SEMESTER I

Paper I

Molecular Symmetry and Molecular Vibrations

1. **Molecular Symmetry:**
   - **a)** Symmetry elements and symmetry operations with special reference to water, ammonia and ethane.
   - **b)** Classification of molecules/ ions based on their symmetry properties.
   - **c)** Derivation of matrices for rotation, reflection, rotation-reflection and inversion operations.
   - **d)** Direct products.
   - **e)** Symmetry point groups applied to all type of molecules (C_{nh}, D_{nh}, C_{nv}, T_d, O_h and I_h).
   - f) Group multiplication basis, matrix representation, character of an operation, orthogonality, projection and shift operators, character tables, reducible and irreducible representations, groups subgroups, and classes.
   - g) Symmetry of orbital: orbital symmetry properties, projection to get symmetry orbitals, projection operators, basis functions and hybrid orbitals with example.

2. **Molecular Vibrations:**
   - **a)** Internal and symmetry coordinates, symmetry adapted linear combinations (SALCs), symmetry of normal vibrations, mixing of internal coordinates in normal modes, determination of symmetry types of the normal modes.
   - **b)** Polyatomic molecular vibrations, vibrational spectroscopy, selection rules for IR and Raman spectroscopy, depolarization effects, analysis of vibration spectra of 1,2 – dichloroethylene.
   - **c)** Normal coordinate analysis of water and ammonia molecules.

3. **Symmetry and Chemical reactivity**
   - **a)** Symmetry control of Chemical reactions.
   - **b)** Symmetry considerations: electro cyclic and cycloaddition reactions.

Books Recommended:

1. DM Bishop, “Group theory and Chemistry” Dover Publications.
2. Cotton, “Chemical Applications of Group Theory”, John Wiley.
3. M. Hamaresh, “Group theory and its Applications to Physical Problems” Addison- Wisley
4. R.L. Flurry, “Symmetry Groups”
5. Hanna “Quantum Mechanics in Chemistry”.
6. McWeeny, “Symmetry - An Introduction to Group Theory”, Pergamon Press.
7. Lowell H. Hall “Group Theory and Symmetry in Chemistry”, McGraw Hill Book Company, New York.

Paper II
Physical Chemistry
(Quantum Chemistry)

1. **Fundamentals**
   a. Limitations of classical machines
   b. Postulates of quantum machines
   c. Quantum mechanicaloperators and classical variables
   d. Operators and matrices
   e. Hermitian Operators and orthogonality
2. **Schrödinger equation and particle in a box**
   a. Schrödinger equation
   b. Linear operator in quantum mechanics
   c. Eigen value problem in quantum mechanics
   d. Wave function and probability
   e. Normalized wave functions
   f. Average quantities
   g. Particle in one and three-dimensional box and degeneracy of state.
3. **Quantum mechanical treatment of a harmonic oscillator**
   a. Classical harmonic oscillator
   b. Harmonic oscillator model of a diatomic molecule
   c. Harmonic oscillator approximation
   d. Energy levels of a harmonic oscillator
4. **Quantum mechanical treatment of a rigid rotor**
   a. Energy levels of a rigid rotor
   b. Rigid rotor model of a diatomic molecule
   c. Rotational vibrational spectra
   d. A non-rigid rotor
   e. Rigid rotor selection rule
5. **Schrödinger equation for H and He- atom**
   a. s-orbital
   b. p-orbital
   c. Electron spin
6. **Atomic structure**
   a. H-F Theory
   b. Two electron problem
   c. Hartree Product
   d. Antisymmetry and Slater determinant
7. **Approximation methods**
   a. The variation method
   b. Perturbation method
   c. First order perturbation theory

Books recommended :

1. Modern quantum chemistry : An introduction to Advance Electronic Structure Theory by a Szabo and NS Ostland
2. Quantum Chemistry by Donald A. Mcquarrie

3. Molecular Quantum Mechanics by P.W. Atkins and R.S. Friedman

SEMESTER I
Paper III
INORGANIC CHEMISTRY
(Main Group Elements)

1. **Stereochemistry of Bonding in Main Group Components**
   Walsh diagram, dπ – pπ bonds, Bents rule, Energetics of hybridization
2. **Preparation, Structure, Bonding and Technical Applications of**
   (a) Polyether complexes of alkali and alkaline earth metals
   (b) polyphasphazenes
   (c) Thiazyl and its polymers, tetrasulfur dinitride.
3. **Structure and bonding of Borane anions**
4. **Structure of Silicons and Silicates**
5. **Synthesis and structure of:**
   (a) Carbides
   (b) Polyions of Ge, Sn, Pb, Sb, Bi and Mg
6. **Preparation, Properties, Structure and Applications of**
   Alkyl and aryls of Lithium, Beryllium, Magnesium, Aluminum, Mercury and Tin.

Books Recommended :

1. Advance Inorganic Chemistry, 6th Edition, Cotton and Wilkinson
2. Inorganic Chemistry, 4th Edition, Principles of Structure and Reactivity by J.F. Huheey, E.A. Keiter and R.L. Keiter, 1993
3. Chemistry of Elements by N.N. Greenwood and A. Ernshaw, Butterworths 1997
4. Organometallic Chemistry: A Unified Approach by R.C. Mehrotra and A.K. Singh
5. Comprehensive Coordination Chemistry Vol.3 by G. Wilkinson, R.D. Gillard, And J.A. McCleverty, Pergamon Press 1987.

SEMESTER I
Paper IV
ORGANIC CHEMISTRY
(Aromaticity and Reaction Mechanism)

Section A

Aromaticity: Concept of aromaticity, antiaromaticity, nonaromaticity and homoaromaticity, Alternant and nonalternant systems, Aromaticity in nonbenzenoids (tropolone, azulene, annulenes, ferrocene and fullerene).

Basic Principles of organic reaction mechanism: potential energy diagram, transition states and intermediates, methods of determination of organic reaction mechanism, Kinetic isotopic effect and its importance in determination of reaction mechanism.

Section B

Substitution Reaction:

Aliphatic Nucleophillic Substitution at Saturated Carbon Atom:

Mechanism and stereochemistry of SN^1, SN^2, SN^1 and SN^2 reactions. Role of structure of substrate, nucleophile, leaving group and solvent on SN reactions, nucleophillic substitution in bridged systems.

Neighbouring Group Participation:

Evidence for NGP, Participation by phenyl group, π and σ bonds, Anchimeric assistance.

Aromatic Nucleophillic Substitution:

aromatic SN^1 and SN^2 reaction (ArSN). Addition –Elimination (ipso) and elimination- addition (benzyne) mechanisms, Effect of substrates structure, nucleophile and leaving group.

Aromatic Electrophillic Substitution:

General view, energy profile diagram, Arenium ion mechanism (ArSE), ortho/ para ratio and ipso substitution.

Elimination Reaction:

E1, E2 and E1Cb mechanism, orientation (Satzef and Hoffman Rule), Pyrolytic (syn), elimination (Chugaev and Hoffman) , stereochemistry of E2 elimination, E1, E2 and E1Cb spectrum, factors affecting E1, E2 and E1Cb reactions. Competition between substitution and elimination.

Books Recommended:

1. Advance Organic Chemistry – Structure and Mechanism, J. March, John Wiley
2. Advance Organic Chemistry, by F.J. Carey and R.J. Sundberg, Plenum
3. Organic Chemistry, Vol.1, I.L. Finar, ELBS.

