VISVA-BHARATI
DEPARTMENT OF CHEMISTRY
M. Sc. SEMESTER-WISE COURSE AND CREDIT STRUCTURE

M. Sc. First Year, Semester I (5T+1P), (Total Marks: 300)

Couse No.	Subject	Marks	CP	No. of Lectures
CH 701	Inorganic Chemistry (core)	50 (40 + 10)	4	50 L
CH 702	Inorganic Chemistry (core)	50 (40 + 10)	4	50 L
CH 703	Organic Chemistry (core)	50 (40 + 10)	4	50 L
CH 704	Organic Chemistry (core)	50 (40 + 10)	4	50 L
CH 705	Physical Chemistry (core)	50 (40 + 10)	4	50 L
CH 706	Physical **Practical (core)**	50 (40 + 10)	4	-

M. Sc. First Year, Semester II (4T +2P), (Total Marks: 300)

Couse No.	Subject	Marks	CP	No. of Lectures
CH 807	Inorganic Chemistry (core)	50 (40 + 10)	4	50 L
CH 808	Organic Chemistry (core)	50 (40 + 10)	4	50 L
CH 809	Physical Chemistry (core)	50 (40 + 10)	4	50 L
CH 810	Physical Chemistry (core)	50 (40 + 10)	4	50 L
CH 811	Inorganic **Practical (core)**	50 (40 + 10)	4	-
CH 812	Organic **Practical (core)**	50 (40 + 10)	4	-

M. Sc. Second Year, Semester III (2ET + 3OT +1OP) (Total Marks: 300)

Couse No.	Subject	Marks	CP	No. of Lectures
CH 913	Elective-1(Inorganic)	50 (40 + 10)	4	50 L
CH 914	Elective-2(Organic)	50 (40 + 10)	4	50 L
CH 915	Optional	50 (40 + 10)	4	50 L
CH 916	Optional	50 (40 + 10)	4	50 L
CH 917	Optional	50 (40 + 10)	4	50 L
CH 918	Optional **Practical**	50 (40 + 10)	4	-

M. Sc. Second Year, Semester IV (1ET + 3OT + 1 Project) (Total Marks: 300)

Couse No.	Subject	Marks	CP	No. of Lectures
CH 1019	Elective-3 (Physical)	50 (40 + 10)	4	50 L
CH 1020	Optional	50 (40 + 10)	4	50 L
CH 1021	Optional	50 (40 + 10)	4	50 L
CH 1022	Optional	50 (40 + 10)	4	50 L
CH 1023	***Project**	100 (80 + 20)	8	-

N.B. [T= Theory; P= Practical; ET= Elective theory; OT= Optional theory; OP=Optional Practical; CP=Credit point]

*** Project to be executed from Semester III and it will be evaluated in Semester IV**

M. Sc. Semester-I
Theoretical
CH 701: Inorganic Chemistry (Core)
Full Marks: 50 (40 + 10); Credit point: 4

1. **Coordination Chemistry-bonding, stereochemistry and structure** **(13L)**

Symmetry and Isomerism; Ligand field theory and molecular orbital theory; nephelauxetic series, structural distortion and lowering of symmetry, electronic, steric and Jahn-Teller effects on energy levels, conformation of chelate ring, structural equilibrium, magnetic properties

2. **Complexes in aqueous solutions** **(12L)**

Metal ligand stability constant and its controlling factors, different tools of study (pH-potentiometric, polarographic, spectrophotomectric, volumetric) and methods of measuring stability constants of complexes, Bjerrun half ň method, stability of mixed ligand complexes and calculations, determination of composition (Jobs, mole ratio and slope ratio methods), evaluation of thermodynamic parameters

3. **Molecular magnetism-I** **(13L)**

Basic concepts of magnetism, magnetization and magnetic susceptibility, Types magnetic behavior (dia-, para-, ferro-, ferri- and antiferro-) and their temperature dependence, Curie and Curie-Weiss laws, temperature independent paramagnetism, Pascal's Constants and its utilities, Determination of χ_M in solution, Usefulness of μ_s and μ_j equation respectively for transition and inner transition series, Van Vleck's equation and its applications, spin-orbit coupling, zero-field splitting, quenching of orbital angular momentum, High-spin/Low-spin Equilibrium, types of exchange interactions

4. **Electronic spectra of transition metal complexes** **(12L)**

Russel-Saunders (R-S) terms-Inter electronic repulsion parameters (B), Splitting of R-S Terms in Different Geometries, Orgel and Tanabe Sugano diagram, Selection rules for spectral transitions, calculation of Dq, B and β parameters, Different types of d-d bands and their assignment, Charge transfer bands

M. Sc. Semester-I
Theoretical
CH 702: Inorganic Chemistry (Core)
Full Marks: 50 (40 + 10); Credit point: 4

1. **Cage, Metal clusters and ring compounds** **(13L)**

Cage compounds- higher boron hydrides- structure and reactivity, equation of balance-styx numbers, Lipscomb topological diagrams, Wades rules, Jemmis' unifying electron counting rule, carboranes, metallocarborane, metalloborranes and heteroboranes, phosphorous cage compounds; Metal clusters- clusters in elemental states, cluster classification, skeletal electron counting, bonding in metal clusters, polyhedral skeleton electron pair theory (PSEPT), Zintl ions, Silicates-pyroxene, amphiboles, talc, clay, zeolite, ultramarine

2. Polymer Chemistry-1 **(12L)**

Basics: Importance of polymers, Basic concepts of monomers, repeat units, degree of polymerization, linear, branched and network polymers, classification of polymers, polymerization-condensation, addition, radical chain-ionic and coordination, copolymerization; Polymer characterization- number, weight and viscosity average molecular weights, polydispersity index and molecular weight distribution, measurement of molecular weight by viscosity method; Structure and property- the glass transition temperature, relationship between T_g and T_m, factors controlling T_g; Functional polymers-fire retarding polymers and electrically conducting polymers; Biomedical polymers- contact lens, dental polymers, artificial heart, kidney, skin and blood cells

3. Organometallic Chemistry-1 **(13L)**

Alkyls and aryls of transition metals– types, routes of synthesis, stability and decomposition pathways, agostic interactions, organocopper in organic synthesis; Compounds of transition metal-carbon multiple bonds: alkilidenes, alkylidynes, low valent carbenes and carbynes-synthesis, nature of bonds, structural characteristics, nucleophilic and electrophilic reactions on the ligands, role in organic synthesis

4. Electro-analytical method-1 **(12L)**

Decomposition and discharge potential, current voltage diagram, linear sweep voltametry (LSV), reversible and irreversible systems, Cottrell equation (qualitative), excitation and switching potential, cyclic voltametry and its application; Coulometry and amperometry – analytical applications

M. Sc. Semester-I
Theoretical
CH 703: Organic Chemistry (Core)
Full Marks: 50 (40 + 10); Credit point: 4

I. Static Stereochemistry **(12 L)**

Molecular symmetry and chirality, Conformation of acyclic and cyclic systems (3 to 5 and 7 to 8 members ring), conformations of rings with multiple double bond, conformations of 3 to 6-membered heterocycles, stereoelectronic effects in heterocycles. Optically active compounds with no asymmetric carbon (allene, biphenyls, spirans etc.), Baldwin's rule, stereochemistry of fused ring and bridged ring compounds (with special reference to decalin and phenanthrene systems)

2. Dynamic Stereochemistry **(13 L)**

Conformation and reactivity, Curtin-Hammett principle and Wenstein-Eliel equations

Conformation, reactivity & mechanism: Acyclic and cyclic system (nucleophilic substitution reaction, formation and cleavage of epoxide ring, addition reactions to double bonds, Elimination reactions, pyrolytic syn-elimination, oxidation of cyclohexanols, neighbouring group participation reactions etc.), Stereoelectronic effects, Elementary idea about asymmetric synthesis

