sundberg, Photochemistry in Advanced Organic Chemistry (3rd Ed.) Plenum Press, 1990.
4. N. J. Turro, Modern Molecular Photochemistry, University Science Books, Sausalito, 1991.

AC 9201H MEDICINAL CHEMISTRY

L	T	P	Cr
3	0	0	3

Course Objective: To introduce the fundamental principles of Development of new drugs, Pharmacokinetics, Pharmacodynamics, role of alkylating agents and antimetabolites in treatment of cancer

UNIT-I

Drug Design: Development of new drugs, procedures followed in drug design, concepts of lead compound and lead modification, concepts of pro-drugs and soft- drugs, structure-activity relationship (SAR), factors affecting bioactivity, resonance, inductive effect, isosterism, bio-isosterism, spatial considerations. Theories of drug activity: occupancy theory, rate theory, induced fit theory. Quantitative structure activity relationship. History and development of QSAR. Concepts of drug receptors. Elementary treatment of drug receptor interactions Physico-

UNIT-II

Cardiovascular Drugs: Introduction, cardiovascular diseases, drug inhibitors of peripheral sympathetic function, central intervention of cardiovascular output. Direct acting arteriolar dilators.Synthesis of amyl nitrate, sorbitrate, diltiazem, quinidine, verapamil, methyldopa, atenolol, oxyprenolol. **(4 hr)**
Local Antiinfective Drugs: Introduction and general mode of action. Synthesis of sulphonamides, furazolidone, nalidixic acid, ciprofloxacin, norfloxacin, dapsone, amino salicylic acid, isoniazid, ethionamide, ethambutal, fluconazole, econozole, griseofulvin, chloroquin and primaquin. **(4 hr)**
Psychoactive Drugs: Introduction, neurotransmitters, CNS depressants, general anaesthetics, mode of action of hypnotics, sedatives, anti-anxiety drugs, benzodiazipines, buspirone, neurochemistry of mental diseases. **(4 hr)**
Antipsychotic drugs - the neuroleptics, antidepressants, butyrophenones, serendipity and drug development, stereochemical aspects of psychotropic drugs. Synthesis of diazepam, oxazepam, chlorazepam, alprazolam, phenytoin, ethosuximde, trimethadione, barbiturates, thiopental sodium, glutethimide **(4 hr)**
Antibiotics: Cell wall biosynthesis, inhibitors, β-lactam rings, antibiotics inhibiting protein synthesis. Synthesis of penicillin G, penicillin V, ampicillin, amoxycillin, chloramphenicol, cephalosporin, tetracyclin and streptomycin. **(6 hr)**

Learning outcomes: Upon successfully completion of this course the students will be able to

1. Knowledge of drug design and Concepts of drug receptors
2. Understanding of important pharmacokinetic parameters
3. Knowledge of drug metabolism, xenobiotics, biotransformation
4. Knowledge of Antibiotics.

References:

1. G.L. Patrick, An Introduction to Medicinal Chemistry, Oxford University Press, 2013.
2. V. Alagarsamy, Textbook of Medicinal Chemistry, CBS Publishers, 2019.
3. R. B. Silverman, The Organic Chemistry of Drug Design and Drug Action, Elsevier, 2015.
4. D. Lednicer, Strategies for Organic Drug Synthesis and Design, Wiley, 1998

AC 9201I MOLECULAR MODELING IN CHEMISTRY

L	T	P	Cr
3	0	0	3

Course Objective: This introductory course in computational chemistry will discuss molecular mechanics, semiempirical, and particularly ab-initio approaches. The course will be practical/project-based, and students will be encouraged to pursue projects related to their own research if possible. The course will highlight the computational algorithms used to implement the theoretical methods. High-level quantum mechanics is not required, but students will need to become familiar with some basic concepts from quantum chemistry such as eigenvectors and eigen values, the Schrödinger equation, orbitals, and variational and perturbational methods.

UNIT-I

Introduction: Molecular Modeling, Historical background. **(2 hr)**

Molecular Modeling methods: Molecular mechanics, Quantum mechanics, Hartree-Fock Calculation, Semi-Empirical Approaches, Density Functional Theory and other methods, idea of hybrid methods may be given. **(5 hr)**

Molecular mechanics: Parameterization, Approximations and limitations, Computation, Multiple minima problems, Molecular Dynamics, Monte Carlo method and conformational search. **(5 hr)**

Applications of Molecular mechanics: Structural Aspects, predicting molecular geometry, Determination of bond length, bond angle, dihedral angle, spectroscopic and other properties. **(5 hr)**

Semi-Empirical methods: Semiempirical Philosophy, Extended Huckel theory, CNDO, INDO, NDDO formalism, General performance of NDDO models, Ongoing development in semi-empirical theory. **(5 hr)**

Application of Semiempirical method: Geometry prediction and properties calculation including thermodynamic properties and spectra.

UNIT-II

Ab-initio and DFT method: Theoretical aspects, Calculations of simple molecules using abintio and DFT method

Software packages: Use of common software packages like Gamess, Hyperchem, Gaussian, CAChe, Spartan, ADF, ChemOffice etc. **(10 hr)**

Applications: Application of molecular modeling for biomolecules, polymers, bioinorganic compounds. **(10 hr)**

(This course is a theory-cum-lab class)

Learning Outcome After passing the course the student shall be able to

1. identify and explain the main similarities and differences between theoretical approaches such as HF (Hartree-Fock), DFT (Density Functional Theory), semi-empirical methods and force field methods.
2. describe and identify the various methods advantages / disadvantages of modelling various scientific issues.
3. able to correlate the electronic and non-electronic properties of known and unknown organic and inorganic compounds.

References:

1. C.J. Carmer, Essentials of Computational Chemistry: Theories and Models, Wiley, 2004.
2. P. Comba and T.W. Hambley, Molecular Modeling of Inorganic Compounds: Wiley, 2009.
3. F. Jensen, Introduction to Computational Chemistry, Wiley,1999.
4. A. Leach, Molecular Modelling: Principles and Applications, Longman,1996

AC 9202A INORGANIC PHOTOCHEMISTRY

L	T	P	Cr
3	0	0	3

UNIT-I

Course Objective: To introduce the fundamental principles of photochemistry, photo-induced reactions of metal-containing complexes including metal carbonyls and their mechanistic pathways.