PRACTICAL
Marks 100: Time 12 hours in two days
Marks distribution

Physical: 20

Inorganic: 20

Organic: 20

Viva: 15

Record:5

Mid-term examination:20

(Marks obtained by students in mid-semester examination will be submitted to the head of the department and it will be sent to the Controller of exams with the marks of the final semester practical examination)

Physical practical exercises:

1. Determine the solubility of benzoic acid in water at different temperatures and calculate the heat of solution.
2. Determine the distribution coefficient of benzoic acid between benzene and water.
3. Determine the distribution coefficient of acetic acid between benzene and water.
4. Determine the distribution coefficient of iodine between carbon tetra chloride and water.
5. Study the adsorption of acetic acid on charcoal and draw the Freundlich isotherm.
6. Show that the order of reaction between acetone and iodine is zero with respect to iodine.

Inorganic exercises

1. Qualitative analysis of an inorganic mixture of seven radicals including Tl, W, Se, Te, V, Be, U, Ti, Zr, Th, Ce and Li, in addition to the radicals prescribed for the B.Sc. Course. Semi micro analysis is to be done.
2. Chromatographic separation of metal ions given in any one of the following combinations:
    (a) Pb^{2+}, Ag^{+}, Hg_2^{2+}
    (a) Co^{2+}, Ni^{2+}, Cu^{2+}
    (a) Fe^{3+}, Cr^{3+}, Al^{3+}
    (a) Ba^{2+}, Sr^{2+}, Ca^{2+}

Organic exercises:

1. Analysis of primary binary organic mixture (liquid-liquid, liquid-solid, solid-solid)
2. Determination of equivalent weight of organic acids by direct titration method

Semester II
Paper 1
Analytical chemistry

1. **Electroanalytical Techniques:**

   (a) Conductometric: Discussion of the nature of the curves of acid-base (including mixtures of acids), precipitation and complexometric titrations.
   (b) Potentiometric: different types of electrodes, discussion of nature of the curves for oxidation- reduction and acid-base titrations, comparison with the conductometric method.
   (c) Voltametry, Cyclic voltametry
   (d) Polarography: Dropping mercury electrons and its advantages, polarographically active species, concept of residual, diffusion and limiting current of half-wave potential, Ilkovic equation and factors affecting diffusion current.

2. **Thermoanalytical Methods:**

   (a) Thermogravimetry: apparatus, factors affecting TGA, interpretation of TG curves of $CaC_2O_4.H_2O$ and $MgC_2O_4.2H_2O$
   (b) Differential Thermal Analysis and Differential scanning Calorimetry: Apparatus, factors affecting DTA/DSC curves with Special reference to heating rate, Particle size and packing, measurement of heat of transition, heat of reaction and heat of dehydration of salts of metal hydrates.
3. **Radiochemical methods:**
   (a) Isotope Method
   (b) Inverse Isotopic Dilution
   (c) Neutron activation technique.
4. **Chromatographic Method:**
   (a) Gas Chromatography: GLC and GC
   (b) HPLC
5. **Spectral Methods:**
   (a) Nephleometry
   (b) Turbidimetry
   (c) Flame Photometry

Books Recommended:

1. Fundamentals of analytical chemistry, D.A. Skoog, D.M. West and F.J. Holler

2. Quantitative inorganic analysis, A.I. Vogel
3. Instrumental Methods of Chemical Analysis, B.K. Sharma
4. Instrumental Methods of Chemical Analysis, H. Kaur
5. Analytical Chemistry, Gary D. Christian

SEMESTER II
Paper II
PHYSICAL CHEMISTRY
Thermodynamics and Electrochemistry

1. Thermodynamics

Joule Thomson's effect, temperature dependence of free energy; Gibbs Helmholtz equation and its application, The Clausius Claypeyron equation. Thermodynamics relations; The Maxwell's relation, Thermodynamic equation of state, Relationship between E or H and P,V,T, partial molar quantities; partial molar volume and partial molar Gibbs energy, Experimental determination of excess molar volume, Chemical potential and its variation with T and P, applications of Chemical Potential, Gibbs Duhem equation, fugacity and activity coefficient and its determination. The third law of thermodynamics, The Nernst heat theorem and entropy calculations, The residual entropy.

2. Electrochemistry

Brief description of ion- association, Wein effect and Debye – Falkenhagen effect, Effect of ionic strength on the rate of ionic reactions. The Electrical double layer, electro kinetic phenomena, Electrode Processes: Concentration polarization, deposition and decomposition potentials, Overvoltage, Limiting current density and Dropping Mercury Electrode.

SEMESTER II
INORGANIC CHEMISTRY
Transition Elements

1. **Structures of 2 to 8 Coordinate Metal Complexes**

   Cation-anion ratio in various polyhedral, Hybrid orbitals and preferred conditions of formation of the complexes of following geometries :
   C.N.2 - Linear
   C.N.3 - Trigonal planar, Trigonal pyramidal
   C.N.4 - Tetrahedral, Square planar
   C.N.5 - Trigonal bipyramidal, Square pyramidal, pentagonal.
   C.N.6 - Octahedral, Trigonal prism
   C.N.7 - Pentagonal bipyramidal, Capped octahedral, Capped trigonal prism.
   C.N.8 - Cubic, Tetragonal antiprismatic, Dodecahedral, Hexagonal bipyramidal, and Bicapped trigonal prism,
   Stereochemical non-rigidity in four to eight coordinate Complexes.

2. **Stereoisomerism** in six coordinate octahedral complexes (Ma3bcd, Ma2bcde, Mabcdef and complexes containing bi-and ter- dentate ligands, Intermolecular and intramolecular rearrangements (Bailar and Ray Dutta twist only), mechanism of racemisation in tris (chelate) octahedral complexes, Methods of resolution of optical isomers.

3. **Kinetics and mechanism** of substitution reactions in octahedral Co (III) and square planar Pt (II) complexes.

4. **Electron Transfer Reactions:**
   Mechanism of one electron transfer reactions (inner and outer sphere mechanisms), Factors affecting the rates of direct electron transfer reactions and the Marcus equation, Two electron transfer reactions.

5. **Metal Ligand Equilibria in Solution :**
   Step wise and overall formation constants and their relations, Factors affecting the stability of metal complexes with reference to the nature of metal ions and ligands, determination of stability constants by pH-metric and spectroscopic methods.

Books Recommended:

1. Inorganic Chemistry, 4th Edition, Principles of Structure and Relativity by J.E. Huheey, E.A. Keiter and R.L. Keiter, 1993
2. Chemistry of Elements by N.N. Greenwood and A. Ernshaw, Butterworths, 1997
3. Mechanism of Inorganic Reactions; A Study Of Metal Complexes in Solution by F. Bosolo and R.G. Pearson
4. Ligand Field Theory And Its Application by B.N. Figgis and M.A. Hitchman, Wiley, NewYork, 2000.

SEMESTER II
PAPER IV
ORGANIC CHEMISTRY
Natural Products and Organic Photochemistry

Section A

Biogenesis of Natural Products: The acetate hypothesis, isoprene rule, mevolonic acid fromacetyl coenzyme A, Biogenesis of terpenoids, Shikmic acid pathway of biogenesis of aromatic ring, General biosynthesis of alkaloids.

Alkaloids: Structure elucidation of alkaloids – a general account, structure and synthesis of – nicotine, Quinine, Morphine and reserpine.

Terpenoids: General structure determination of terpenoids, structure of synthesis of terpenoid, camphor, abietic acid, squalene and taxol (Synthesis only).

Alicyclic Compounds: General methods for preparation of medium and large ring alicyclic compounds. Baeyer strain theory, theory of strainless rings.

Section B

Organic Photochemistry: electronically excited states, spin multiplicity, Jabonskil diagram, Intersystem crossing.