3. Reactions Mechanism: Substitution reactions and Free-radical reactions **(12 L)**

Substitution reactions: Aliphatic nucleophilic substitution — S_N1, S_N2, mixed S_N1 and S_N2, SET mechanisms; neighbouring group mechanism, neighbouring group participation by pi and sigma bonds, anchimeric assistance; 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, Aromatic nucleophilic substitution — S_NAr, benzyne and $S_{RN}1$ mechanisms; reactivity effects of substrate structure, leaving group and attacking nucleophile, Aliphatic electrophilic substitution — S_E1, S_E2, and S_E^i mechanisms; electrophilic substitution accompanied by double bond shifts; effects of substrates, leaving group and solvent polarity on the reactivity, Aromatic electrophilic substitution — the arenium ion mechanism; orientation and reactivity; energy profile diagrams; the ortho/para ratio; orientation in other ring systems; *ipso* attack; *Free radical reactions*: Types of free radical reactions; free radical substitution mechanism; mechanism at an aromatic substrate; neighbouring group assistance; reactivity for aliphatic and aromatic substrates at a bridgehead; reactivity in the attacking radicals; effects of solvents on reactivity; allyllic halogenation (NBS), oxidation of aldehydes to carboxylic acids; auto-oxidation; free radical rearrangements

4. Reactions Mechanism: Elimination, Addition and Rearrangement reactions (12L)

Elimination reactions: E1, E2 and E1cB mechanisms; product stereochemistry; effects of substrate structures, attacking base, leaving group and the medium on reactivity; mechanism and orientation in pyrolytic elimination; *Addition reactions*: Addition to carbon–carbon multiple bonds — mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals; region- and chemoselectivity; orientation and reactivity; 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 and organolithium reagents to carbonyl and unsaturated carbonyl compounds; Mechanism of condensation reactions involving enolates- Aldol, Knoevenagel, Claisen, Perkin and Stobbe reactions; *Rearrangement reactions*: Formation and stability of carbonium ions, carbanion, carbenes, nitrenes, radicals and arynes. Rearrangement involving carbocation (Wagner-Meerwein, Pinacol-Pinacolone rearrangement), reaction involving acyl cation, PPA cyclization and Fries rearrangement, rearrangement of carbenes (Wolff & Arndst-Eistert synthesis), rearrangement of nitrenes (Hoffmann, Curtius, Schmidt, Lossen, Beckmann rearrangement); sigmatropic rearrangements

M. Sc. Semester-I
Theoretical
CH 704: Organic Chemistry (Core)
Full Marks: 50 (40 + 10); Credit point: 4

I. Heterocyclic chemistry of 1,2- & 1,3-azoles (15L)

1,2- and 1,3-azoles: Synthesis/ reactions/ applications, Comparison of azoles (1,2- / 1,3-) with other related mono-heterocycles.

2. Green Chemistry (10 L)

The need of green chemistry, Principles of green chemistry, Concept of atom economy Tools of green Chemistry – microwave, ultra sound, ionic liquids, supercritical H_20 and CO_2 as solvents, etc. Green Chemistry in real world cases and planning green synthesis in chemical laboratory

3. Some selective name reactions: Part-A (12 L)

Shapiro reaction, Mitsunobu reaction, Hofmann-Loffler-Freytag reaction, Barton reaction, Ene reaction, Mannich reaction, Stork enamine reaction, Michael addition, Robinson annulation, Barton decarboxylation and deoxygenation reaction, Sharpless asymmetric epoxidation.

4. Some selective name reactions: Part-B (13 L)

Birch reduction, Aldol condensation, Wittig reaction, Prevost reaction, Simmons-Smith cyclopropanation, Nef reaction, Favorskii reaction, Baeyer-Villiger oxidation, Claisen rearrangement, Beckmann rearrangement etc

M. Sc. Semester-I
Theoretical
CH 705: Physical Chemistry (core)
Full Marks: 50 (40 + 10); Credit point: 4

1. Introduction to Quantum Mechanics **(10L)**

Wave-particle duality. Uncertainty principle. Postulates of Quantum Mechanics. Schrodinger wave equation and its solution. Wavefunction and its probabilistic interpretation. Orthogonality and normalization of wavefunctions.

2. Operator Algebra **(10L)**

Definition. Linear operators. Hermitian operators. Theorems. Eigenvalue equation. Commutation relation. Operators and observables.

3. Free particle and Particle-in-Box **(15L)**

Free Particle. Particle-in-Box and energy quantization. Selection Rules. Discussion on Bohr's correspondence principle. Checking the validity of Schrodinger wave equation based on correspondence principle and Heisenberg's Uncertainty principle. Tunneling

4. Harmonic Oscillator **(15L)**

Solution of Schrodinger equation of a Harmonic oscillator using the operator method as well as the technique for solution of differential equation. Selection rules for Harmonic oscillator. Checking the validity of Schrodinger wave equation based on correspondence principle Heisenberg's Uncertainty principle.

M. Sc. Semester-I
Practical (core)
CH 706: Physical Chemistry
Full Marks: 50 (40 + 10); Credit point: 4

1. To determine the rate constant of hydrolysis of an ester/ ionic reaction in a micellar media.
2. To verify Ostwald dilution law and determine the K_a of a weak acid.
3. To determine the concentrations of a strong and a weak acid in a given mixture by potentiometry.
4. To determine the formal potential of Fe^{III}/ Fe^{II} couple by potentiometry.
5. To determine the rate constant and salt effect on the rate constant of decomposition of $K_2S_2O_8$ by KI.
6. To determine the composition of a mixture of acetic acid, sodium acetate and ammonium acetate by conductometry.
7. To determine the rate constant and energy of activation of the alkaline hydrolysis of ethyl acetate by conductometry.
8. To determine the dissociation constant of Phenolphthalein indicator by spectrophotometry.
9. To study the kinetics of alkaline hydrolysis of crystal violet by spectrophotometry

M. Sc. Semester-II
Theoretical
CH 807: Inorganic Chemistry (Core)
Full Marks: 50 (40 + 10); Credit point: 4

1. **Inorganic reaction mechanism-I** **(13L)**

Energy profile of a reaction, application of different reaction parameters in understanding reaction mechanism-linear free energy relationship,, effect of leaving group, non-leaving group, entering group, steric hindrance and acceleration; solvent exchange reaction-importance in suggesting reaction mechanism, derivation of some important rate laws, kinetically indistinguishable schemes, techniques of fast kinetics, classification of ligand substitution reaction mechanism-associative, dissociative, interchange, etc., Eigen mechanism, proton ambiguity, internal conjugate base formation

2. **Bioinorganic Chemistry-I** **(12L)**

Metal ions in biology, myoglobin, hemoglobin, heamocyanin, hemeerythrin, cytochromes, rubredoxin, feredoxins; biological fixation of nitrogen, chlorophyll and photosynthesis; PS-I, PS-II, bioenergetics and ATP cycle, glucose storage, Na^+/K^+ ion pump, ionophores

3. **Structure and properties of solids** **(13L)**

Structure of mixed oxides-spinel, inverse spinel, ilmenite, perovskite, OSSE; crystal defects-intrinsic and extrinsic, thermodynamics of crystal defects, Schottkey and Frenkel defects; color centers, dislocations, Burger vectors and Burger circuits, non-stoichometric compounds; electronic properties of solids-conductors, semiconductors, insulators, superconductors; ferroelectricity, antiferroelectricity, piezoelectricity, pyroelectricity, cooperative magnetism, Quantum theory of paramagnetism, photoconductivity.

4. **Solid state reactions and thermo-analytical methods** **(12L)**

General principle and classification of solid state reactions, Experimental procedures to study the reactions-TGA, DTA, DSC; Thermogram, thermal stability, thermal degradation, laws governing nucleation and growth of nuclei, single crystal phase transformation, thermo-chemiluminescence, thermometric titrations, solid state reaction kinetics.

M. Sc. Semester-II
Theoretical
CH 808: Organic Chemistry (Core)
Full Marks: 50 (40 + 10); Credit point: 4

I. Natural Products with special reference to Biosynthesis **(13 L)**

Natural Products: Biosynthesis of a) Non-nitrogenous secondary metabolites from Shikinic acid, flavonoids and related polyphenolics, b) mono- and di-terpenoids from Mevalonic acid c) tri-terpenoids from geranyl pyrophosphate.