1. **Basic Principles**: Photochemical laws – Franck-Condon principle, radiative lifetimes, quantum yields, quenching rates and mechanisms. **(12 hr)**

2. **Photochemistry of Transition Metal Complexes**: Photoreactions of complexes of Cr(III) – photo-aquation, photo-substitution and photo-racemization; Photo-substitution and photo-redox reactions of Co(III) complexes; Ru (II) polypyridyl and dinuclear Rh (I) isocyanide complexes as sensitizers; supra-molecular complexes as antenna. Applications of quenching and sensitization techniques in the identification of reactive state in coordination complexes. **(14 hr)**

UNIT-II

3. **Photochemistry of Transition Metal Carbonyls**: Photochemical substitution reactions of metal carbonyls with each other, n-donors, π-donors and ligands other than CO, Photochemical isomerization- positional isomerization, isomerization of ligands, Photochemical addition and elimination reactions – insertion into M-H, M-C and M-M bonds **(15 hr)**

Learning Outcome Upon successful completion of this course the students will be able to

1. understand basics concepts of inorganic photochemistry.
2. demonstrate the knowledge and understanding of photo-induced reactions of metal complexes.

References:

1. D. M. Roundhill, Photochemistry and Photophysics of Metal Complexes, Plenum Press, 1994.
2. G. J. Ferraudi, Elements of Inorganic Photochemistry, Wiley, 1988.
3. V. Balzani and V. Carassiti, Photochemistry of Coordination Compounds, Academic Press, 1970.

4. O. Horvath and K.L. Stevenson, Charge Transfer Photochemistry of Coordination Complexes, VCH Publishers Inc. 1993.

AC 9202 B SUPRAMOLECULAR CHEMISTRY

L	T	P	Cr
4	0	0	4

Course Objective: This course aims to demonstrate the importance of supramolecular (non-covalent interactions) for the assembly of complex nanomaterials.

UNIT-I

Introduction: Definition, host-guest chemistry, supramolecular interactions, interdisciplinary nature of supramolecular chemistry **(4 hr)**

Host-Guest Chemistry or Molecular Recognition: Classification of host molecules/receptors: cation and anion binding hosts; cation-binding hosts (crown ethers, podands, cryptands, spherands, calixarenes, siderophores), nomenclature, solution behaviour, selectivity of cation complexation, macrocyclic, macrobicyclic and template effects, preorganization and complementarity, soft ligands for soft metal ions, complexation of organic cations, alkalides and electrides; anion-binding hosts **(7 hr)**

Crystal Engineering: Concepts, crystal structure prediction, the cambridge crystallographic structural database, crystal engineering of diamondoid lattices, crystal engineering with H-bonds, H-bonds to carbon monoxide, weak hydrogen bonds, hydrogen bonds to metals and metal hydrides, π-π stacking, other interactions, awkward shapes and mismatch, coordination polymers, biomimetic structures, mixed crystals: hourglass inclusions. **(8 hr)**

UNIT-II

Self-Assembly: Introduction, biochemical self-assembly, self-assembly in synthetic systems, self-assembling coordination compounds, self-assembly of closed complexes by hydrogen bonding, catenanes and rotaxanes, halicates, molecular knots, catalytic and self-replicating systems.
Introduction to metal organic frameworks (MOFs) and covalent organic frameworks (COFs) **(9 hr)**

Molecular Devices: Introduction, supramolecular photochemistry, information and signals: Semiochemistry, molecular electronic devices: switches, wires and rectifiers, machine based on catenanes and rotaxanes, dendrimers. **(7 hr)**

Biological Mimics: Introduction, characteristics of enzymes, cyclodextrins as enzyme mimics, corands as ATPase mimics, cation-binding hosts as Transacylase mimics, metallobiosites, haem analogues, vitamin B_{12} models **(7 hr)**

Learning Outcome: By the end of the course the student should have a clear understanding of the importance of intermolecular forces to define the "chemistry beyond the molecule".
The student should be able to use the basic understanding of such forces to rationalize the formation of complex nanomaterials.
Understand the importance of the bottom-up approach to prepare complex (nanoscale) systems. The student will be able to recognize the main types of supramolecular assemblies and suggest synthetic strategies for their preparation. Furthermore, the student should be able to identify the main supramolecular forces involved in such systems.

References :

1. J. W. Steed and J. L. Atwood, Supramolecular chemistry, Wiley, 2000.
2. F. Vogtle, Supramolecular Chemistry, Wiley, 1991.
3. J. W. Steed, D. R. Turner and K. J. Wallace, Core concepts in supramolecular chemistry and nanochemistry, Wiley, 2007.
4. J.-M. Lehn, Supramolecular Chemistry: Concepts and Perspectives, Wiley, 1995.

AC 9202C PHYSICAL METHODS IN INORGANIC CHEMISTRY

L	T	P	Cr
3	0	0	3

Course objective; Introduce the theory of the various instruments and the signals produced when analyzing compound. Equip the student with enough information to be able to interpret signals from spectroscopic instruments

UNIT-I

General Introduction to spectroscopy: Nature of radiation, energies corresponding to various kind of radiation, energies for atomic and molecular transitions. **(10 hr)**

Infrared Spectroscopy: Theory of IR absorption, types of vibrations, observed number of modes of vibrations, Intensity of absorption bands, theoretical group frequencies, factors affecting group frequencies and band shapes (Physical state, vibrational coupling, electrical effects, resonance, Inductive effects, Ring strain) vibrational-rotational fine-structure. Experimental method. Application of IR to the following:

ii) a) Distinction between Ionic and coordinate anions such as NO_3, SO_4 and SCN b) Lattice and coordinated water.

ii) Mode of bonding of ligands such as urea, dimethylsulphoxide and hexamethylphosphoramide. **(11 hr)**

UNIT-II

Nuclear Magnetic Resonance Spectroscopy:- Historical introduction to magnetic resonances, chemical shift, mechanism of electron shielding and factors contributing to the magnitude of chemical shift, Nuclear overhausser effect, Double resonance, chemcial exchange, Lanthanide shift reagents and NMR spectra of paramagnetic complexes. Experimental technique. NMR of simple molecules containing^{19}F,^{31}P etc.. **(9 hr)**

Stereochemical non-rigidity and fluxionality: Introduction, use of NMR in its detection, its presence in trigonal bipyramidal molecules, Systems with coordination molecules (PF_5, $Ti(acac)_2Cl_2$, $Ti(acac)_2Br_2$, $Ta_2(OMe)_{10}$,). Fluxionality of metal carbonyls using NMR spectroscopy. **(6 hr)**