Photochemistry of Alkenes: Geometrical isomerization, cyclization dimerization and photo-oxidation reactions. Rearrangements of 1,4 and 1,5 – dienes (di-pi methane and related rearrangements).

Photochemistry of Carbonyl Compounds: Reduction, inter and intermolecular addition (Paterno- Buchi), fragmentation (Norrish-1 and Norrish-2), Reactions of saturated acyclic, cyclic and unsaturated carbonyl compounds, Photochemistry of cyclohexanone and cyclohexadienone.

Photochemistry of Carbonyl Compounds: isomerization, skeletal isomerization, Dewar and Prismane isomerization of disubstituted benzenes, Photo-Fries rearrangement.

Books recommended:

1. Fundamentals of Photochemistry, K.K. Rohtagi- Mukherjee, University Press
2. Organic Photochemistry, J. Cox and B. Halton, Cambridge University Press
3. Organic Chemistry, Vol 2, I.L. Finar, ELBS

SEMESTER II
PRACTICAL
Marks 100: Time 12 Hours in two days
Marks distribution

Physical: 20

Inorganic: 20

Organic: 20

Viva: 15

Record: 5

Mid-term examination: 20

(Marks obtained by students in mid-semester examination will be submitted to the head of the department and it will be sent to the Controller of exams with the marks of the final semester practical examination)

Physical practical exercises:

1. Draw the solubility curve for water-acetic acid- chloroform system.
2. Study the adsorption of oxalic acid on charcoal and draw the Freundlich isotherm.
3. Determine the rate constant of the acid-catalyzed hydrolysis of ethyl acetate at laboratory temperature.
4. Determine the rate of constant of the hydrolysis of ethyl acetate by sodium hydroxide at laboratory temperature.
5. Carry out the coductometric titration between the strong acid and strong alkali.
6. Determine the dimerization constant of benzoic acid in benzene medium by partition method.
7. Determine the solubility of salicylic acid in water at different temperatures and calculate the heat of solution.

Inorganic

Either both gravimetric and one volumetric estimation of two metal ions from following mixtures:

(a) Cu^{2+} and Ni^{2+}
(b) Cu^{2+} and Zn^{2+}
(c) Ni^{2+} and Zn^{2+}
(d) Cu^{2+} and Ba^{2+}
(e) Cu^{2+} and Ag^{+}
(f) Fe^{2+} and Ag^{+}
(g) Ba^{2+} and Ag^{+}

Organic

Preparation of organic compounds involving two stages. Emphasis should be given in the following Processes:
Purification, distillation under reduced pressure, steam distillation, and fractional crystallization

SEMESTER III
PAPER I
Spectroscopy- 1

1. UV-Visible Spectroscopy

1.1 Different type of electronic transitions
1.2 Lambert's Beer's law
1.3 Chromophores
1.4 Auxochromes
1.5 Solvent effect
1.6 Red shift and blue shift
1.7 Woodward's rule for conjugated cyclic and acyclic dienes and α, β – unsaturated carbonyl compounds
1.8 Absorption in aromatic compounds (substituted benzene, naphthalene and anthracene)
1.9 Problems related UV-Visible Spectroscopy

2. Infrared Spectroscopy

2.1 Review of linear harmonic oscillator
2.2 Vibrational energies of diatomic molecules
2.3 Zero point energy
2.4 Force constant and bond strength
2.5 Anharmonicity
2.6 Morse potential energy diagram
2.7 Vibration rotation spectroscopy
2.8 P, Q, R branches
2.9 Break down of Born-Oppenheimer approximation
2.10 Selection rules
2.11 Overtones
2.12 Hot Bands
2.13 Absorption by common functional groups
2.14 Brief description of IR and F.T.I.R. instruments
2.15 Problems related I.R. Spectroscopy

3. Raman Spectroscopy

3.1 Theories of Raman Effect
3.2 Conditions of Raman active Vibrations
3.3 Selection rules
3.4 Polarized and Depolarized Raman lines
3.5 Study of : (Simple molecules such as SO_2, CO_2, N_2O and C_2H_2; (b) Hydrogen Bounding and (c) Metal ions in solution.
3.6 Mutual exclusion principle
3.7 Problems related with Raman Spectra and its interpretation

4. Diffraction Methods for Structure determination

4.1 X-ray

SEMESTER III
PAPER II A
PHYSICAL CHEMISTRY
Advanced Quantum Mechanics

1. **Symmetry Properties and Quantum Mechanics:**
   Invariability of SchrÖdinger equation for a molecule with respect to symmetry operations and its consequences, construction of molecular orbitals of ammonia and π–molecular orbitals of naphthalene, The direct product representation and its application in the derivation of selection rules for electronic, vibrational and Raman spectra.

2. **Huckel Molecular Orbital Theory and its Applications:**
   Calculation of -energy levels and delocalisation energy of butadiene, cyclic conjugated polyolefins - cyclopropenyl, cyclobutadiene, cyclopentadienyl, benzene, tropylium radical and cyclooctatetraene, concept of armomaticity and antiaromaticity, Huckel treatment of linear polyenes.

3. **Semi–Empirical and Ab–Initio SCF Theories :**
   Hartee-Fock Self consistent field (SCF) method, Semi–empirical SCF theory (CNDO, INDO & MNDO), Slater and Gaussian type orbitals, configuration interaction and electron correlation, Moeller-Plasset Perturbation methods.

4. **Introduction to density functional theory :**
   Concept of basic sets, exchange-correlation energy and Kohn-Sham orbitals, Local Density Approximation (LDA) and Generalized Gradient Approximation (GGA), Significance of Density Functional Theory.

5. **Introduction to molecular mechanics**

Books Recommended:

1. Chemical Application of Group Theory – F.A. Cotton
2. Introductory Quantum Chemistry – A.K. Chandra
3. An Introduction to Quantum Mechanics of Chemical Systems – R.P. Rastogi and V.K. Srivastava
4. Physical Chemistry – P.W. Atkins
5. Valence Theory – J.N. Murrell, S.F.A. Kettle and J.M. Teddor
6. Chemistry by Ira N. Levine Prentice Hall of India New Delhi 1995.

7 Coulson's volume by R. McWeeny ELBS 1978.

SEMESTER III
PAPER II B
INORGANIC CHEMISTRY
Chemical Application of Symmetry and Group Theory

1. **Symmetry and Point Groups:**
   Definitions, the symmetry point groups, identification of molar point groups, molecules of low symmetry, high symmetry and special symmetry (C_n , S_n, D_n, C_{nv}, and D_{nh} only)
2. **Groups, Sub-Groups and Classes:**
   Definitions, multiplication tables, group generating elements, sub-groups and classes, irreducible representations, the orhtogonality Theorem.
3. **Matrices Representation:**
   Matrix Representations of symmetry elements, block-factorization of larger matrices, matrix representation of C_{3v}, and C_{4v}, point groups, transformation matrices.
4. **Normal Modes of Vibrations:**
   Cartesian Coordinate and internal coordinate methods of normal mode analysis applied to C_{2v} (Symmetric XY_2, ZXY_2), C_{3v} (XY_3), T_d (XY_4) and O_h (XY_6) systems.
5. **Valence Bond treatment :**
   Formation of hybrid orbitals of XY_3 (planar), XY_4 (tetrahedral and square planar),
6. **Crystal Fields:**
   Derivation of 'd' orbital splitting patterns of central atom (M) in ML2, ML3, ML5, and ML7 system (energy calculations are not required). The effect of weak crystal field on S, P, D, F and G spectroscopic terms in Oh and Td point groups.
7. **Molecular Orbitals:**
   A_2 and AB_n (n = 1 to 3) type molecules.