2. Structure and Functions of Proteins & Lipids **(12 L)**

Structure and functions of proteins: Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing. Secondary structure of proteins, Ramachandran Diagram, forces responsible for holding of secondary structures, □-helix, □-sheets. Tertiary structure of protein-folding, quaternary structure, Biosynthesis of peptide chain, *Lipids:* Fatty acids, structure and function of triacylglycerols, glycerophospholipids. Properties of lipid bilayers, Biological membranes, Fluid mosaic model of membrane structure.

3. Structure and Functions of Nucleic acids and Enzymes (13 L)

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; *Enzymes:* Chemical and biological catalysis, Properties of enzymes like catalytic power, specificity and regulation, Concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site-directed mutagenesis; *Mechanism of Enzyme Action:* Transition state theory. Examples of some typical enzyme mechanisms for chymotrypsin, ribonuclease

4. Co-enzyme chemistry (12 L)

Cofactors as derived from vitamins, coenzymes, prostehtic groups, apoenzymes, Structure and biological functions for pyridoxal phosphate, NAD^+, $NADP^+$, FMN, FAD. Mechanisms of reactions catalyzed by the above cofactors

M. Sc. Semester-II
Theoretical
CH 809: Physical Chemistry (core)
Full Marks: 50 (40 + 10); Credit point: 4

1. Group Theory-I (10L)

Introduction to symmetry. Symmetry elements and Symmetry operations. Definition of a Group. Point symmetry groups. Group multiplication tables. Theorems of groups. Conjugate elements and class. Symmetry Operators and their Matrix Representation. Function space. Reducible and irreducible representations. Equivalent representations. Characters of representations.

2. Group Theory-II (14L)

Great Orthogonality Theorem- statement and interpretation. Proof of its corollaries. Character table and its construction. Number of times an irreducible representation occurs in a reducible one. The reduction of reducible representations. Notation of irreducible representations. Representations and quantum mechanics. The invariance of Hamiltonian operator under symmetry transformations. Direct product representation. Molecular vibrations. Symmetry species of the vibrational mode. Selection rules for Infra-red and Raman spectra. Crystal field splitting.

3. Quantum Mechanics of Rotational Motion (12L)

Angular momentum operators and their commutation relations. Operator algebra and Ladder operators for Rotational motion. Solution of Schrodinger equation using the operator method as well as the technique for solution of differential equation. Quantum Mechanics of rigid rotor and its application.

4. Hydrogen Atom (14L)

Separation of translational and internal motion of a two-body problem. Determination of radial part of the wavefunction. Relation among principal, azimuthal and magnetic quantum number. Nodal properties of angular part as well as the radial part of the Hydrogen atom wavefunction. Shape of the orbitals, Space quantization. Selection rules for Hydrogen atom.

M. Sc. Semester-II
Theoretical
CH 810: Physical Chemistry (core)
Full Marks: 50 (40 + 10); Credit point: 4

1. Ion-ion interaction **(12L)**

Ion association, symmetric and asymmetric ion-pair formation, Bjerrum theory, The fraction of ion-pair, Triple ion formation, Determination of ion-association constant, Activity coefficient of electrolytes, Extended Debye-Huckel theory, Pitzer equation for activity coefficient, Experimental determination of mean ionic activity coefficient.

2. Ion-Solvent interaction **(15L)**

Solvation of ions, Solvation number, Frank-Wien model of ionic solvation, Born model, Thermodynamics of ionic solvation, Enthalpy and free energy of solvation of ions, Experimental determination of solvation of ion.

3. Interface and Colloidal Stability **(12L)**

Colloidal aggregates, nanoparticles, stability of colloids and nanoparticles in solution. Surface charge of colloidal particles, Electrical double layer and theories of electrical double layer. Helmholtz- Perrin model, Gouy-Chapman model, Stern model. Zeta-potential, Determination of zeta potential. Streaming potential, sedimentation potential. DLVO theory, Optical properties of colloids and nanoparticle.

4. Biophysical Chemistry **(14L)**

Hydrophobic hydration, micelle formation, hydrophobic interaction, stabilization and denaturation of protein. Water structure alternation theory of denaturation of protein, protein–lipid interaction, Transport of ions and small molecules through membranes. Ion channels.

M. Sc. Semester-II
Practical (Core)
CH 811: Inorganic Chemistry
Full Marks: 50 (40 + 10); Credit point: 4

1. Analysis of some ores and alloys
2. Preparation of some complex salts and their characterization
3. Determination of composition and formation constant of a few selected systems by pH and spectrophotometric method
4. Magnetic susceptibility measurements

M. Sc. Semester-II
Practical (Core)
CH 812: Organic Chemistry
Full Marks: 50 (40 + 10); Credit point: 4

1. Separation of components from a mixture of organic compounds followed by their characterization.

M. Sc. Semester-III
Theoretical
CH 913: Elective-1 (Inorganic)
Full Marks: 50 (40 + 10); Credit point: 4

1. **Nuclear properties and structure** **(13L)**

Nuclear stability–different factors, nuclear models-Fermi gas model, Liquid drop model, nuclear shell model, nuclear magic number and its derivation from nuclear potential well, nuclear spin, nuclear configuration and parity, nuclear isomerizaion and non-optical transitions, nuclear temperature and entropy; models of disintegration-radiation emission (fluorescence) and electron emission (Auger effect), Theory of radioactivity decay-golden rule and selection rule, radioactive equilibrium.

2. Nuclear reactions **(12L)**

General features, types of nuclear reactions, conservation laws, Q-value and cross-section of nuclear reaction, mechanism of nuclear reactions, resonance and non-resonance reaction, nuclear fission-discovery, characteristics, fission yields, reproduction factor, four factor formula, critical size, atom bomb; nuclear reactors, breeder reactor, natural fission reactor; calculation of fission probability from Bohr-Wheeler's theory; nuclear fusion- characteristics, hydrogen bomb, stellar energy, controlled fusion reaction.

3. Inorganic photochemistry-1 (**13L)**

Basics of photochemistry- absorption, excitation, photochemical laws, quantum yield, lifetime of excited states, Flash photolysis, stopped flow techniques. Energy dissipation by radiative and non-radiative process, absorption spectra, Franck-Condon principles, photochemical stages- primary and secondary process; Properties of excited states- structure, dipole moment, acid-base strength, reactivity; Photochemical kinetics- calculation of rates of radiative process; Bimolecular deactivation- quenching; Excited states of metal complexes-comparison with organic compounds, electronically excited states of metal complexes, charge transfer excitation.

4. **Supramolecular Chemistry-I** **(12L)**

Basic concepts and principles, molecular recognition and host-guest interactions, anion coordination and recognition of anionic substrates, organometallic receptors and their host-guest complexes, spherical recognition, podand, podate, cyrptand, cryptate, coronand, coronate, molecular devices and supramolecular assemblies, supramolecular orbital, supramolecular arrays: ribbon. Ladder, rack, braded, grid; harnessing non-covalent forces to design functional materials

M. Sc. Semester-III
Theoretical
CH 914: Elective-2 (Organic)
Full Marks: 50 (40 + 10); Credit point: 4

1. NMR Part A **(13L)**

Nuclear Magnetic Resonance (NMR) 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 (alcohol, 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 curve-variation of coupling constant with dihedral angles; simplification of complex spectra — nuclear magnetic double resonance, contact of shift reagent, solvent effect; Fourier transform technique; nuclear Overhauser effect (NOE); resonance of other nuclei — F, P;

2. **NMR Part B** **(13L)**
Carbon-13 NMR Spectroscopy — general considerations; chemical shift values (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon); coupling constant; Two Dimensional NMR Spectroscopy — COSY, NOESY, DEPT, INEPT, APT and INADEQUATE techniques.