Mossbauer Spectroscopy: - Basic concepts (Radiation Source, Mossbauer Nuclei, Recoiless gamma resonance fluorescence. Use of the Doppler effect of vary the γ-ray energy). The effect of Isomeric shift, quadrupole hyperfine interaction and magnetic hyperfine interaction on MB spectra, MB experiment, Application of MB spectroscopy in structural determination of the following:

i) High spin Fe (II) and Fe (III) halides FeF_2, $FeCl_2.2H_2O$, FeF_3, $FeCl_3.6H_2O$. Low spin Fe(II) and Fe(III) Complexes-Ferrocyanides, Ferricyanides, Prussian Blue.

ii) Iron carbonyls. $Fe(CO)_5$, $Fe_2(CO)_9$ and $Fe_3(CO)_{12}$

iii) Inorganic Sn(II) and Sn(IV) halides. **(6 hr)**

Learning Outcomes

1. Study the spectra of compounds and propose structures for compounds.(Skills)
2. Study spectra of compounds,determine functional groups and write structures

References:.

1. R.S. Drago, Physical Methods for Chemistry (2nd Ed.), East West Press Pvt. Ltd. 2016.
2. K. Nakamoto, Infrared and Raman Spectra: Inorganic and Coordination Compounds (6th Ed.), Wiley, 2008.
3. F.A. Cotton, Basic Inorganic Chemistry, Wiley, 1995.
4. J.D.Lee, A New Concise Inorganic Chemistry, Oxford University Press, 2008.
5. E. D. Olsen, Modern Optical methods of Analysis, Mc-Graw Hill, 1975.

6. C.N.R. Rao and J.R. Ferraro, Spectroscopy in Inorganic Chemistry, Elsevier, 1971.

AC 9202D SPECIAL TOPICS IN INORGANIC CHEMISTRY

L	T	P	Cr
3	0	0	3

Course Objective: To impart basic knowledge of macrocyclic complexes, supramolecular chemistry, metallomesogens, molecular magnetism and techniques in magnetic characterization.

UNIT-I

Macrocyclic Complexes: Types of macrocyclic ligands – design and synthesis by coordination template effect, di- and poly-nuclear macrocyclic complexes; applications of macrocyclic complexes. **(8 hr)**

Supramolecular Chemistry: Concept of supra-molecular chemistry, molecular recognition, nomenclature, design of supra-molecular through non-covalent interactions and their applications in transport processes. **(8 Hr)**

Molecular Magnetic Materials : Basic concepts of molecular magnetism, types of magnetic interactions, recent techniques of magnetic susceptibility measurements, inorganic and organic ferro-magnetic materials, low-spin – high-spin transitions, isotropic interactions in dinuclear compounds (dipolar, anisotropic and anti-symmetric interactions), trinuclear compounds and compounds of high nuclearity, magnetic chain compounds, magnetic long-range ordering in molecular compounds: design of molecular magnets, physical investigations and applications. **(8 hr)**

UNIT-II

Metallomesogens: Basic concepts, types of meso-phases, synthetic strategies, characterization and applications. **(8 hr)**

Inorganic Polymers: Classification, Types of Inorganic Polymerization, Comparison with organic polymers, Boron-oxygen and boron-nitrogen polymers, silicones, coordination polymers, sulfur-nitrogen, sulfur-nitrogen-fluorine compounds, chalcogenide clusters – binary and multi-component systems, homolytic inorganic systems. **(10 hr)**

Learning Outcome Upon successful completion of this course the students will be able to

1. classify macrocyclic ligands and synthesize macrocyclic complexes.
2. understand basics concepts of supramolecular chemistry and its applications.
3. acquire the knowledge and understanding of molecular magnetism and its measurements.
4. have basic understanding of metallomesogens and their synthesis and characterization.

References:

1. J.-M. Lehn, Supramolecular Chemistry, VCH, Weinheim, 1995.
2. J. L. Serrano, Metallomesogens: Synthesis, Properties and Applications, Wiley, 2008.
3. O. Kahn, Molecular Magnetism, VCH, Weinheim (1993).
4. F.A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, Advanced Inorganic Chemistry, Wiley, 2021..

AC-9202E INORGANIC POLYMERS

L	T	P	Cr
3	0	0	3

Unit-I

Inorganic Polymers: Introduction, different types of Inorganic Polymers and their importance, Characterization: Molecular Weights, Molecular Weight Distributions, Other Structural Features Chain Statistics, Solubility, Crystallinity, Mechanical Properties.

(6 h)

Polysiloxanes and Related Polymers: Introduction, Nomenclature, Preparation, General Properties, Reactive Homopolymers, Elastomeric Networks, Characterization Techniques, Applications of polysiloxane.

(8 h)

Polyphosphazenes: Introduction, Alternative Synthesis Routes to Linear Polymers: Ring-opening polymerization and Condensation polymerizations. Surface Reactions of Polyphosphazenes, Hybrid Systems through: Block, Comb, or Ring-Linked Copolymers, Composites, Organometallic Polyphosphazenes, Applications of Polyphosphazenes, Optical and Photonic Polymers. **(8 h)**

Unit-II

Polysilanes and Related Polymers: Introduction, History, Synthesis, Chemical Modification of Polysilanes, Physical and Electronic Properties of Polysilanes, Electrical Conductivity and Photoconductivity, Luminescence of Polysilane, Photodegradation of Polysilanes. **(8 h)**

Miscellaneous Inorganic Polymers: Introduction, Ferrocene-Based Polymers, and Additional Phosphorus- and Boron-Containing Polymers, Other Silicon-Containing Polymers, Polygermanes, Polymeric Sulfur and Selenium, Other Sulfur-Containing Polymers, Aluminum- Containing Polymers, Tin-Containing Polymers, Arsenic-Containing Polymers, Metal Coordination Polymers. **(12 h)**

References:

1. J. E. Mark, H. R. Allcock, R. West, Inorganic Polymers, Oxford University Press, 2005.
2. P.B. Saxena, Inorganic Polymers, Discovery Publishing House, 2007.
3. R. De Jaeger, M. Gleria , Inorganic Polymers, Nova Science Publishers, 2007
4. R. D. Archer, Inorganic And Organometallic Polymers, John Wiley & Sons, 2001.
5. N.P.S. Chauhan and N.P. Chundawat, Inorganic and Organometallic Polymers, De Gruyter & GmbH Co. 2019.