Books Recommended:

1. Chemical applications of group theory. F. A. Cotton. 2nd Ed.. Wiley Eastern. 1971.

2. Group theory and symmetry in chemistry. L. H. Hall. McGraw Hill Inc.. 1969.

3. Symmetry, Orbitals and Spectra. M. Orchin and H. H. Jaffe. Wiley interscience. 1971.

4. Molecular Orbital Theory. C.J. Ballhausen and H. B. Gray. W. A. Benzamin Inc. 1965

SEMESTER III
Paper II C
ORGANIC CHEMISTRY
Stereochemistry

1. **Stereochemistry with chiral center**
   Elements of symmetry, chirality, molecules with more than one chiral center, threo and erythro isomers, Interconversion of Fischer, Newmann and Saw-Horse projections, configurational projections, R/S and E/Z
2. **Stereomerism with axial/ planar chirality and Helicity**
   Principle of axial and planar chirality, optical isomerism of biphenyl, alkenes and spiranes, optical activity due to intramolecular overcrowding, absolute configuration.
3. **Topocity and Prostereoisomerism**
   (a). Introduction
   (b). Homotopic, enantiotopic and destereotopic atoms, groups and faces
   (c). Nomenclature and symbols
4. **Asymmetric synthesis**
   (a). Regeoslsctivity, stereoselestivity and stereospecificity
   (b). Asymmetric synthesis involving chiral, auxillary chiral reagent and chiral catalysis
   (c). Enantiomeric excess i.e. quasirecemate and optical purity.
5. **Stereochemistry of compounds containing S and P atoms,** Geometrical isomerism of compounds containing C=N and –N=N- bonds.
6. **Cyclostereoisomerism**
   Configuration,c conformation and stability of mono and disubstituted cyclohexanes and cyclohaxenones, chirality of distributed cyclohexanes.

SEMESTER III
Paper III A
PHYSICAL CHEMISTRY

1. **Conductance in non–aqueous media :**
   Ion association, its effect on conductance, diffusion of electrolytes, measurements of coefficient, diffusion in relation to conductance.
2. **Electro Kinetic Phenomena :**
   Quantitative treatment of electro–osmosis, electro phoresis and streaming potential, electrical layer theories
3. **Electrodics :**
   The equilibrium exchange current density, Butler–Volmer Equation Tafel plot, high field and low field approximation
7. **Corrosion :**
   The mechanism of corrosion of metals, corrosion current and corrosion potential, electro-chemical corrosion theory, estimation of corrosion rates, corrosion prevention, polarization resistance, electro-eposition.

Books Recommended:

1. S. Glasston : Electro Chemistry
2. Robinson & Stokes : Electrolytic Solutions
3. Potter : Electro chemistry
4. Bockris and Reddy: Modern Electrochemistry Vol I and II
5. Mc Donald : Electro Chemical impedence spectroscopy

SEMESTER III
Paper III B
INORGANIC CHEMISTRY
Coordination Chemistry

1. **Energy levels in an atom :**
   Relation between electronic configuration and energy terms, Hund's rules and ground state energy terms. Inter electron repulsion parameter. Variation of Racah B and C parameters in different transition series. Spin orbit coupling parameters.
2. **Free ions in crystal fields :**
   Effect of weak crystal field on free ion terms in octahedral, square planar and tetrahedral symmetries. Orgel diagrams, Mixing of terms, Medium and strong field approximation in Oh point group, transition from weak to strong field and correlation diagram for only d^2 case, Non-crossing rule, Tanabe Sugano diagrams.
3. **Electronic spectra of complexes :**
   Interpretation of the spectra of aqueous solution of $M[H2O]_6^{n+}$, calculation of Dq, B and β parameters, Jahn Teller distortion and its effect on electronic spectra,
4. **Magnetic properties of Complexes :**
   Dia, para, ferro and antiferromagnetism, Quenching of orbital angular momentum by ligand . The magnetic properties of A, E and T terms.
5. **Metal-ligand Bonding**
   Limitations of CFT, Nephelauxetic series, molecular orbital energy level diagram of octahedral, tetrahedral and square planner complexes.

Books recommended:

1. B.N. Figgis, M.A. Hitchman, Ligand Field Theory and Its Applications, Willey, New York, 2000

2. D. Sutton, Electronics Spectra of Transition Metal Complexes.
3. K. Veera Reddy, Symmetry and Spectroscopy of Molecules.

SEMESTER III
Paper III C
ORGANIC CHEMISTRY
Organic Reaction Mechanism

1. **Molecular Rearrangements:**

   Mechanism and application of :

   Favorskil, Sommetet-Hauser, Stevens, Baeyer-Villinger, Demjanov, Hoffman, Curtious, Schmidt, Wolf bentenzidine and dinone-phenol rearrangement.

2. **Pericyclic reactions**

   2.1 Introduction, classification and characteristics

   2.2 Conservation of Molecular orbital symmetry.

   2.3 Use of correlation diagrams: FMO and PMO approaches to study of:

   2.3.1 Electrocyclic reactions of linear conjugated diene, triene and allyl systems.

   2.3.2 Cycloaddition reactions involving [2+2] and [4+2] systems.

   2.3.3 Sigmatropic rearrangements ([1,3], [1,5] and [3,3]).

   2.3.4 Group transfer reactions.

3. **Addition Reactions:**

   3.1 Carbon-Carbon double bond addition:

   Mechanism and stereochemistry of addition of halogen acids to alkane, 1,2-Bishydroxylation, epoxidation, hydroboration and oxymercuration-demercuration, sharpless asym-epoxidation.

   3.2 Carbon-heterobond addition:

   Mechanism of addition to C=O bonds, Cram's rule, condensation reaction involving enolares e.g., Aldol, Cannizzaro, Stobe and Claisen.

SEMESTER III
Paper IV A
PHYSICAL CHEMISTRY
Thermodynamics and Intermolecular Forces

1. **Intermolecular Forces :**

   Dispersion, dipole, induction and Charge transfer forces. The hydrogen bond

2. **Thermodynamics of Mixtures :**

   Excess thermodynamic functions, Regular solution, solutions, solutions of macromolecules, Activity coefficients determination by **NRTL** (Non Random Two Liquids Model) and **UNQUAC** (Universal Quasi Chemical Approach) Models. **ASOG** (Analytical Solvents of groups) and **UNIFAC** (Universal Functional Activity Coefficient) Methods.

3. **Phase Equilibria :**

   Thermodynamic relations at λ–point. Thermodynamic interpretation of phase diagrams : eutectic systems, Systems exhibiting complete miscibility in solid and liquid phases. Mixtures having a congruent melting point, Critical solution mixing.

4. **Liquid State :**

   Configurational entropy and free energy. Cell theory of liquid state, Hole theory, Molecular theory of liquid viscosity, Mesomorphism.

5. **Thermodynamics of Irreversible Processes :**

   Entropy production in irreversible processes, Entropy equation for heat flow, relation between fluxes and forces. Non-equilibrium stationary states, Linear phenomenological equations, Onsager's reciprocity relation, non-linear thermodynamics treatment of electro-kinetic phenomena, thermo-osmosis and reverse osmosis.