3. **Mass Spectroscopy** **(13L)**
Mass Spectroscopy: 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 spectrometry; examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

4. Identification of organic compounds by Spectroscopic techniques **(12L)**
Applications of spectroscopic techniques (UV, FT-IR, NMR and Mass) in a combined manner to solve structural problems of unknown organic compounds.

M. Sc. Semester-III
Theoretical
CH 915: Optional (Inorganic)
Full Marks: 50 (40 + 10); Credit point: 4

1. **Metal ion promoted reactions** **(13L)**
Important reactions-oxidative addition, reductive elimination, oxidative coupling, insertion, electrophilic and nucleophilic attack on the ligand; catalytic cycle, Tolman catalytic loop; Homogeneous/heterogeneous catalysis: hydrogenation by Wilkinson's catalyst, water gas shift reaction, Fisher-Tropsch synthesis, isomerization, alkene polymerization, Wacker-Smidt synthesis, hydroformylation, hydrosilation, hydrophosphylation, hydroamination, hydrocyanation and hydroboration reactions, Monsanto acetic acid synthesis, Heck reaction, oxopalladation reactions, Mobil process, synthesis of methanol.

2. Physical characterization of inorganic compounds by spectral analysis-I **(12L)**
Electron spin resonance spectroscopy (ESR)- Basic principle and spectral display, standard material for ESPR spectroscopy (dpph), details understanding on hyperfine coupling constant, significance of g-tensors, application to detect free radicals (H, CH_3, C_6H_5, NH_2, CD_3, PH_4, F_2^-, $[BH_3]^-$, etc) and various transition metal complexes having one unpaired electron, charge transfer spectra and its application

3. Organometallic Chemistry-II **(13L)**
Transition metal pi complexex-transition metal complexex with alkenes, alkynes, allyl, diene, dienyl, arene and trienyl complexes: preparations, properties, nature of bonding and structural features, important reactions relating to nucleophilic and electrophilic attack on the ligands and to organic synthesis; transmetallation and cyclisation reactions, fluxional organnometallic compounds.

4. **Nuclear detection techniques and spectroscopy** **(12L)**

Mossbauer spectroscopy: Mossbauer effect, nuclear recoil, Doppler effect, instrumentation, chemical shift-examples, quadruple effect, effect of magnetic field, effect of simultaneous electric and magnetic fields, typical spectra of iron and tin compounds, application of Mossbauer spectroscopy-nature of metal ligand bond, coordination number, structure, oxidation state; NQR.

M. Sc. Semester-III
Theoretical
CH 915: Optional (Organic)
Full Marks: 50 (40 + 10); Credit point: 4

1. Supramolecular Chemistry: Basic concept **(12 L)**

Definitions of supramolecular chemistry, Host-guest chemistry, Chelate and macrocyclic effects, Preorganisation, Thermodynamic and kinetic selectivity, supramolecular interactions (i..e. cation –π, π-π etc.), *Cation, Anion and Neutral molecule binding*: Crown ethers, podands/ lariat ethers, spherands, cryptands, complexation of organic cations, calixarenes, cation host to anion host, shape selectivity, guanidinium receptors, coordination interactions, *cavitands***:** cyclodextrins and moleculartweezers. Molecular switches.

2. Supramolecular Chemistry: Applications **(13 L)**

Catenanes, rotaxanes and molecular knots: Self assembly and templates, strict self assembly and self assembly with covalent modification, electrostatic and H-bonding effects in templating, catenanes/ catenands/ catenates, rotaxanes/ pseudo-rotaxanes, metal templates for catenanes (Sauvage), π stacking in catenane and rotaxane formation (Stoddart), helicates and molecular knots*; Molecular devices:* History and future of nanoscale machines, Relation to host-guest chemistry (definition of supramolecular device), Supramolecular photochemistry, Photo- and electro-chemical sensors, Dendrimers, Molecular device components, Machines based on catenanes/ rotaxanes, Chemically assembled electronic nanocomputing.

3. Advanced Heterocyclic chemistry: Part-A **(12 L)**

Nomenclature of heterocycles - replacement and systematic nomenclature (Hantzsch-Widman system) for monocyclic, fused and bridged heterocycles; aromatic heterocycles — tautomerism in heterocyclic systems, reactivity of aromatic heterocycles; non-aromatic heterocycles — conformation of six-membered heterocycles with reference to molecular geometry, barrier to ring inversion, pyramidal inversion and 1,3-diaxial interaction, anomeric and related effects, hydrogen bonding and intermolecular nucleophilic-electrophilic interactions; meso-ionic systems — general classification, chemistry of some important meso-ionic heterocycles of type A and B and their applications.

4. Advanced Heterocyclic chemistry: Part-B **(13 L)**

Heterocyclic synthesis - principles of heterocyclic synthesis involving cyclization reactions and cycloaddition reactions; synthesis and reactivity of 3-, 4-, 5- 6- & 7-membered heterocycles with one, two or more heteroatoms (aziridines, oxiranes, thiiranes, azetidines, oxetanes, thietanes, diazines, triazines, thiazines, azepines, oxepines); benzo-fused five and six-membered heterocycles — synthesis and reactions including medicinal applications of benzopyrroles, benzofurans, benzothiophenes, quinolizinium and benzopyrylium salts, coumarins and chromones; heterocycles in pharmaceutical industry.

M. Sc. Semester-III
Theoretical
CH 915: optional (Physical)
Full Marks: 50 (40 + 10); Credit point: 4

1. Revisiting Classical Mechanics (13L)

Motion of a classical particle: definition of velocity, acceleration and mass. Central problem of mechanics. Newtons' prescription for classical mechanics. Laws of motion: law of inertia, law of causality, law of reciprocity. Superposition principle of force. Introduction to the idea of law of force for motion. Application of Newton's prescription to translation, rotation and vibrational motion. Time reversible symmetry. Work-energy theorem and definition of kinetic energy. Conservative and non-conservative force. Definition of potential energy. Conservation of total mechanical energy for conservative system and its implication in the context of first law of thermodynamics. Generalized coordinate systems. Lagrangian equation of motion and definition of generalized momentum. Hamiltonian equation of motion. Definition of phase space.

2. Wave Motion (12L)

Wave equation. Sinusoidal waves, boundary condition, reflection and transmission, polarization. Electromagnetic waves in vacuum. Wave equation for electric and magnetic fields. Monochromatic plane waves. Transport of energy and momentum in electromagnetic waves. Interference of waves. Young's double-slit experiment, determination of wave length.

3. Early age of Quantum Mechanics (13L)

Definition of ideal blackbody and blackbody radiation, Characteristics of the radiation, calculation of number of modes, necessity of new fundamental constant and quantization of energy of electromagnetic oscillator. Temperature dependence of heat capacity of solids. Einstein's theory of heat capacity of solids. Photoelectric effect and Einstein's theory. Compton effect and its theory. Model of atom. Franck-Hertz experiment. deBroglie hypothesis. Double-slit experiment, superposition principle and instruction to formulate Quantum Mechanics.

4. Revisiting the basic principles of Quantum Mechanics (12L)

Understanding Schrodinger's idea of wavefunction and the postulates of quantum mechanics. Interpretation of wavefunction and its consequences. Definition of current in quantum mechanics. Dirac representation of state. Schrodinger and Heisenberg pictures of quantum mechanics. Heisenberg's uncertainty principle. Generic features of quantum mechanics such as tunneling and selection rule. Quantum-classical correspondence.