AC-9203A MACROMOLECULES AND SURFACE CHEMISTRY

L	T	P	Cr
3	0	0	3

Course Objective: To introduce the fundamental principles of kinetic study of polymerization, thermal decomposition of initiators, molecular weight determination by different methods, surface phenomenon, adsorption of gas on solid surface and catalysis.

UNIT-I

Introduction:

Classification and nomenclature of polymers, composition and polymerization mechanism. Step Polymerization: Reactivity of functional groups, basis for analysis of polymerization, kinetics of step polymerization, self catalysed polymerization, external catalysis of polymerization, step polymerization other than polyesterification non-equivalence of functional groups in polyfunctional reagents. Radical chain ploymerization: Overall kinetics of chain polymerization, initiation, thermal decomposition of initiators, types of initiators, kinetics of initiation and polymerization, dependence of polymerization rate on monomer, photochemical initiation, initiation by ionizing radiation, pure thermal initiation, redox initiation. **(12 hr)**

Co-polymerization and emulsion polymerization: The composition of addition copolymers, kinetics of chain propagation in co-polymerization, qualitative and quantitative theories of emulsion. Polymerization rate, degree and number of polymer particles in emulsion polymerization. Molecular weight average and viscosity average molecular weight, molecular weight determination by osmotic method, light scattering method, sedimentation method, diffusion constant, sedimentation equilibrium, viscosity method.
Statistics of Linear polymers Molecular weight, molecular weight distribution, polydispersity index, average and end to end distance, average radius of gyration. (**12 hr)**

UNIT-II

Surface Chemistry

Adsorption: Adsorption, Adsorption of gases, influence of temperature and pressure, nature of adsorption and adsorbed gases, unimolecular layers, types of adsorption, Langmuir adsorption isotherm and BET adsorption equation and their derivation, estimation of surface area of adsorption, Gibbs adsorption equation and its verification. (**10 hr)**

*

Kinetics of heterogeneous reaction at solid surfaces: Gas reaction on solids, single reacting gas, retardation of reaction products, two reacting gases, retardation by reactants and products, adsorption and desorption as rate determining, absolute rate theory of heterogeneous reactions. (**8 hr)**

Catalysis: Catalysts and Criteria of catalysis and initiation of a reaction. Catalytic activity and its determination, salt effects (Primary and Secondary). (**6 hr)**

Learning outcomes: Upon successfully completion of this course the students will be able to

1. Kinetic study of polymerization.
2. Explain various methods to determine molecular mass of polymer.
3. Knowledge of adsorption phenomenon & Kinetics of heterogeneous reaction at solid surfaces
4. Understanding catalytic activity, salt effects (Primary and Secondary)

References:

1. G. Odian, Principles of Polymerization, Wiley, 1991.
2. P. J. Flory, Principles of Polymer Chemistry, Asian Books Pvt. Ltd. 2007.
3. C.H. Chan, C.H. Chia and S. Thomas, Apple Academic Press, 2021.
4. G. M. Barrow , Physical Chemistry, Mc-Graw Hill, 1996.
5. A. W. Adamson Physical Chemistry of Surfaces, Wiley, 1997.

AC-9203B ADVANCED STATISTICAL THERMODYNAMICS

L	T	P	Cr
3	0	0	3

Course Objective: To introduce the fundamental principles of Statistical thermodynamics, Statics of photon and electron gases, gaseous state, solid state, chemical system, fluctuations and irreversible processes

UNIT-I

Quantum Statistics

Recapitulation of classical statistics and partition function, comparison between Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics, thermodynamic probability, statistics of monatomic ideal gas, principle of equipartition of energy, barometric equation, theory of paramagnetism, statistics of photon and electron gases, velocity, speed and energy distribution functions, thermionic emission. (**12 hr)**

Gaseous State

Classical and quantum mechanical treatments of specific heats of ideal diatomic gases, vibrational, rotational and electronic contributions to the specific heats of diatomic gases, fine correction due to rotation-vibration coupling for diatomic gases, ortho and para hydrogens, polyatomic gases, gas mixture and entropy of mixing, non ideal gases, equation of state of non ideal gases, Lennard-Jones potential energy equation compressed gases.

(12 hr)

UNIT-II

Solid State

Classical treatment of specific heat of solids, Einstein and Debye theories of specific heats, Debye's T3 law, entropy of solids, equation of state of solids, order and disorder and the melting point. **(6 hr)**

Chemical Systems

Law of mass action, chemical equilibrium, dissociation, equilibrium constants and their computation.

(**6 hr)**

Fluctuations

Means distribution, mean square deviation, fluctuations in energy in a canonical ensemble, density fluctuation in a gas. Theory of Brownian motion and Brownian motion of galvanometer. (**6 hr)**

Irreversible Processes

Introduction, entropy production, coupled phenomena, transport parameters, thermoelectric phenomena, The Seebeck effect, Peltier effect and Thomson effect. (**6 hr)**

Learning outcomes: Upon successfully completion of this course the students will be able to

1. Understand basic and advances statistical thermodynamics.
2. Understand solid and gases state & laws.
3. Understanding of basic concepts in irreversible processes.

References:

1. T.L. Hill, Introduction to Statistical Thermodynamics, Dover Publication, 2012.
2. M.C. Gupta, Statistical Thermodynamics , New Age International Publishers, 2007.
3. F. Reif, Fundamental of Statistical and Thermal Physics, Mc-Graw Hill, 1985.
4. R. K. Pathria, Statistical Mechanics, Butterworth-Heinemann, 1999.

AC 9203C PHYSICAL METHODS IN CHEMISTRY

L T P Cr

3 0 0 3

Course Objective: To introduce the fundamental principles of electrochemical technique and its application, IR, Raman and photoelectron spectroscopy and their applications, Diffraction technique, Thermal analysis and its application

UNIT-I

Electrochemical Techniques: Impedance technique -- its application for studying electrode kinetics and corrosion. Application of Rotating Disc Electrode (RDE) for measurement of electrochemical rate constant. **(4 hr)**
Vibrational Spectroscopy: Vibration of polyatomic molecules. Introduction to normal coordinate analysis. IR and Raman transitions. Applications to surface studies. Reflectionabsorption Infrared spectroscopy (RAIRS). Electron energy loss spectroscopy (EELS). **(8 hr)**
Photoelectron Spectroscopy and Related Techniques: Principle and applications to studies of molecules and surface. UPES and XPS. Auger electron and X-ray fluorescence spectroscopy (AES and XRF). **(8 hr)**

UNIT-II

Techniques for Studying Surface Structure: Low energy electron diffraction (LEED). Scanning tunneling and atomic force microscopy (STM and AFM). **(6 hr)**
Diffraction Techniques: Principle and applications of X-ray powder diffraction, single crystal X-ray diffraction, elctron and neutron diffraction. **(10 hr)**
Thermal Analysis: Thermogravimetric analysis, Differential thermal analysis and differential scanning calorimetry, Applications of DTA, DSC and TGA. **(6 hr)**

Learning Outcome: Upon successful completion of this course the students will be able to

1. understand application for studying electrode kinetics and corrosion.
2. explain IR and Raman transition.
3. demonstrate knowledge and understanding of basic concepts in X-ray diffraction, electron and neutron diffraction.
4. understand Thermogravimetric analysis and related techniques.