SEMESTER III
Paper IV B
INORGANIC CHEMISTRY
Supramolecular Chemistry

1. **Definition, classification** of supramolecular host-guest compounds, nature of supramolecula rinteractions, Chelate and macrocyclic effects.
2. **General principles** of molecular recognition, complex formation and host design, templates and self assembly.
3. **Host-Guest Chemistry**
   - (a) Cation Binding hosts
     - (i) Crown ethers
     - (ii) Cryptands
     - (iii) Spherands
     - (iv) Podants
   - (b) Anion binding hosts:
     - (i) Expanded porphyrins
     - (ii) Guanidinium Based reseptors
   - (c) Netural Molecules binding hosts:
     - (i) Solid State Clatharates
     - (ii) Zeolites
4. **Selected Applications in:**

1. Supramolecular Chemistry: concepts and perspectives
2. Supramolecular Chemistry by JW Steel and JL Atwood
3. Principles and Methods in Supramolecular Chemistry by H Scheneider and A Yatsimirsky
4. Supramolecular Chemistry: an Introduction by F Vogtle.
5. Perspectives in Supramolecular Chemistry, Vol.2, Crystal Engineering and molecular recognition by Desiraju (Ed.)

SEMESTER III
Paper IV C
INORGANIC CHEMISTRY
Biomolecules

1. **Vitamins:**

   Chemistry and Physiological functions of the followings:

   c. Thiamine : Riboflavin, Pyridoxin and Pantothenic acid
   d. Vitamin D : Calciferol
   e. Vitamin E : Tocoferol
   f. Vitamin K, A and C

2. **Hormones:**

   (a). Sex Hormones (Stroidel Hormones)

   (i). General introduction to estrogens and androgens

   (ii). Estrone : Structure and synthesis, relationship to estradiol

   (iii). Progesterone: Preparation from steroid and physiological functions

   (b). Non-Stroidel Hormones:

   Structure and functions of Theroxine and Andernalin.

3. **Steroids:**

   Diel's hydrocarbon, Determination of ring system, positions of hydroxyl group, angular methyl group, double bond and nature and position of side chain in cholesterol.

4. **Carticoids:**

   Chemistry and therapeutic uses of cartistone.

M. Sc. (Final)
Physical chemistry Practical
Semester III
Marks 100: Time 12 Hours in two days (10:00 AM to 4:00 PM)
Marks distribution

Practical-2 : 60 marks (two practical of 30 marks each)

Viva: 10

Record: 10

Mid-term examination: 20

(Marks obtained by students in mid-semester examination will be submitted to the head of the department and it will be sent to the Controller of exams with the marks of the final semester practical examination)

Excercises:

1. **pH-Metry :**

   1.1 Determination of strength of strong acid and strong base.
   1.2 Determination of strength of weak acid by pH titration with a strong base.
   1.3 Varification of hendersons's equation.

2. **Conductometry**

Equivalent conductance of strong electrolytes at infinite dilution.
Conductometric trtration of strong acid with strong base
Conductometric titration of weak acid with strong base
Titration of mixtures of acids
Precipitation titration
Verification of Ostwald's dilution law
Verification of Kohlrausch's Law

3. **Potentiometry**

M. Sc. (Final)
INORGANIC chemistry Practical
Semester III
Marks 100: Time 12 Hours in two days (10:00 AM to 4:00 PM)
Marks distribution

Practical-2 : 60 marks (two practical of 30 marks each)

Viva: 10

Record: 10

Mid-term examination: 20

(Marks obtained by students in mid-semester examination will be submitted to the head of the department and it will be sent to the Controller of exams with the marks of the final semester practical examination)

1. Gravimetry estimation of three metal ions from following:

   Ag^{+}, Cu^{++}, Ni^{++}, Zn^{++}, Fe^{+++}, Al^{+++}, Ba^{++} and Mg^{++}

2. EDTA Titration:

   Estimation of Mg^{++}, Zn^{++}, and Mg^{++} and Ca^{++} in admixture.

3. Preparation and Characterization of some metal complexes.

M. Sc. (Final)
ORGANIC chemistry Practical
Semester III
Marks 100: Time 12 Hours in two days (10:00 AM to 4:00 PM)
Marks distribution

Practical-2 : 60 marks (two practical of 30 marks each)

Viva: 10

Record: 10

Mid-term examination: 20

(Marks obtained by students in mid-semester examination will be submitted to the head of the department and it will be sent to the Controller of exams with the marks of the final semester practical examination)

Practicals:

1. Multistep synthesis of organic compounds
2. Estimation of sulfur in organic compounds
3. Estimation of glycine

SEMESTER IV
Paper I
Spectroscopy II

1. **Mass Spectrometry :**

   Measurement technique (El, Cl, FD and FAB), Molecular base and molecular ions, various class of organic molecules, McLafferty re-Arrangement and retro-Diels-Alder Fragmentation, nitrogen rule and determination of molecular composition of organic compounds from mass spectra data.

2. **PMR**

   The spinning nuclei, Chemical shift and its measurement, factors affecting chemical shifts, anisotropic effect and shielding mechanism, interpretation of protons spin-spin coupling, coupling constant, simple, virtual and complex coupling, Chemical and magnetic equivalence, first and non-first order spectra, Analysis of AB, AMX and ABX systems, Simplification of complex spectra and NOE deuterium exchange, hinderd rotation and rate process, NMR studies of other neuclei e.g., 19F and 31P. application in structural determination of simple organic and inorganic molecules.

3. **CMR**

   General introduction, peak assignments, chemical shift, ^{13}C-^{1}H coupling, Off-resonance Decoupling, Deuterium, fluorine and phosphorus coupling, NOE and DEPT, 2D NMR: COSY, NOSY and NETCOR. Application to simple organic and inorganic molecules.

4. **Electron Spin Resonance Spectroscopy**

   Basic principle, factor affecting value, isotropic and anisotropic hyperfine coupling constant, Application to organic free radical, Methyl Free Radical, Naphthalene and Bennzene free radicals, CID NP.

5. **Mossobauer Spectroscopy**

Theory, Instrumentation, Applications - isomer shift, nuclear quadrupole coupling and hyperfine interaction, Problems related to Mossobauer Spectroscopy

6. **Problems:** Structural elucidation based on spectra.

SEMESTER IV
PAPER II A
PHYSICAL CHEMISTRY
Chemical Kinetics and Reaction Dynamics

Chemical Kinetics:

1.1 Homogeneous Processes

1.1.1 The study of fast reactions:

Flow systems, Relaxations and shock tube methods, Flash Photolysis

1.1.2 Oscillatory Chemical Reactions:

Autocatalysis, Autocatalytic Mechanisms of oscillatory chemical reactions: The Lotka - Volterra mechanism, The Brusselator, the Oregonator, Bistability and Chemical chaos.

1.2 Heterogeneous Processes

Mechanism of surface reactions:

(i) Unimolecular surface reactions

(ii) Biomolecular surface reactions with special reference to

(a) Reaction between two adsorbed molecules, and

(b) Reaction between a gas molecule and an adsorbed molecule

2. Statistical Treatment of Unimolecular reactions, Limitation of Lindemann theory, Hinshelwood treatment, reaction scheme for Hinshelwood treatment, shortcomings on Hinshelwood treatment, RRK theory, salient features and limitations, RRKM theory and advances made by Slater, Decomposition of diatomic molecule and linear triatomic molecules .

3. Reaction Dynamics:

Collision cross-section and inter-molecular potential. Potential energy surfaces, Elastic molecular collisions, Photo fragment spectroscopy, Crossed-molecular beam.

SEMESTER IV

PAPER II B
INORGANIC CHEMISTRY
Bioinorganic Chemistry

1. **Metalloenzymes**

   Zinc enzymes - carboxypeptidase, carbonic anhydrase; Copper enzymes - superoxide dismutase; Mobybdenum - xanthine oxidase; Coenzyme vitamin B_{12} .

2. **Bioenergetics and ATP cycle**

   Glucose storage, metal complexes in transmission of energy, chlorophylls, Photosystem I and II in cleavage of water.