M. Sc. Semester-III
Theoretical
CH 916: Optional (Inorganic)
Full Marks: 50 (40 + 10); Credit point: 4

1. **Bioinorganic Chemistry-II** **(12L)**

Metal-protein interaction-storage, transfer and activity; study of metalloprotein and metalloenzyme-catalase, peroxidase, ceruloplasmin, cytochrome c oxidase, carbonic anhydrase, carboxypeptidase, metallothionine, xanthine oxidase, sulphite oxidase, nitrate reductase, superoxide dismutase, chemistry of respiration; Vitamin B_{12} and B_{12} co-enzyme; metal deficiency and diseases, Toxic effects of metals, detoxification of metal ions

2. **Inorganic reaction mechanism-II** **(13L)**

Ligand substitution reaction of octahedral complexes-different types, isomerization and racemization; Substitution reactions of square planar complexes-different theories of trans and cis effects, nucleophilicity scale, kinetics of chelate formation; Substitution reaction of tetrahedral complexes, studies of fast reactions, kinetic and activation parameters-tools to propose plausible mechanism; Streochemical changes: racemisation in octahedral complexes types of ligand rearrangements, isomerization in 4, 5 and 6 coordinates complexes; reactions of coordinated ligands; template reactions.

3. Molecular magnetism-II **(13L)**

Magnetic orbital and exchange pathways in polynuclear systems, Quantitative approach to exchange interactions, Bleaney-Bower's equation, orthogonality and Accidental orthogonality phenomenon, deliberate synthetic approaches to ferromagnetically coupled systems, magnetization versus field studies, calculation of ground state and spin manifold, canting/hidden canting and weak ferromagnetism, spin frustration, polynuclear transition metal complexes: magneto-structural correlations, magnetism without metals and magnetic materials.

4. Supramolecular Chemistry-II **(12L)**

Receptors and receptor-substrate complexes, coreceptor molecules and multiple recognition, supramolecular reactivity and catalysis, supramolecular electronic, ionic and photonic devices, catenanes and rotaxanes, systematic approach towards supramolecular architecture, self assembly and self processes.

M. Sc. Semester-III
Theoretical
CH 916: Optional (Organic)
Full Marks: 50 (40 + 10); Credit point: 4

1. Protection and Deprotection **(12 L)**

The role of Protective groups in organic synthesis, Principle of protection and deprotection, Different procedure for protection and deprotection of hydroxyl (including 1,2- and 1,3- dihydroxy), phenols, amines, carbonyls and carboxylic groups.

2. Organic Synthesis I **(13 L)**

The disconnection approach, Basic principles, Guidelines for disconnection with special emphasis on chemoselective, regioselective, stereoselective and stereospecific reactions, Functional group inter conversion, synthon and reagent, synthetic equivalent, illogical electrophile and illogical nucleophile, Umpolong synthesis.

3. Organic Synthesis II **(12L)**

Designing synthesis of some target molecules with proper retrosyntheic analysis : Eg Menthol, Taxol, Penicillin V, Reserpine, Progesterone, Estrone, Periplanone B, L-Hexoses etc..

4. Special techniques in Organic Synthesis **(13 L)**

The background of organic synthesis, Reactions with solid-supported reagents and catalyst, solid phase synthesis, Phase transfer reactions, Sonochemistry, Microwave in organic synthesis, Ionic liquid in organic synthesis, , Electro organic synthesis, Concept of organocatalyst.

M. Sc. Semester-III
Theoretical
CH 916: Optional (Physical)
Full Marks: 50 (40 + 10); Credit point: 4

1. Approximate Methods and their Applications **(12L)**

Variation theorem, Linear variation method, Applicability of variation method to excited states. Time-independent perturbation theory for nondegenerate states, Perturbation of a two-level system, Many level systems, Degenerate perturbation theory and their applications, Eckert's Theorem. Hydrogen and Helium atoms. Hellman-Feynman and Virial Theorems. Time-dependent perturbation theory, Rabi Oscillation, Many level system; the variation of constants, the effect of slowly switched constant perturbation, The effect of oscillating perturbation, Transition rates to continuum, Radiation-matter interaction. Fermi Golden rule, Einstein transition probabilities, lifetime and energy uncertainty.

2. Spin and Many Electron Wavefunctions **(13L)**

Introduction to spin. Operator algebra for spin. Construction of matrix representation of spin operators, Eigenvalues and eigenfunctions of spin operators. Non-relativistic wavefunction for Hydrogen atom. Many-electron wavefunctions- examples with 2 and 3 electron systems, Slater determinants. Projection Operators. Parity Operator and Pauli Principle, The Pauli exclusion principle. Introduction of core, Coulomb, and exchange integrals with their properties- example of He atom.

3. Theory of Many-electron Systems and their Applications **(13L)**

The Born-Oppenheimer approximation, Hartree self consistent field method, Koopman's theorem, Hartree-Fock method for many-electron systems. Coulomb operators, Exchange operators, Coulomb and Fermi hole, Restricted and unrestricted Hartree-Fock calculations, The Roothan equation. Correlation energy, Basis sets for electronic structure calculations. Spin-orbit interaction, The Condon-Slater rules.

4. Density- Functional and Semiempirical Methods in Quantum Chemistry **(12L)**

Introduction to density functional, Hohenberg-Kohn variation theorem, Kohn-Sham equations, Exchange-correlation energy, Local density approximation, Generalized gradient approximation. Semiempirical MO treatments of Planar Conjugated Molecules, The Free-electron MO method, The Huckel and Extended Huckel MO method, The Pariser-Parr-Pople method, General semiempirical MO methods.

M. Sc. Semester-III
Theoretical
CH 917: Optional (Inorganic)
Full Marks: 50 (40 + 10); Credit point: 4

1. Errors and Evaluation (12L)

Precision- standard deviation, relative standard deviation; Accuracy- absolute error, relative error; Types of error in experimental data- systematic (determinants), random (indeterminate) and gross; Source of errors and the effects upon the analytical results; Methods of reporting analytical data, Statistical evaluation of data.

1. Inorganic photochemistry-II (13L)

Ligand field photochemistry- photosubstitution, photooxidation and photoreduction, ground state and excited state, energy content of the excited state, development of redox potentials of the excited states; Redox reactions by excited metal complexes- energy transfer, exciplex formation, conditions of the excited states to be useful redox reactants, excited electron transfer, photochemical reactions of Cr, Fe and Ru complexes, role of spin-orbit coupling in the lifetime of the complexes, Application of redox process for catalytic purposes, transformation of low energy reactants into high energy products, chemical energy into light; Sensitization and metal complex sensitizers; inorganic photochemistry in biological process and their model studies, solar-energy conservation and storage.

3. Electro-analytical methods-II (12L)

Fundamentals, electrode-solution interface layer, electrolytic process, three electrode system; supporting electrolyte, DME; Ilkovic equation, Ilkovic-Heyrolsky equation, test of reversibility, current-voltage diagram, DC and AC Polarography, stripping voltametry

4. Physical characterization of inorganic compounds by spectral analysis-II (13L)

Application NMR spectroscopy-fundamentals, the contact and pseudo contact shifts, factors affecting nuclear relaxation, application of H-1, C-13, P-31 and F-19 NMR towards the structural elucidation of metal-organic complexes, an overview of metal nucleides with emphasis on Pt-195 and Sn-119 NMR

M. Sc. Semester-III
Theoretical
CH 917: Optional (Organic)
Full Marks: 50 (40 + 10); Credit point: 4

1. Oxidation reactions in Organic Synthesis (12 L)

Fundamental Concepts of Redox reactions in Organic Chemistry, Oxidation of alcohols: By Chromium and Manganese Reagents, Silver carbonate, oxidation via alkoxysulphonium salts and other methods, *Oxidation of Carbon-Carbon double bonds:* Dihydroxylation, epoxidation, Sharpless Epoxidation, Diastereoselective epoxidation of homoallylic alcohols, Ozonolysis, Photosensitized oxidation of alkenes, Pd-catalyzed oxidation of alkenes, *Oxidation of Carbonyl Compounds:* Baeyer-Villiger oxidation of ketones and related reactions, Conversion to α , β-unsaturated ketones, other methods, Use of Ruthenium tetroxide and Thallium (III) nitrate as oxidizing agents for organic substrate, other oxidizing agents.

2. Reduction reactions in Organic Synthesis **(13 L)**

Catalytic Hydrogenation: Concept of hydrogenation and hydrogenolysis, Heterogeneous and Homogeneous Catalytic Hydrogenation (the Catalyst used, selectivity of the reduction, reduction of functional groups, stereochemistry and mechanism), Transfer Hydrogenation.