References:

1. A.J. Bard and L.R. Faulkner, Electrochemical Methods: Fundamentals and Applications, Wiley, 2001.
2. J.M. Hollas, Modern Spectroscopy, Wiley, 2004.
3. C.N. Banwell and E.M. Mc Cash, Fundamentals of Molecular Spectroscopy, Tata Mc-Graw Hill, New Delhi, 1994.
4. E.M. Mc Cash, Surface Chemistry, Oxford University Press, 2001.
5. A.K. Cheetham and P. Day, Solid State Chemistry Techniques, Oxford University Press, 1988

AC9203D-ELECTROCHEMISTRY & CHEMICAL KINETICS

L T P Cr

3 0 0 3

Course Objective: To introduce the fundamental principles of Debye-Hückel theory of ion-ion interaction and activity coefficient, Modification of DHO theory, Electrical Double Layer at Metal/Semiconductor-Electrolyte Interface, Electrode Kinetics, Electrocatalysis, Experimental Techniques for Fast Reaction, Transition State Theory, Reactions in Solution, Homogeneous Catalysis and Kinetics of Polymerisation Reactions

UNIT-I

Activity Coefficient and Ionic Migration in Electrolyte Solutions: Quantitative treatment of Debye-Hückel theory of ion-ion interaction and activity coefficient, applicability and limitations of Debye-Hückel limiting law, its modification for finite-sized ions, effect of ion- solvent interaction on activity coefficient. Debye-Hückel-Onsagar (D-H-O) theory of conductance of electrolyte solution, its applicability and limitations, Pair-wise association of ions (Bjerrum and Fuoss treatment), Modification of D-H-O theory to account for ion-pair formation, Determination of association constant (KA) from conductance data. **(9 hr)**

Electrical Double Layer at Metal/Semiconductor-Electrolyte Interface: Thermodynamics of double layer, Electrocapillary equation, Determination of surface excess and other electrical parameters- electrocapillarity, excess charge capacitance, and relative surface excesses. Metal/water interaction- Contact adsorption, its influence on capacity of interface, Complete capacity-potential curve, Constant capacity region hump. Specific adsorption-extent of specific adsorption, Semiconductor/ electrolyte interface, Capacity of space- charge, Mott-Schottky plot. **(8 hr)**

Electrode Kinetics: Review of Butler-Volmer treatment. Polarizable and non-polarizable interfaces. Multistep reactions- a near equilibrium relation between current density and over potential, Concept of rate determining step. Determination of reaction order. Stochiometric number, and transfer coefficient. Electrocatalysis--comparison of electrocatalytic activity. Importance of oxygen reduction and hydrogen evolution reactions and their mechanisms. **(5 hr)**

UNIT-II

CHEMICAL KINETICS

Experimental Techniques for Fast Reaction: Flow techniques, relaxation methods, flash photolysis.

Transition State Theory: Application of statistical mechanics to transition state theory, Comparison of transition state theory with experimental results. Thermodynamic treatment of TST. Theories of unimolecular reactions--treatments of Lindmann, Hinshelwood, Rice-Ramsperger- Kassel (RRK), and Rice- Ramsperger-Kassel-Marcus (RRKM). **(6 hr)**

Reactions in Solution: Reaction between ions; Effect of solvent (single & double sphere models), interpretation of frequency factor and entropy of activation, influence of ionic strength, salt effect and reaction mechanisms, Reactions involving dipoles. Influence of pressure on reaction rates in solution. Significance of value of activation parameters. Influence of substituents on reaction rates Electronic theories of organic reactivity. Linear free energy relationships, The Hammett equation, significance of σ^* and ρ^* The Taft equation. **(8 hr)**

Homogeneous Catalysis: General catalytic mechanism, Mechanism of acid-base catalysis (protolytic and prototropic). Bronsted catalytic law. **(4 hr)**

Kinetics of Polymerisation Reactions: Condensation and Addition (free radical, ionic, coordination) Polymerisation. Co-polymerization. **(2 hr)**

Learning Outcome Upon successful completion of this course the students will be able to

1. understand ion-ion interaction and activity coefficient, Determination of association constant (KA)
2. explain Debye-Hückel-Onsagar (D-H-O) theory and its applicability
3. demonstrate knowledge and understanding of basic concepts in Electrical Double Layer at Metal/Semiconductor-Electrolyte Interface, Electrode Kinetics.
4. understand significance of chemical kinetics, catalysis and Kinetics of Polymerisation Reactions.

References:

1. J.O' M. Bockris and A.K.N. Reddy, Modern Electrochemistry, Vol. 1 & 2A and 2 B, Plenum Press, New York ,1998.
2. M. J. Pilling and A.P.W, Seakins, Reaction Kinetics, Oxford Science Publication, New York,1998.
3. C. Vallance, An Introduction to Chemical Kinetics, Morgan and Claypool Publishers, 2017.
4. G. Cox, Modern Liquid Phase Kinetics, Oxford University Press, 1994.