3. **Transport and Storage of Dioxygen**

   Heme proteins and oxygen uptake, Structure and function of hemoglobin, myoglobin, hemocyanins and hemerythrin, model synthetic complexes of iron.

4. **Electron Transfer in Biology**

   Structure and function of metalloproteins in electron transport process - cytochromes and iron - sulphur proteins, synthetic models.

5. **Nitrogenase**

   Biological nitrogen fixation, molybdenum nitrogenase, other nitrogenase model systems.

6. **Metal Storage, Transport and Biomineralization**

   Ferritin, transferrin and siderophores

7. **Metals in Medicine**

   Metal deficiency and diseases, toxic effects of metals, metals used for diagnosis and chemotherapy with particular reference to anticancer drugs.

Books Recommended:

1. Bioinorganic Chemistry. R. N. Hay. Wiley. 1984.

2. The Inorganic Chemistry of Biological Processes. M. M. Hughes. Wiley 1981.

3. An Introduction to bioinorganic Chemistry. El Ichiro ochai. Allyn. 1977.

4. Inorganic Chemistry : Principles of structure and reactivity. J.E. Huheey Harper. 1983.

5. Advanced inorganic Chemistry. F.A. Cotton and G. Wilkinson. Wiley. 1999.

SEMESTER IV

PAPER II C
ORGANIC CHEMISTRY
Organic Synthesis

1. **Protection and Deprotection of groups**:
   Principles of protection and deprotection of alcohols, thiols, 1,2- and 1,3-diols, amines, carbonyls and carboxyl groups in organic synthesis.
2. **Selective name reactions and their application in organic synthesis**
   Reformatsky, Robinson annulations, Michael addition, Shapiro, Mannch, ene, Barton, Hoffman - Loffter - Frytag reaction, Birch reduction and woodward - Prevost hydroxylation.
3. **Oxidation:**
   Scopes of the following reagents with following application and mechanisms
   DDQ, SeO_2, Jones reagent and thallium nitrate TI $(NO_3)_3$
4. Mechanism and stereochemistry of reduction with following reagents:
   $NaBH_4$, LAH, DIBAL, diborane, di-isoamyl borane and 9BBN, mechanism of metal hydride reduction of saturated / unsaturated compounds.
5. **Retero-Synthesis:**
   Introduction to synthones and synthetic equivalents, disconnection approach, functional group interconversions. One group C-X and two groups C-X disconnection, Chemiselectivity.

SEMESTER IV
PAPER III A
PHYSICAL CHEMISTRY
Statistical Mechanics

1. **Basis of Classical Statistical Mechanics :**
   Phase space, Ensembles, Ensemble–average, Liouvilles theorem, Quantum Picture, Basic postulates, classical limit, Quantisation of phase space.
2. **Distribution laws :**
   Energy levels, Boltzmann distribution law, Fermi – Dirac statistics Bose – Einstein Statistics.
3. **Distributions & Thermodynamics:**
   The partition function, relation of the partition function to the thermodynamic function.
4. **Determination of Partition functions:**
   Localised and non–localised systems, Separation of the partition function. Translational partition function, The Sackur Tetrode – equation, Rotational partition function, vibrational partition functions, Electronic partition function. Derivation of thermodynamic properties of ideal gases from partition functions.
5. **Applications :**
   Equilibrium Constants from partition function for: Isomerisation equilibrium, Ionisation– equilibrium ($H \leftrightarrow H^+ + e$), and Dissociation equilibrium ($Na_2 \leftrightarrow 2Na$)

SEMESTER IV
PAPER III B
INORGANIC CHEMISTRY
Organotransition Metal Chemistry

1. **Alkyls and Aryls of Transition Metals**

   Types, General Synthetic Routes, Stability and Decomposition pathways.

2. **Compounds of Transition Metal - Carbon Multiple Bond: Carbenes and Carbynes**

   Low valent carbenes and carbines ,synthesis, nature of bond and Structural Characteristics.

3. **Transition Metal π- Complexes**

   (a) Preparations, Important reactions relating on the ligands, Structural features and bonding of alkenes, allynes, alkyls, diene, dienyl, arene complexes, MO approach of bonding in ferrocene and bis (benzene) chromium.

   (b) Ligand behaviour of $C_3Ph_3^+$, $C_7H_7^+$ and $C_8H_8^{2-}$ in different organometallic compounds.

4. (a) Nature of M-C and C-O bonds. Preparation, properties and structures of platinum metal carbonyls, substitution reactions using σ-donor, σ-donor and **π** -acceptor and **π** -donor ligands.

   (B) **Metal Clustures:** condition of formation of metal-metal bond. Carbonyl type clusture. Electron count in metal clustures.

5. **Catalysis involving organometallic compounds**

   Olefin hydrogenation. Oxo reaction. Fischer Tropsch process. Wacker process. Polymerisation of olefins.

6. **Fluxional Organometallic Compounds**

   Fluxionality and dynamic equilibria in compounds such as η^3 - allyl and η^3 dienyl complex.

Books Recommended:

1. Comprehensive Organometallic Chemistry, Ed. E.W. Abel, Abel, F.G.A. Stone and G. Wilkinson, Pergamon, 1982.

2. Advnaced Inorganic Chemistry, F.A. Cotton and G. Wilkinson, `Wiley, 1999.

3. The chemistry of elements, N.N. Greenwood and A. Earnshaw, 1997.

4. Inorganic Chemistry, principles of structure and reactivity. J.E. Huheey, Harper, 1983.

5. Organometallic Chemistry (A unified approach), R.C. Mehrotra and A. Singh, Wiley Eastern, 1991

SEMESTER IV
PAPER III C
ORGANIC CHEMISTRY
Select Topics in Organic Chemistry

1. **Hetercycles**
   a. General introduction and nomenclature
   b. Chemistry of
      (i) Five membered: Pyrazole and imidazole, oxadiazole and thiadiazole and thiazole
      (ii) Six membered: Pyrazine, pyrimidine and pyridiazine
2. **Reagents**
   Preparation and application in organic synthesis of following:
      (i) DCC, DDQ, CH_2N_2, LDA, R_2CuLi, Trimethylsilyl iodide and 1:3 dithane
      (ii) Wilkinson's catalyst, Banker yeast and Phase-transfer catalyst.
      (iii) Sulphur, nitrogen (ethamine) and phosphorous ylides
3. **Nucleic acids:** General structure of RNA and DNA
4. **Carbohydrates:** Structure, function and configuration of
      (i) Disaccharides: Lactose, maltose, sucrose
      (ii) Polysaccharides: Cellulose, Starch and Glycogens.