Reduction by Dissolving Metals: Reduction with Metal and acid (reduction of carbonyl compounds), reduction with metal in liq. Ammonia, Reductive fission of alcohols and halides; *Reduction by Hydride Transfer reagents:* Aluminium alkoxides, lithium aluminium hydride and sodium borohydride and their modified reagents (selectivity of the reduction, reduction of functional groups, stereochemistry and mechanism). Reductions with Boranes and dialkylboranes.

Wolff-Kishner reduction, Desulphurisation of thio-acetals, Reduction of organic compounds by di-imide, low-valent Titanium reagents, trialkyltin hydrides, trialkylsilanes and other reagents.

3. Organometallic Chemistry: Part-A **(12 L)**

Preparation, Properties and Reactions of Organomagnesium, Organolithium and Organozinc reagents in synthesis. The role of Boron, Silicon, Sulphur and Phosphorus in organic synthesis.

4. Organometallic Chemistry: Part-B **(13 L)**

Principle, preparation, properties and application of some transition metals in organic synthesis with special ref. to Copper, Palladium, Cobalt, Titanium and Nickel.

M. Sc. Semester-III
Theoretical
CH 917: Optional (Physical)
Full Marks: 50 (40 + 10); Credit point: 4

1. Connection between Thermodynamics and Statistical Mechanics **(12L)**

Definition of Microstates and Macrostates. Boltzmann's definition of entropy. Formula for calculation of thermodynamic properties in terms of number of microstates. Determination of number of microstates for classical ideal gas. Connection among the properties of ideal gas, Gibbs paradox, Sackur-Tetrode equation.

2. Ensemble Method and its Application **(13L)**

Definition of ensemble. A priori probability. Gibbs postulate in Statistical mechanics. Ergodic hypothesis. Prescription for studying of thermodynamic systems based on ensemble method. Preparation of equilibrium ensemble corresponding to given thermodynamic system (isolated, closed and open). Determination of distribution function. Partition function. Calculation of thermodynamic properties in terms of partition function. Theory of Fluctuations. Calculation of fluctuation in energy, number of particles, density, entropy, volume, temperature etc.

3. Boltzmann, Fermi-Dirac and Bose-Einstein Statistics **(13L)**

Canonical partition function for non-interacting distinguishable and non-identical particles. Boltzmann Statistics. Grand canonical partition function for non-interacting identical particles. Fermi-Dirac and Bose-Einstein statistics and their limiting behavior. Ideal monoatomic gas. The translational partition function. The electric and nuclear partition function. Thermodynamic function. Ideal diatomic gases. The rigid rotor-Harmonic oscillator approximation. The vibrational partition function. The rotational partition function of a heteronuclear molecule. The symmetry requirement of the total wave function of a homonuclear diatomic molecule. The rotational partition function of a homonuclear diatomic molecule. Thermodynamic function.

4. Classical and Quantum Statistics **(12L)**

The classical partition function. Phase space and the Liouville equation. Equipartition of energy. Ideal polyatomic gas. The vibrational and the rotational partition functions. Thermodynamic function. Hindered rotation. A weakly degenerate ideal Fermi-Dirac Gas. A strongly degenerate ideal Fermi-Dirac gas. A weakly degenerate ideal Bose-Einstein gas. A strongly degenerate ideal Bose-Einstein gas. An ideal gas of photons. The density matrix. The classical limit from the Quantum mechanical expression for Q.

M. Sc. Semester-III
Practical
CH 918: Optional (Inorganic)
Full Marks: 50 (40 + 10); Credit point: 4

1. Separation by chromatographic techniques.
2. Colorimetric estimation of some metal ions.
3. Measurement of some water quality parameters.
4. Green synthesis of some inorganic compounds.

M. Sc. Semester-III
Practical
CH 918: Optional (Organic)
Full Marks: 50 (40 + 10); Credit point: 4

1. Preparation of organic compoundsby conventional and green chemical methods followed by purification and characterization by spectroscopic technique.
2. Quantitative Estimation of:
   (a) Sugars (Glucose, Cane sugar) (b) Phenol (c) Aniline (d) Nitrogen by Kjldahl method
   (e) Saponification and Iodine value.

M. Sc. Semester-III
Practical
CH 918: Optional (Physical)
Full Marks: 50 (40 + 10); Credit point: 4

1. To determine the effect of change of (i) temperature and (ii) concentration on the rate constant of hydrolysis of an ester.
2. To study the conductance behavior of strong and weak electrolytes.
3. To determine the cmc of SDS in Water and Water-Ethanol (1:1) mixture using conductometry.
4. To determine the hydrolysis constant of aniline hydrochloride by conductometry.
5. To study the titration of H_3PO_4 by NaOH using potentiometry .
6. To determine the concentration of different halides in a mixture by potentiometry.
7. To study the iodination of aniline at different pH.
8. To determine the rate constant of oxidation of iodide ions by hydrogen peroxide studying the kinetics as a clock reaction.
9. To determine the order and rate constant of the reaction between $HBrO_3$ and HI.

M. Sc. Semester-IV
Theoretical
CH 1019: Elective-3(Physical)
Full Marks: 50 (40 + 10); Credit point: 4

1. Solid State Chemistry (16L)

Crystalline and amorphous structures. Lattice vector and reciprocal lattice vector. Defects in the solid state. Band theory of solids. Band theory – Quantum mechanical aspect. Brillouin zone. Free electron gas theory of metal. Fermi energy. Electrical and thermal conductivity of metals. Semiconductor Hall effect and Hall co-efficient.

2. Electric and Magnetic properties of Matter (8L)

Molecular response parameters – Polarizability. Dispersion forces. Bulk electrical properties – Permittivity and Susceptibility. Refractive index. Dielectric relaxation. Optical activity and Circular birefringence. Conduction in dielectrics. Magnetic susceptibility. Paramegnetism and Diamagenetism. Vector potential and current density. Shielding constants. The g-value. Spin-spin coupling and Hyperfine Interactions.

3. Physcial Chemistry of Polymers (18L)

Polymerization reaction, kinetics of free radical and condensation polymer. Graft polymerization. Morphology and crystallinity of polymer by TGA and SEM analysis. Molecular weight determination of polymer by light scattering method and GPC method.
Criteria for polymer solubility. Thermodynamics of polymer solutions. Good and bad solvents. Theta temperature. Flory-Huggins model, dilute polymer solution. Excluded volume.

4. Photoexcited Processes (8L)

Excitation of molecules – Singlet and Triplet states. Radiative and Non-radiative relaxations. Franck-Condon principle. Absorption, emission and excitation spectra - mirror symmetry. Quenching of Fluorescence. Excited state processes – proton transfer, electron transfer and energy transfer. Marcus Theory. Solvent effect in spectroscopy. Solvation dynamics. Non-linear optical processes. Stimulated emission of radiation. Principles of Laser action. Applications of Lasers.

M. Sc. Semester-IV
Theoretical
CH 1020: Optional (Inorganic)
Full Marks: 50 (40 + 10); Credit point: 4

1. Environmental chemistry (12L)

Biochemical effects of As, Pb, Cd, Hg, Cr, and their chemical speciation, monitoring and remedial measures; eutrophication, wastewater treatment, control of air pollution: different methods, role of plants, various source of soil pollution; noise pollution, Agricultural and industrial pollution, Green solution to various environmental hazards.

2. Lanthanides, actinides and super-heavy elements **(13L)**

Coordination chemistry, magnetic and spectral properties, comparison of general properties of lanthanides and actinides, comparison with d-block elements, Organo lanthanides and actinides, separation of lanthanides and actinides, analytical application of lanthanides and actinides-lanthanides as shift reagents and high temperature super conductors, manmade elements-theoretical background, production, separation and predicted properties.