AC 9203E PHOTO PHYSICAL CHEMISTRY

L T P Cr

3 0 0 3

Course Objective: To introduce the fundamental principles of Photophysical Processes in Electronically Excited Molecules, phosphorescence and fluorescence, Photophysical Kinetics of Bimolecular Processes, Photochemical Primary Processes and Current Topics in Photochemistry

UNIT-I

Photophysical Processes in Electronically Excited Molecules: Radiationless transitionfluorescence emission. Triplet states and phosphorescence emission. Photophysical kinetics of unimolecular prosesses. Delayed fluorescence. **(6 hr)**

Photophysical Kinetics of Bimolecular Processes: Bimolecular collisions in gases and vapours and the mechanism of fluorescence quenching. Kinetics of collision quenching – Stern-Volmer equation. Concentration dependence of quenching and excimer formation. Mechanism of quenching. **(8 hr)**

UNIT-II

Photochemical Primary Processes : Rate constant and lifetime of reactive energy states. Types of photochemical reactions. **(8 hr)**

Techniques : Measurement of emission characteristics – fluorescence, phosphorescence, and chemiluminescence. Techniques for the study of transient species in photochemical reactions. Lasers in photochemical kinetics. **(12 hr)**

Some Current Topics in Photochemistry : Chemistry of stratospheric ozone. Plant photosynthesis. Photodynamic therapy of tumor. **(8 hr)**

Learning Outcome Upon successful completion of this course the students will be able to

1. understandphosphorescence emission. Photophysical kinetics of unimolecular processes. Delayed fluorescence.
2. Explain Kinetics and Mechanism of collision quenching.
3. demonstrate knowledge and understanding of basic concepts in Photophysical Processes and kinetics of Bimolecular Processes.
4. understand significance of fluorescence, phosphorescence, and chemiluminescence
5. demonstrate knowledge and understanding of Plant Photosynthesis Photodynamic therapy of tumor.

References:

1. S. Mondal, S. Saha, Photochemistry and Photophysics, IntechOpen, 2018
2. K. K. Rohtagi, Fundamentals of Photochemistry, New Age International, New Delhi, 2017.
3. R. P. Wayne, Principles and Applications of Photochemistry, Oxford University Press, 1988.
4. N. J. Turro, Modern Molecular Photochemistry, University Science Books, Sansalito,1991.

AC9203F MOLECULAR REACTION DYNAMICS

L	T	P	Cr
3	0	0	3

Course Objective: To introduce the fundamental principles of Reaction kinetics and dynamics, energy threshold, opacity function, potential energy surfaces. Motion over the surface.

UNIT-I

Introduction: Reaction kinetics and dynamics. From Cross-sections to rate coefficients. Impact parameter, centrifugal barrier, energy threshold, opacity function **(8 hr)**

Potential Energy Surfaces: Types of potential energy surface. Experimental probes for potential energy surfaces. Motion over the surface: a theoretical approach. **(12 hr)**

UNIT-II

The Differential Cross-Section: Elastic Scattering. Reactive Scattering. Case Studies. Stereochemistry. **(10 hr)**

State-Specific Cross Sections: Experimental considerations- Molecular beam and Spectroscopic experiments. Models of energy utilization and disposal. Kinematic constraints. Case Studies. Rate coefficients and illustrative experiments: Femtosecond chemistry, predissociation of NaI. **(10 hr)**

Learning Outcome: Upon successful completion of this course the students will be able to

1. Understanding of reaction kinetics, opacity function
2. Knowledge of potential energy surfaces
3. Understanding of Elastic Scattering. Reactive Scattering.
4. Understanding of Models of energy utilization and disposal. Kinematic constraints.

References:

1. M. Brouard, Reaction Dynamics, Oxford University Press, 1998.
2. R.D. Levine and R.B. Bernstein, Molecular Reaction Dynamics and Chemical Reactivity, Oxford University Press, 1987.
3. R.D. Levine, Molecular Reaction Dynamics, Cambridge University Press, 2009.
4. N.E. Henriksen and F.Y. Hansen, Theories of Molecular Reaction Dynamics, Oxford University Press, 2018.

AC-9203G BIOPHYSICAL CHEMISTRY

L	T	P	Cr
3	0	0	3

Course Objective: To introduce the fundamental principles of biological process, biopolymers, photosynthesis, vision mechanism, kinetic property of muscle.

UNIT-I

Chemistry and Biology

Amino acids , proteins , enzymes , DNA & RNA in living systems , electrolytes, the chirality of biological molecules, the biochemical process , weak and strong interactions, macromolecules and rubber elasticity, polyelectrolytes, biopolymers. **(12 hr)**

Physical aspects of biopolymers:

X-ray diffraction, electronic absorption & luminescence Spectroscopy, optical activity , magnetic activity, magnetic-optical activity. Osmosis, hydrophobic hydration and interactions. The properties of amino acids and their aqueous solutions. **(12 hr)**

UNIT-II

Photo biological Process: Photosynthesis, mechanism of vision , the molecular mechanism of photoreceptor **(10 hr)**

Mechano-chemical processes: Introduction, thermodynamics, nerve conduction and membrane equilibria, muscle and muscle proteins, their chemistry and physics, kinetic properties of muscle, mechano- chemical systems, biomachanics. **(14 hr)**

Learning outcomes: Upon successfully completion of this course the students will be able to

1. Understand biological molecules and their chemical processes.
2. Knowledge of vision mechanism and photoreceptor mechanism
3. Demonstrate knowledge of osmosis, photosynthesis and muscle protein.

References:

1. S.J. Lippard and J.M. Berg, Principles of Bioinorganic Chemistry, University Science Books, 1994.
2. M.V. Volkenshtein, General Biophysics, Academic Press, 1983.
3. P. Narayan, Essentials of Biophysics, New Age International Publishers, 2000.
4. A. L. Lehninger and M.M. Cox, Principles of Biochemistry (8th Ed.), Macmillan Learning, 2021.

AC 8151 ORGANIC CHEMISTRY LAB

L	T	P	Cr
0	0	6	3.0

Quantitative Organic Analyses:

Synthesis: Synthesis, purification and identification of organic compounds by recrystallization/functional group

i. Oxidation: Adipic acid from cyclohexanol
ii. Aldol condensation: Dibenzal acetone from benzaldehyde
iii. Cannizzaro reaction: Benzyl alcohol and benzoic acid from benzaldehyde
iv. Aromatic electrophilic substitutions: p-nitroaniline from aniline
v. Beckmann Rearrangement: Benzanilide ← Benzophenone oxime ← Benzaldehyde
vi. Reduction: Benzhydrol from benzophenone [$NaBH_4$ reduction]
vii. Esterification: Methyl benzoate from benzoic acid
viii. Haloform reaction: Iodoform synthesis from acetone / ethyl alcohol
ix. Sublimation: Synthesis/purification of Phthalic anhydride from Phthalic acid

As per curriculum requirements the course coordinator can device/modify any Two experiments.