SEMESTER IV
PAPER IV A
Science of Materials

1. **Introduction**
   Materials Science and Engineering, Classification of Materials, Advanced Materials, Materials of the future.
2. **The structure of crystalline solids**
   Fundamental concepts, Unit cells, Crystal Systems, Metallic crystal structures, packing of solids, space groups, X-ray diffraction and crystal structures.
3. **Imperfection in Crystals**
   Point defects and colour centres, Edge and screw dislocations, dislocation and crystal growth, Grain boundary.
4. **Phase diagrams and Phase transformations**
   Gibbs phase rule and phase diagrams showing the formation of eutectics, Congruent melting, incongruent melting and peritectic type Compounds. Phase diagrams of Iron-Carbon systems and their microstructures. Phase transformations, type and kinetics of phase transformations and their study.
5. **Solid State Reactions**
   Introduction, Classification, Methods for study of kinetics of solid state reactions, solid state reactions with special reference to spinel formation. Intercalation Chemistry, Organic solid state reactions: Thermal and photo reactions, Solvent fee reactions.
6. **Mechanical properties of metals and alloys**
   Stress and strain, Elastic properties, Elastic deformation, Fracture, Fatigue, creep, Ferrous and non ferrous alloys and their mechanical properties.
7. **Magnetic properties of materials**
   Introduction, Diamagnetism, Paramagnetism, Ferromagnetism, Antiferromagnetism and Ferrimagnetism. Soft and Hard magnetic materials.
8. **Optical properties of materials**
   Introduction, Optical properties of metals and non-metals, Luminescence, Photoconductivity, Lasers, non linear optical materials and optical fibers in communications.
9. **Electrical properties of materials**
   Electrical conduction, Conduction in term of free electron and band theory. Semiconductors -Intrinsic and Extrinsic semiconductors and semiconductor devices.
10. **Super Conductors**
    Introduction, High Tc super conductivity in Cuparates, preparation and characterization of 1-2-3 and 2-1-4 materials, Theory of superconductivity. Application of high Tc materials.
11. **Nano Materials**

Introduction, preparation of nano materials, size property relationship, Carbon nanotubes,

Discussion of some nano particles such as barium titrate, gold application of nano materials.

SEMESTER IV
PAPER IV B
Solid State Chemistry

1. **Crystal Structures**
   Rock Salt, Zinc Blende, Wurtzite, Diamond, Graphite, Fluorite, Sesquoxide, Spinel (Normal/inverse), ReO3, Perovskite, Amorphous state, Cuasi-crystals, Icosahedron, Silicates, Zeolites.
2. **Imperfections in crystals**
   Point defects : Schottky and Frenkel defects. Colour centres Line defects : Edge and screw dislocations. Burger's Vector. dislocation densities. dislocation multiplicity and slip dislocation and crystal growth.
   Surface imperfection : Grain boundaries
3.. **Free electron theory of metals**
   Deficiencies of the classical theory. the free electron approximation. the Fermi- Dirac distribution.
4. **Band theory of solids**
5. **Semiconductors :** Intrinsic and impurity semiconductors. Carrier concentrations. Effect of temperature on electrical conductivity and mobility of electrons in semiconductors. Hall effect. Seebeck coefficient. p-n junctions. Organic semiconductors.
6. **Superconductivity :** Zero resistance and the transition tempeature. Superconductivity and periodic table. Magnetic properties. Theory of superconductivity (BCS theory). Type I and Type II superconductors. Hard superconductors. Surface energy. Superconducting magnets. Preparation of superconducting materials. Recent developments in superconductivity and their applications.
7. **Phase Transformations in Solids :** Classification and thermodynamic of phase transformations in solids. Kinetics of thermal phase transformations. Experimental methods of the study of phase transformations. Phase transformations in metals, Martensitic to Austenite, Order disorder, liquid crystals, Nucleation and Growth Mechanism. Alloys. some compounds such as titanium dioxide. aluminium oxide. dicalcium and tricalcium silicate.
8. **Nucleation and Crystal growth :** Homogeneous and heterogeneous nucleation. Equilibrium conditions for a curved interface. Critical nuclei. Theory of nucleation rate. crystallisation of lamellar eutectics. Dendritic growth and peritectic solidification.
   Preparation of single crystals from vapour. melt and solution.
9. **Solid State Reactions :** Classification. Nature of solid state reactions. Reaction involving single solid phase. solid-gas reaction. solid-solid reaction. solid-liquid reaction. intercalation chemistry. Reaction of organic solids. factors affecting solid state reactivity. experimental methods for the study of solid state reaction.

Books Recommended:

1. Solid state chemistry and applications by A.R. West.
2. Phase Transition in Solids by K.J. Rao and C.N. R. Rao.
3. Solid state chemistry by N.B. Hanni.
4. Solid state chemistry by D.K. Chakrawati

SEMESTER IV
PAPER IV C
Polymer Chemistry

1. **The Science of Large Molecules**

   Basic concepts, Types, Classification of polymers and General definitions.

2. **Polymerization**

   Kinetics and mechanism of Condensation, Addition (Radical chain and Ionic chain), Coordination and Copolymerization,

3. **Polymer Characterization**

   Concept of average molecular weights in polymers: Number, Weight , Viscosity average and sedimentation average molecular weights, Concepts of Monodispersity, Polydispersity and Molecular Weight Distribution Curves,

4. **Degradation of Polymers**

   Types of degradation – Random degradation and Chain depolymerization, A general idea of thermal, mechanical and oxidative degradations, Antioxidants and stabilizers.

5. **Rheology of Polymers:**

   Viscous flow (Newtonian and Non-Newtonian fluids), Rubber elasticity (thermodynamic and entropy elasticity), Visco-elasticity, The glassy state and glass transition temperature.

6. **Polymer Processing:**

   Plastic Technology: A general idea of Moulding and Extrusion techniques, Thermoforming and Thermofoaming,

   Fiber Technology: A brief idea of textile and fabric terms and properties, Fiber Spinning techniques (melt, wet and dry spinnings).

SEMESTER IV
PAPER IV D

Nuclear and Radiation Chemistry

1. **The Atomic Nucleus**
   The atom, Units used in nuclear chemistry. The nucleus and the outer sphere, Classification of nuclides, nuclear stability, atomic energy.
2. **Nuclear Models**
   Historical, The shell model, The liquid drop model, The Fermi gas model, The collective model, The optical model.
3. **Radioactivity**
   Discovery, Radioactive elements, General characteristics of radioactive decay, Decay kinetics, Parent-daughter decay-growth relationships, Alpha decay, Beta decay, Nuclear deexcitation, gamma emission, artificial radioactivity.
4. **Nuclear Reactions**
   Bethe's notation, types of nuclear reactions, conservation in nuclear reactions, reaction cross-section, the compound nucleus theory, experimental evidence of Bohr's theory, Experiments of Ghoshal, Alexander and Simonoff, Specific nuclear reactions, Photonuclear reactions, Direct nuclear reactions, Thermonuclear reactions, The origin and evolution of elements.
5. **Nuclear fission**
   The process of nuclear fission, Fission fragments and their mass distribution, Charge distribution, Ionic charge of fission fragments, Fission energy, Fission cross-sections and thresholds, Fission neutrons, Theory of nuclear fission, Other types of fission, Neutron evaporation and spallation.
6. **Nuclear Reactors**
   The fission energy, The natural uranium reactor, The four factor formula: The reproduction factor k, The classification of reactors, Reactor power, Critical size of a thermal reactor, Excess reactivity and control, The breeder reactor, Nuclear reactors in India, Reprocessing of spent fuels: Recovery of uranium and plutonium, Nature's nuclear reactor.
7. **Applications of Radioactivity**
   Probing by isotopes, typical reactions involved in the preparation of radioisotopes, the Szilard-Chalmers' reaction, Use of charged plates in the collection of radioisotopes, Radiochemical principles in the use of tracers, Typical applications of radioisotopes as tracers, Uses of nuclear radiations, Radioisotopes as a source of electricity.