3. **Nanomaterials** **(12L)**

Nanoparticles: zero dimensional nanostructure, homogeneous and heterogeneous nucleation, metallic nanoparticles- synthesis and applications; Nanowires and nanorods: one dimensional nanostructures, spontaneous growth, VLS, electro spinning, lithography; Thin film: two-dimensional nanostructure- preparation techniques; Langmuir-Blodgette (LB) film-growth techniques, photolithography properties and applications.

4. **Physical characterization of inorganic compounds by spectral analysis-III** **(13L)**

Basic concept of Raman Spectroscopy, application of vibration spectroscopy- symmetry and shapes of AB_2, AB_3, AB_4, AB_5 and AB_6, mode of bonding of ambident ligands, ethylenediamine and diketo complexes, Resonance Raman spectroscopy, surface enhanced Raman spectroscopy (SERS).

M. Sc. Semester-IV
Theoretical
CH 1020: Optional (Organic)
Full Marks: 50 (40 + 10); Credit point: 4

1. Organic Photochemistry **(13L)**

Basic Principles, Jablonski diagram, Excited state (S1 and T1) of some organic molecules, *Cis-trans* mechanism, Photo chemical reactions of carbonyl compounds, olefins and conjugated carboyl compounds, Photo induced functionalisation of organic molecules involving Norrish type I, Norrish type II, Paterno Buchi Reaction, di-π- methane rearrangement, Bartron reaction, Photo reduction of ketones, Substitution in aromatic system.

2. Radical Reaction in Organic Chemistry **(12L)**

Definition, Generation of free radicals, detection, shapes and stability, stable free radicals. Example of addition , substitution, oxidation, cyclization and rearrangement involving radical reaction mechanism.

3. Pericyclic reaction Part A **(13L)**

Introduction, phase and symmetry of orbitals, types of pericyclic reactions; *Cycloaddition reactions:* Definition, FMO-approach, Co-relation diagram, Dewar's PMO-approach for cycloaddition (2+2 and 4+2) reactions, Woodward-Hoffmann selection rules, Regioselectivity, secondary orbital interaction, Lewis acid catalysis, Site selectivity, Periselectivity. Regioselectivity in 1,3-Dipolar cycloadditions, *Electrocyclic reactions:* Definition, FMO-approach, Dewar's PMO-approach for electrocyclic reactions, electroreversion, stereochemical effects, Woodward-Hoffmann rules,

4. Pericyclic reaction Part B **(12L)**

Chelotropic reactions: Definition, FMO-approach for cholatropic reactions, Woodward-Hoffmann rules, Stereochemical outcome, *Sigmatropic rearrangement:* Definition, types of sigmatropic reactions, Hydrogen shifts and carbon shifts ([1, j] and [i, j]), FMO-approach, Dewar's aromatic transition state approach, selection rules, Claisen and Cope rearrangements, *Ene reaction:* Definition, FMO-approach for ene reactions, Effects of Lewis acids.

M. Sc. Semester-IV
Theoretical
CH 1020: Optional (Physical)
Full Marks: 50 (40 + 10); Credit point: 4

1. **Modeling of artificial photo synthesis (13L)**

Photo Natural solar energy conversion process (reaction of photo synthesis) , photolysis of water, modeling and mimicking of photo synthesis process

2. **Details of artificial photo synthesis (12L)**

Photo physical and photo chemical process of semiconductor based material and dye sensitized photo galvanic cells in solar energy conversion. Theoretical aspects of this conversion process

3. **Molecular Reaction dynamics (MRD)-I (13L)**

Motivation, important vocabularies of MRD, Energy partitioning, A simple model of energy partitioning, Molecular collisions and free path phenomena, collision cross-section and the inter molecular potential

4. **Molecular Reaction dynamics (MRD)-II (12L)**

Dynamics of elastic molecular collisions, the reaction cross-section, the reaction probability, elastic scattering as a probe of the interaction potential, inter molecular potential from experiment and theory, angular distribution in direct reactive collisions.

M. Sc. Semester-IV
Theoretical
CH 1021: optional (Inorganic)
Full Marks: 50 (40 + 10); Credit point: 4

1. **Polymer Chemistry-II (12L)**

Inorganic polymers- coordination polymers, polyphosphazenes, silicones, inorganic rubber, sulfur-nitrogen polymers, polyatomic ions of Sn, Pb, S, Se and Te, homopoly and heteropoly acids and salts; Organo-metallic Polymers- different types; Polymerization: Metal ion initiated polymerization and coordination polymerization, olefin metathesis and metathesis polymerization, ring opening polymerization (ROP), Zieglar-Natta catalysts and green catalysts; Polymer metal complexes and their role in analytical chemistry

2. **Redox reactions and its mechanism (13L)**

Classification, kinetics and mechanism, outer-sphere electron transfer reactions-controlling factors, self-exchange rate, electron tunneling hypothesis, hetero-nuclear redox reaction and simplified Marcus theory; Marcus cross relationship and its application, solvated electron; Inner-sphere electron transfer reaction-characteristics and controlling factors, ligand transfer, role of bridging ligand, chemical mechanism of electron transfer, complementary and non-complimentary redox reactions.

3. **Physical characterization of inorganic compounds by spectral analysis-IV (13L)**

Electron paramagnetic resonance- Zero field splitting factor and its importance in napthyl radical and various metal centers having more than one odd/even number unpaired electrons, spin polarization for atoms and transition metal ions, spin orbit coupling, EPR activity and application to metal-ligand complex with paramagnetic metal ions and paramagnetic ligands, Isotropic and anisotropic EPR spectra of metal complexes, Electronic spectra for chemical analysis (ESCA)- basic principle and applications

4. **Advanced Inorganic materials (12L)**

Synthesis and characterization, Magnetoresistance, Colossal magnetoresistive materials (CMR), Double exchange, Superexchange, Goodenough-Kanamori-Anderson rules (GKA), Phase separation: homogeneous, inhomogeneous, structural and electronic, Charge ordering (CO), orbital ordering (OO), effect of ionic radius on the physical properties of these functional materials, Chemical pressure, Size disorder, Thermoelectric oxides.

M. Sc. Semester-IV
Theoretical
CH 1021: Optional (Organic)
Full Marks: 50 (40 + 10); Credit point: 4

1. **Concept on M.O. and V.B. theory (12 L)**

Introduction to Huckel molecular orbital (MO) method as a mean to explain modern theoretical methods. Advanced techniques in PMO and FMO theory. Molecular mechanics, semi empirical methods and Ab Initio methods. Pictorial Representation of MOs for molecules, Qualitative Application of MO Theory to reactivity, Valence bond configuration mixing diagrams. Relationship between VB configuration mixing and resonance theory. Reaction profiles. Potential energy diagrams.

2. **Structural effects on reactivity (13 L)**

Linear free energy relationships (LFER). The Hammett equation, substitutent constants, theories of substitutent effects. Interpretation of σ-values. Reaction constant *ρ*. Deviations from Hammett equation. Dual - parameter correlations, inductive substituent constant. The Taft equation.

3. **Natural Products: Structure and Stereochemistry (12 L)**

Natural Products: Structure and stereochemistry of Alkaloids (Atropine/ Quinine); Terpenoids (Abietic acid/ β-Carotene); Steroids (Cholesterol)

4. **Natural Products: Bio-synthesis (13 L)**

Natural Products: Biosynthesis of Atropine, Quinine, Abietic acid, β-Carotene, Cholesterol.

M. Sc. Semester-IV
Theoretical
CH 1021: Optional (Physical)
Full Marks: 50 (40 + 10); Credit point: 4

1. **Electrode kinetics (12L)**

Butler-Volmer equation and its application. Tafel equation from Volmer equation. Equilibrium exchange current density and its determination. Current potential reaction for reversible electrode. Doss rectification. Electrokinetics of Corrosion reaction. Pourbaix diagrams. Corrosion current and corrosion potential. Evans diagrams.

2. Theory of semiconductor – electrolyte interface **(12L)**

The structure of the semiconductor–electrolyte interface. Analogies between semiconductors and electrolytic solutions. The Garrett-Brattain space charge. Differential capacity. Mott-Schottky equation. Flat band potential. Application of semiconductor electrode in photoelectric device.