References:

1. D. Pasto, C. Johnson and M. Miller, Experiments and Techniques in Organic Chemistry, Pearson, 1991.
2. A. R. Tatchell, Vogel's Textbook of Practical Organic Chemistry, Prentice Hall, 1989.
3. R.C. Das and B. Behera, Experimental Physical Chemistry, Tata McGraw Hill, 1983.
4. J. Leonard, B. Lygo and G. Procter, Advanced Practical Organic Chemistry, CRC Press, 2013.
5. D.V. Liskin and P. Chaloner. Advanced Organic Synthesis: A Laboratory Manual, CRC Press, 2016.

AC 8152 INORGANIC CHEMISTRY LAB

L	T	P	Cr
0	0	6	3.0

Course Objectives: To study the principle of distribution of common and rare metals ions in different groups; to know inter and intra-group precipitation and separation of metal ions; to improve the skill in the qualitative analysis of rare metal ions in different groups; to identify the methodology to analyse a metal ion in the presence of other metal ion; to impart the skill in estimation of metal ions by colorimetric and complexometric methods and to identify the methodology to estimate a metal ion in the presence of other metal ion.

Qualitative Analysis:
Mixture containing 8 ions (4 cations and 4 anions) including the complex ions and interfering anions, insoluble salts (like AgCl and $BaSO_4$ etc.) and two rare cations; Group-I: W and Tl; Group-II: Se, Te and Mo, Group-III: Ti, Ce, Th, Zr and V.

Quantitative Analysis

Quantitative determination of metal ions using complexometric, Gravimetric and Titrimetric method

Determination of manganese in the presence of iron
Determination of nickel in the presence of iron
Determination of nickel by gravimetric and copper by titrimetric in a mixture
Determination of barium by gravimetric and calcium by complexometric in a mixture

NB: About 50% of the time should be spent in qualitative analysis

Learning outcome: Upon successful completion of this course the students will be able to identify each component in an inorganic mixture including insoluble salts, rare cations, and complex anions and interfering anions. The students should be able to determine qualitatively the cations in a complex mixture or alloy.

As per curriculum requirements the course coordinator can device/modify any Two experiments.

References:

1. Vogel's Text book of Inorganic Qualitative Analysis, 4th Ed, ELBS, London, 1974.
2. G.H. Jeffery, J. Bassett, J. Mendham and R.C. Denney, Vogel's Text book of Quantitative Chemical Analysis, Longman Scientific and Technical, 1989.
3. G.N. Mukherjee, Advanced Experiments in Inorganic Chemistry, U.N. Dhur & Sons Pvt. Ltd. 2018.
4. G. Raj, Advanced Practical Inorganic Chemistry, Goel Publishing House, 2019.

AC 8251 PHYSICAL CHEMISTRY LAB

L	T	P	Cr
0	0	6	3.0

Measurement of viscosity

1. To determine the molar mass of polyvinyl chloride soluble in water by viscosity measurements.

Optical measurement

2. Determine the refractive indices of given liquids by Abbe's refractometer and calculate their refractions.
3. Determine molar refractivity of ethyl acetate, methyl acetate, ethylene chlorine and chloroform and calculate the atomic refractivity's of C, H and Cl.
4. To determine the composition of two sugar solution X and Y of unknown concentrations by using refractometer.

Adsorptions on solid surfaces

5. To verify the Freudlich and Langmuir isotherms for adsorption of acetic acid on activated charcoal.

Order of reaction

6. To determine the rate constant for the acid-catalyzed hydrolysis of methyl acetate.
7. Comparison of strengths of two acids, say hydrochloric acid and sulphuric acid, used in equal concentration for hydrolysis of methyl acetate.

Molar mass

8. Determination of the molar mass of urea (non-electrolyte) by Beckmann's freezing point method.

Distribution of solutes in adjacent phases

9. Determine the partition coefficient of Succinic acid between ether and water at room temperature.

Colorimetry & Photometry

10. Verify Beer's law $KMnO_4$ and $K_2Cr_2O_4$ solutions using photoelectric spectrophotometer and measure concentrations in their solutions of unknown concentrations.

Polarimetry

11. Determination of the specific and molecular rotation of sucrose at a number of concentrations and to obtain the value of intrinsic rotation for sucrose.

Phase equilibria

12. To construct the mutual solubility curve of a binary two-phase liquid system (for example, 1 butanol/water or methanol/cyclohexane).

Potentiometric measurement

13. Determine solubility and solubility product of silver chloride in water.
14. Titrate 0.1N Mohr salt with 0.1 N $KMnO_4$ potentiometrically.

As per curriculum requirements the course coordinator can device/modify any Two experiments.

References:

1. A. M. James and F. E. Prichard, Practical Physical Chemistry, Prentice Hall, 1974.
2. R.C. Das and B. Behera, Experimental Physical Chemistry, Tata McGraw Hill, 1983.
3. D. P. Shoemaker, C. W. Garland and J. W. Niber, Experimental Physical Chemistry, Mc-Graw Hill, 1998.
4. J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2016.

AC 8252 ANALYTICAL CHEMISTRY LAB

L	T	P	Cr
0	0	6	3

Course Objective: To practice the concepts of various analytical techniques, to evaluate data and statistical evaluation. To gain fundamental concept for instrumentation and non-instrumentation analysis and applications.

1. **Estimation of two metal ions by separating them from a mixture and find out the percentage of error.**
   (a) Copper and Nickel (Gravimetric).
   (b) Nickel and Zinc (Gravimetric).
   (c) Copper and Iron (Copper by gravimetric and Iron by volumetric/gravimetric).

2. **Precipitation Titration.**
   (a) Determination of Ag^+orCl^- by Volhard's method.
   (b) Determination of Cl^- by Mohr's/Fajan's method.

3. **Complexometric titration /redox titration**
   (a) Determination of Ca^{2+} & Mg^{2+} in a mixture (or hardness in tap water) by EDTA method.
   (b) Determination of iron in iron ore/ Ca in Limestone ($KMnO_4$ method).
   (c) Determination of Copper in brass (Iodometry).
   (d) Determination of Ascorbic acid in Vitamin-C tablets by titration using bromate bromide mixture.

4. **Electrochemical method.**
   (a) Potentiometric titration of copper with EDTA.
   (b) Determination of K_a of polybasic acid (phosphoric acid) by potentiometric method.
   (c) Electrogravimetric method: Electrogravimetric determination of Copper and Lead in brass.
   (d) Coulometric Titration: Coulometric Titration of cyclohexane.
   (e) Voltametry: (i) Polarometric determination of Copper and Zinc in brass.
   (ii) Amperometric titration of Lead.