Books Recommended:

Essentials of Nuclear Chemistry 2nd Edition by Hari Jeevan Arnikar

SEMESTER IV
PAPER IV E
Drugs and Agrochemicals

1. **Drug Design**: Development of new drugs, Structure activity relationship (SAR), Factors affecting bioactivity, 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-chemical parameters: Lipophilicity, partition-coefficient, electronic ionization constants, steric, Shelton and surface activity parameters and redox potentials.
2. **Antibiotics**: Synthesis of penicillin-G, penicillin-V, ampicillin, chloramphenicol, streptomycine and cephalosporin-C.
3. **Synthetic Drugs:** A general study of important synthetic drugs of the following types:
   (i) Sulpha drugs: Sulphanilamide derivatives, sulphathiazole, sulphathalidine, sulphasuccidine, sulphaguanidine, sulphadiazine.
   (ii) Antimalarials: 4-Aminoquinoline derivatives, chloroquine, santoquine, camaquin, 8-aminoquinoline.
   (iii) Anti-cancer agents: Nitrogen mustards, antimetabolites in cancer chemotherapy.
   (iv) Psychopharmacological agents: Reserpine, promazine, chloropromazine, mepazine.
   (v) Antitubercular agents: PAS, Thiosemicarbazones, hydrazides and thiocarbanilides.
4. **Insecticides:**
   (i) A brief reference to natural insecticides, tobacco alkaloid, pyrothrins and rotonoids (detailed chemistry not required).
   (ii) Organophosphorus insecticides, OMPA, Parathion, Paroxon, diazinon, malathion, and related compounds.
   (iii) Halogenated insecticides, halogenated alkanes, gammexane, Aldrin, Dieldrin, DDT and important analogs (DFDT, DMDT, DDD).
5. **New breed of pesticides:**
   (i) JH analogues and anti JH compounds in pest control (detailed structure not required).
   (ii) Use of sex pheromones in pest control
6. **Fungicides:**
   Halogenated phenols and quinones, dithiocarbamates, Zineb, Maneb, Ferbam and organomercurials.
7. **Herbicides:** 2,4-D and related compounds, substituted urea carbamates.

SEMESTER IV
PAPER IV F
Biophysical Chemistry

1. **Biological Membranes** :
   Mechanism of facilitated diffusion of glucose, chloride ion and biocarbonate ion through erythrocytes, Mechanism of active transport of Na^+, K^+, Ca^{++} and proton through membrane, co-transport : Symport and antiport, Brief description of Na^+ channel protein and transport antibiotics. Brief description of molecular assembly and LB films.
2. **Nucleic Acids :**
   Conformation of DNA and RNA (A, B and Z forms) Genetic code and gene – protein relationship, DNA cloaning and principle of protein engineering. DNA damage and repair mechanism.
3. **Proteins :**
   Conformation of polypeptide chain, periodic structures in proteins – α–helix, β- pleated sheet, collagen helix and β- turn, principle of protein folding and forces involved in protein folding.
   Structures and functions of myoglobin, hemoglobin, lysozyme and carboxypeptidase A.
4. **Bioenergetics :**
   The mechanism of oxidative phosphorylation – chemical coupling hypothesis, the conformational coupling hypothesis and chemi - osmotic coupling hypothesis.
5. **Biological Regulations :**
   Prostagladins, cyclic AMP and its role in hormone action, Interferons.
6. **Enzyme Kinetics and Therory of Enzyme Catalysis:**
   Presteady state kinetics, steady state kinetics, kinetics of enzyme inhibitors and determination K_I, kinetics of multisubstrate enzymes- compulsory order, random order and double displacement type mechanism, non-linear enzyme kinetics.

Books Recommended:

1. Biophysics by M.V. Vallenstein, MIR publication, Moscow.
2. Biochemistry by L. Stryer, Freeman and Co, San Fransisco, (Indian Print CBS Publications and Distributors Delhi).
3. Biophysical Chemistry Part I, II, III by C.R. Cantor and P.R. Schimmel, Freeman and Co, San Francisco.
4. Principles of biochemistry by Lehninger, Neloson, and COX, Worth Publishers Inc, USA (Indian print, CBS Publishers and Distributers, Delhi)
5. Enzyme Kinetics by P.C.Engel, Chapman And Hall London

6. Enzyme Structure and Mechanism by A. Ferst, Freeman and Company, San Francisco, USA

SEMESTER IV
PAPER IV G
Computational Chemistry

1. Introduction to Internet and Computer
2. Historical perspectives of computational chemistry
3. Computable quantities
    a. Structure
    b. Potential energy surface
    c. Chemical properties
4. Construction of z-matrix
    a. Diatomic molecules
    b. Polyatomic molecules
    c. Ring systems
5. Force Field/Molecular Mechanics
    a. Potential Energy Functional Forms
        (i) Common force fields viz., Harmonic, LJ (6-12), L.J (10-12) and Morse
        (ii) Existing force fields in popular packages viz., AMBER, CHARMM, DREIDING and MM.n
6. Ab- initio HF calculations:
    a. Geometry optimization and calculation of HF energy
    b. Basis sets
    c. Density function theory
        (i) Basic theory
        (ii) Advantage over ab-initio approach
        (iii) Implementation into popular quantum mechanical package
        (iv) Applicationszs
7. Introduction to QSPR and QSAR
8. Application to Real systems
    a. Biomolecule
        (i) Methods for modeling Biomolecules
        (ii) Site-specific interaction
        (iii) Introduction to computer aided - Drug – design (CADD)
    b. Synthesis Route prediction
    c. Polymers
    d. Transition metals
9. Software Packages; Introduction to available software packages. Suitability of packages for specific calculations. The following packages may be introduced.
    a. semi-empirical software such as AMPAC, MOPAC, MacroModel.
    b. Molecular mechanics/Molecular Dynamics. MOE & PC MODEL
    c. Ab--Initio and DFT Software - Gaussian, GAMESS. MOLPRO
    d. Graphics Packages - GaussView and Molden

Books Recommended:

1. Introduction to Computational Chemistry by Frank. Jensen
2. Computational Chemistry by C. J. Cramer

M.SC. (Final)
Physical Chemistry Practical
Semester IV
Marks 100: Time 12 Hours in two days
Marks Distribution

Practical-2 : 60 marks (two practical of 30 marks each)

Viva-10

Record: 10

Project: 20

Practicals:

1. **Chemical Kinetics:**

   1.1 Determination of rate constant of acid Hydrolysis of ester
   1.2 Relative Strength of strong acids by studying the kinetics of hydrolysis of ester
   1.3 Kinetics of reactions between Potassium Persulphate and Potassium iodide.
   1.4 Kinetics of iodination of acetone

2. **Optical Methods:**

   2.1 Colorimetry : Verification of Lambert's Beer Law
   2.2 Refractometry
   2.3 Spectroscopic methods of analysis: UV-Visible, IR
   2.4 Polarimetry

3. **Computational Experiments:**

   3.1 Geometry optimization and energy calculation

4. **Project work**

M.SC. (Final)
Inorganic Chemistry Practical
Semester IV
Marks 100: Time 12 Hours in two days
Marks Distribution

Practical-2 : 60 marks (two practical of 30 marks each)

Viva-10

Record: 10

Project: 20

Practicals:

A. Any two of the following exercises:

1. **Potentiometry:**

   a. Acid-Base, Redox Titrations.

   b. Determination of stability constants of suitable complex systems.

2. **Conductometry**
   Acid-Base and precipitation Titrations
3. **Colorimetry and Spectrophotometry:**
   Estimation of the following metals in solution V, Cr, Mo, Fe and Ni.
4. **Flame Photometry:**
   a. Estimation of sodium and potassium in admixture.
   b. Estimation of magnesium and calcium in tap water.
   c. Estimation of calcium in calcium salt solution.

B. Project Work

M.SC. (Final)
Organic Chemistry Practical
Semester IV
Marks 100: Time 12 Hours in two days
Marks Distribution

Practical-2 : 60 marks (two practical of 30 marks each)

Viva-10

Record: 10

Project: 20

Practicals:

1. Analysis of ternary organic mixture
2. Estimation of glucose
3. Project work