3. Non-equilibrium Statistical Mechanics **(13L)**

Brownian motion: Einstein's theory. Irregular movement of particles suspended in a liquid and its relation to diffusion. Diffusion and mobility. Determination of Avogadro number. Experimental confirmation. Theoretical observation on Brownian motion and the existence of a random force. Langevin description of Brownian motion: general expression for mean square displacement (i) short time limit and (ii) long time limit. Relation between random and viscous force: the fluctuation-dissipation theorem. Brownian motion in velocity space: Fokker Planck equation. Calculation of M_1 (v), calculation of M_2 (v). Brownian motion in phase space (motion in a force field): Kramers' equation. Kramers' equation as a generalization of Liouville equation and connection to equilibrium statistical mechanics, Kramers theory of activated process (i) calculation of j and (ii) calculation of n_a. A simple connection to transition state theory. Overdamped motion: Smoluchowski equation and diffusion over a barrier. The master equation: applications in (i) unidirectional random walk, and (ii) quantized harmonic oscillator interacting with a radiation field.

4. Irreversible Thermodynamics **(13L)**

Thermodynamic criteria for Non-equilibrium states. Entropy production and Entropy balance equations. Generalized flux and forces. Stationary states. Phenomenological equations. Microscopic reversibility and Onsager equation. Applications in physico-chemical and biological phenomena. Coupled reactions.

M. Sc. Semester-IV
Theoretical
CH 1022: Optional (Inorganic)
Full Marks: 50 (40 + 10); Credit point: 4

2. Radio tracers and hot atom chemistry **(10L)**

Szilard-Chalmer reaction and retention of activity, primary and secondary retention, synthesis of labeled compounds, isotopes dilution, DIDA, IIDA and substoichometric methods of analysis, application and numerical problems, Nuclear activation analysis, secondary particle activation analysis, charged particle activation analysis, problems and application

3. **Radiation chemistry** **(14L)**

Ionizing radiation and its physical and chemical effect in target, water radiolysis, Definition of different units in radiation chemistry, calculation of radiation dose, biological effects, lethal dose, permissible level of radiation dose, primary radiological products of water and their characterization, dosimetric concepts and quantities, different types of chemical dosimeter, thermo-luminescence and lyo-luminescence, different unusual reactions by lyo-luminescence

4. **Atomic spectroscopy** **(10L)**

Basis principle, instrumentation and applications of Atomic Absorption Spectroscopy (AAS), Atomic Emission Spectroscopy (AES), Flame Emission Spectroscopy (FES), Inductively Coupled Plasma Mass Spectroscopy (ICPMS) and Fluorometry

4. Separation techniques **(16L)**

Solvent extraction: principle, distribution ratio and partition coefficient, successive extraction and separation; different methods of extraction systems; Craig extraction and counter current distribution; problems; Chromatography: general principle; classification, mathematical relations of capacity, selectivity factor, distribution constant and retention time; chromatogram, evaluation in column chromatography: band broadening and column efficiency; Van Deemeter equation; column resolution, numerical problems, GC, LC, TLC, PC, SEC

M. Sc. Semester-IV
Theoretical
CH 1022: Optional (Organic)
Full Marks: 50 (40 + 10); Credit point: 4

1. Drug design and Antineoplastic agent **(12 L)**

Drug Design: Concept of Pharmacodynamics, Drug targets: Enzymes, Receptors, nucleic acids. Concept on Pharmacokinetics: Drug Absorption, Distribution, Metabolism and Excretion. Concept on lead compound and lead modification, Pharmacophore. Concept of prodrug and soft drug. Structure activity relationship (SAR), factors affecting bioactivity; *Antineoplastic agents:* **S**ynthesis and mode of action of mechlorethamine, cyclophosphamide, melphalan, and 6-mercaptopurine.

2. Cardiovascular, Antiinfective and Antibiotics **(13 L)**

Cardiovascular drugs: Introduction to cardiovascular diseases, Synthesis and mode of action of amyl nitrate, sorbitrate, diltiazem, quinidine, verapamil, methyl dopa; *Local antiinfective drugs and antibiotics:* Synthesis and mode of action of sulphonamides, nalidixic acid, norfloxacin, aminosalicyclic acid, ethinamide, fluconazole, chloroquin and premaquin; *Antibiotics:* Cell wall biosynthesis, inhibitors, β-lactam rings, Synthesis of penicillin.

3. Asymmetric Synthesis: Part-A **(12 L)**

Introduction, kinetic and thermodynamic principles to asymmetric synthesis, diastereoselective & enantioselective synthesis; *Methods of asymmetric synthesis:* Resolution, use of chiral pool, chiral auxiliaries, use of stoichiometric chiral reagents, asymmetric catalysis.

4. Asymmetric Synthesis: Part-B **(13 L)**

Asymmetric hydrogenation with special reference to Ru-BINAP catalysts, asymmetric reduction of prochiral ketones with Baker's Yeast & CBS-catalyst, asymmetric epoxidation with special reference to Sharpless and Jacobsen epoxidation, asymmetric diethylzinc addition to carbonyl compounds, asymmetric aldol reactions, asymmetric Michael reaction; Few important industrial applications of asymmetric synthesis

M. Sc. Semester-IV
Theoretical
CH 1022: Optional (Physical)
Full Marks: 50 (40 + 10); Credit point: 4

1. Excitation of Molecules and Motion in Excited State (10L)

Theory of Electromagnetic Radiation. Interaction between Matter and Electromagnetic Radiation – Semiclassical treatment using Time-dependent perturbation Theory. Fermi golden rule, Transition probabilities and rates, Spectral shapes. Decoupling of the nuclear and electronic motions in a molecule: Born-Oppenheimer approximation.

2. Rotational, Vibrational and Raman Spectroscopy (15L)

Rigid & Non-rigid Rotors. Vibrational spectroscopy – Harmonic and Anharmonic Oscillators. Normal coordinates. Effects of Anharmonicity. Vibration-rotation transitions. Raman and Rayleigh scattering – Classical and Quantum Mechanical treatments. Polarization of scattered light. Rotational and Vibrational Raman spectroscopy. Resonance Raman effect. Selection rules of rotational, vibrational and Raman spectroscopy. Instrumentation of microwave, IR and Raman spectroscopy.

3. Electronic Spectroscopy (15L)

Atomic structure: vector model, spin-orbit coupling, atomic states and term symbols. Many-electron atoms – Hund's rules. Selection rules for atomic electronic transitions. Diatomic molecules – Hund's coupling cases. Rotational and vibrational structures of diatomic electronic transitions. Franck-Condon principle. Dissociation, Photodissociation and Predissociation. Polyatomic molecules – orbitals and electronic states. Chromophores. Vibronic transitions. Spin-orbit coupling and singlet – triplet transitions. Selection rules for molecular electronic transitions. Photoelectron spectroscopy. Rotational structure of some polyatomic electronic transitions. Instrumentation of UV-visible absorption and emission spectroscopy.

4. Spin Spectroscopy – NMR and ESR (10L)

Nuclear magnetic moment and response in an external magnetic field. Classical and Quantum Mechanical perspectives of nuclear magnetic resonance (NMR). Bloch equations. Spin-spin and spin-lattice relaxation and spectral shapes. Free induction decay and FT-NMR technique. Chemical shift and nuclear shielding. Spin magnetic moment of electrons and electron spin resonance signal (ESR). The g-factor and hyperfine splitting – interaction between nuclear spin and electron spin. Applications and instrumentation of NMR and ESR. Multi-dimensional NMR spectroscopy. Nuclear quadrupole resonance.

M. Sc. Semester-IV
Project
CH 1023: Optional (Project)
Full Marks: 100 (80 + 20); Credit point: 8

Topic selection in consultation with the teacher, literature search from different reference books and using internet search, typed written-up with proper tables, structures, figures and literature to be submitted, seminar lecture on this topic to be delivered in presence of external expert and sectional teachers