(5) Spectrometry
   (a) Determination of iron in natural water by UV-vis spectrophotometric method.
   (b) Determination of manganese in steel.
   (c) Simultaneous determination of manganese and chromium in a mixture.
   (d) Determination of Na^+, K^+, Ca^+ in mineral water by AES.
   (e) Determination of Lead in brass by AAS.

(6) **Thermal Analysis**: TGA/DTA analysis of $CuSO_4$or calcium oxalate.

Learning Outcome Upon successful completion of this course the students will be able to
1. perform the experiments and calculate error, precision and accuracy.
2. get through practical knowledge on instrumental and non-instrumental method analysis.

As per curriculum requirements the course coordinator can device/modify any Two experiments.

References:

1. D.A. Skoog, F. Holler, S. Crouch, Principles of Instrumental Analysis, Brooks/Cole, 2017.
2. G.H. Jeffery, J. Bassett, J. Mendham and R.C. Denney, Vogel's Text book of Quantitative Chemical Analysis, Longman Scientific and Technical, 1989.
3. A. R. Tatchell, Vogel's Textbook of Practical Organic Chemistry, Prentice Hall, 1989.
4. J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2016.

AC 9151A ADVANCED LAB TECHNIQUES (ORGANIC)

L	T	P	Cr
0	0	6	3.0

Chromatography: Separation of mixtures using TLC.

Spectroscopy

Preparation, separation and purification of organic compounds, and their characterization by spectral techniques (UV, IR, PMR, CMR and MS)

(i) Acetylation: Acetylation of cholesterol and separation of cholesteryl acetate by column chromatography
(ii) Benzilic acid rearrangement: Benzilic acid from benzoin (Benzoin → Benzil → Benzilic acid)
(iii) Skraup synthesis: Preparation of quinoline from aniline,
(iv) Malonic ester Synthesis: Synthesis of Barbiturate
(v) Diels-Alder reaction: Maleic anhydride with anthracene

Extraction of Organic Compounds from Natural Sources

(i) Isolation of caffeine from tea leaves.
(ii) Isolation of piperine from black pepper

GREEN CHEMISTRY EXPERIMENTS

Enzymatic synthesis: Reduction of ethyl acetoacetate using Bakers' yeast to yield enantiomeric excess of S (+) ethyl-3-hydroxy-butanoate and determine its optical purity by polarimeter.

Synthesis using Microwave/Sonicator

(i) Alkylation of diethyl malonate with benzyl chloride.
(ii) Synthesis of Heterocyclic compounds using multi component reactions

Synthesis using Ionic liquids

(i) Preparation of ionic liquid
(ii) Synthesis of chiral compounds using ionic liquids and determination of optical activity of the product by polarimeter

As per curriculum requirements the course coordinator can device/modify any Two experiments.

References:

1. D. Pasto, C. Johnson and M. Miller, Experiments and Techniques in Organic Chemistry, Pearson, 1991.
2. A. R. Tatchell, Vogel's Textbook of Practical Organic Chemistry, Prentice Hall, 1989.
3. J. Leonard, B. Lygo and G. Procter, Advanced Practical Organic Chemistry, CRC Press, 2013.
4. D.V. Liskin and P. Chaloner. Advanced Organic Synthesis: A Laboratory Manual, CRC Press, 2016.

AC 9151B ADVANCED LAB. TECHNIQUE I

L	T	P	Cr
0	0	6	3

Course Objectives: To study the principle of distribution of common and rare metal ions in different groups; to know inter- and intra-group precipitation and separation of metal ions; to improve the skill in the qualitative analysis of rare metal ions in different groups; to identify the methodology to analyse a metal ion in the presence of another metal ion; to impart the skill in estimation of metal ions by colorimetric and complexometric methods and to identify the methodology to estimate a metal ion in the presence of another metal ion.

1. **Synthesis and characterization of metal complex**
   $[Co(NH_3)_4CO_3]NO_3$ and $[Co(NH_3)_5Cl_2]Cl_2$
2. **Study of isomerism in metal complexes (linkage isomerism, cis-trans and enantiomers)**
   Synthesis of and $[Co(NH_3)_5ONO]Cl_2$ and $[Co(NH_3)_5NO_2]Cl_2$
   Synthesis of enantiomers $[Co(en)_3]Cl_3$
3. **Organometallics**
   Synthesis of Ferrocence, Nicalocene or $TiCl_2$(□-$C_5H_5)_2$
4. **Inorganic polymers**
   Preparation of S_4N_4, $(PNCl_2)_n$ and/or $B_3H_3N_3Me_3$
5. **Solvent extraction and preparation of metal complex with unusual valence sate and uncommon OS**
   Preparation of Fe(dtc)NO: characterization by element analysis, Uv-visble, FT-IR, magnetic moment, and EPR

6. Synthesis of macrocyclic complex and its coordination chemistry

7. Synthesis of air sensitive compounds: Inert atmosphere and vacuum line preparation
8. Reaction of coordinated ligand
9. ESR and electrochemical station studies of metal complex
   [Fe(bp)3][BF4]2
10. Determination of stability constant by pH and UV-vis spectrophotometry
11. Composition of complex by Jobs method
12. Influence of ligand field strength upon spectra of Cu(II) complex

NB: Some experiments require more time; at least 8 experiments should be performed in a semester. Individual experiment may be changed as per the need.

Learning Outcome
Demonstrate the ability to apply basic mathematics (arithmetic and algebra) and basic chemical principles to find solutions to simple quantitative problems and situations. Enhance and broaden your repertoire of synthesis and characterization techniques as related to inorganic chemistry. Perform laboratory experiments that are based on fundamental chemical principles and adhere to departmental standards of laboratory safety. Apply logical thought processes and background knowledge to draw appropriate conclusions from chemically related information and data. Infer conclusions and consequences from experimental data.

As per curriculum requirements the course coordinator can device/modify any Two experiments.

References

1. J.D. Woollins, Inorganic Experiments, Wiley, 2010.
2. G.Pass, and H.Sutcliffe, Practical Inorganic Chemistry, Chapman Hall, 1965.
3. W.G.Palmer, Experimental Inorganic Chemistry, Cambridge University Press, 1954.
4. D. M. Adams and J. B. Raynor, Advanced Inorganic Practical Chemistry, Wiley, 1965.
5. G.N. Mukherjee, Advanced Experiments in Inorganic Chemistry, U.N. Dhur & Sons Pvt. Ltd. 2018.