M. Sc. (Previous)
Paper–I, Physical Chemistry–I
(Quantum Mechanics, States of Matter and Diffraction Techniques)

1. Quantum Mechanics :

(a) General Theory

Operators and computational relations, Postulates of quantum mechanics and Schrödinger wave Equation, Free particle, Particle in one dimensional, two dimensional, and three dimensional boxes, degeneracy, brief description of quantum mechanical tunneling, Harmonic Oscillator, rigid rotor and the hydrogen atom. Angular momentum including spin coupling of angular–momentum including spin–orbit coupling.

(b) Approximate methods for treating multi–electron atoms

Perturbation method and variation theorem, calculation of first order correction to wave function and energy by perturbation method, application to He atom, Antisymmetry and exclusion principle, Slater determinantal wave function and Self consistent field orbitals.

(c) Quantum mechanics of chemical bonding

Born-Oppenheimer approximation, V.B. and M.O. treatment of H_2^+, H_2, Huckel Molecular Orbital Calculations of ethylene, calculation of charge density, partial bond order and free valence in allyl system from the given molecular orbitals.

(d) Molecular symmetry and group theory

Symmetry elements and symmetry operations, Definition of a group, Products of symmetry operations and group multiplication table, Similarity transform and classes of a group, Point groups of molecules and their identifications.

Matrix representations of symmetry operations, Representations of point groups, Reducible and irreducible representations, Character table, Direct product representation and its applications, Symmetry adopted linear combinations of orbitals taking water as an example.

2. States of Matter :

(a) Gaseous State

Maxwell–Boltzmann distribution of molecular velocities, its derivation and experimental verification, Derivation of expressions for average, root–mean–square and most–probable velocities.

Transport Properties of a perfect gas : Diffusion, Thermal conduction and viscosity.

(b) Liquid State

Structure of liquids, The radial distribution functions, Monte–Carlo method, Molecular dynamics.

(c) Solid State

Crystal defects and Non–stoichiometry, Point defects, Line and plane defects; Schottky and Frenkel defects, Thermodynamics of Schottky and Frenkel defects formation. Non– Stoichiometric compounds, Band theory of solids, Semiconductor – intrinsic and extrinsic semiconductor, Superconductors, Nanomaterials. Solid–state reactions.

3. Diffraction techniques in molecular structure determinations

(a) X-rays diffraction

General features of diffraction, Powder X-ray diffraction, Single crystal X-rays diffraction - the technique, structure factor, phase problem and structure refinement, brief description of time-resolved X-rays diffraction techniques.

(b) Neutron diffraction

Brief introduction and difference with X-rays diffraction

(c) Electron diffraction

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

Books

1. Physical Chemistry by I. N. Levine Mc Graw-Hill Book company, New Delhi.
2. Physical Chemistry by Atkins, 7^{th} edition Oxford University Press (Indian Print available).
3. Quantum chemistry by I.N. Levine, Mc Graw-Hill Book Company, New Delhi.
4. Introductory Quantum Chemistry by A.K. Chandra, Tata Mc Graw-Hill Publishing Company Ltd., New Delhi

M. Sc. (Previous)

PAPER-II - INORGANIC CHEMISTRY-1
(Main Group Elements)

1. **Stereochemistry and Bonding in Main Group Compounds**
   VSEPR, Walsh diagram, $d\pi - p\pi$ bonds, Bent's rule, Energetics of hybridization, Some simple reactions of covalently bonded molecules.

2. **Bond enthalpy concept and interpretation of the following on the basis of bond enthalpy data :**

   Thermodynamic stability : XeF_n , XeO_n , P_4 over P_2; N_2 over N_4; S_8 over S_2; single bonded structure containing extended arrays of B-O-B of B_2O_3 molecule; N_4O_6 over N_2O_3.

3. **Inorganic solids**

   Lattice energy and its interpretive uses, Explanations for non-existence of $TlCl_2$ and NH_5, Stabilization of high oxidation states of metals by fluorine and oxygen, stabilization of low oxidation states of metals by large anions, non- stoichiometric and interstitial compounds, solid electrolytes.

4. **a.** Preparation, structure, bonding and technical applications of Polyether complexes of alkali and alkaline earth metals, polyphosphazenes, thiazyl and its polymers, tetrasulphur dinitride.
   b. Structure and bonding of : borane anions, metalloboranes and metallocarboranes.
   c. Structures of silicones and silicates.
   d. Polyions of Ge, Sn, Pb, Sb, Bi and Hg

5. Preparation properties, structure and applications of alkyls and aryls of lithium, beryllium, magnesium, aluminium, mercury and tin.

Books

1. Concepts and Models in Inorganic Chemistry, B.D. Douglas, D.H. McDaniel and J.J. Alexander, John Wiley, 1983.
2. Inorganic Chemistry : A Unified Approach, W.W. Porterfield, Addison Wesley, 1984.
3. Some Thermodynamic Aspects of Inorganic Chemistry, D.A. Johnson, 2nd. Ed. Cambridge, 1982.
4. Inorganic Chemistry : K.F. Purcell and J.C. Kotz, Holt Saunders, 1977.5.Inorganic Chemistry concepts : Electrochemistry of Solids, Hans Rickert, springer Vetlag, 1982.

M.Sc. (Previous)
Paper - III: Organic Chemistry - I
(Reactions, Stereochemistry and Aromaticity)

1. Basic principles of organic reaction mechanism

(a) Thermodynamic and kinetic control, Hammond's postulate
(b) Potential energy diagrams, transition states and intermediates
(c) Methods of determination of organic reaction mechanism

2. Nature of bonding in organic molecules

Delocalized chemical bonding, conjugation, cross-conjugation, bonds weaker than covalent: addition compounds, crown ether complexes and cryptands, inclusion compounds, cyclodextrins, catenanes and rotaxanes.

3. Substitution Reactions

(a) Aliphatic nucleophilic substitution (SN^1, SN^2, SN^i, mixed SN^1 and SN^2, and SET mechanisms). Role of substrate structure, attacking reagents, leaving groups and solvents on SN^1 and SN^2 mechanisms. Neighbouring group participation by □ and □ bonds, anchimeric assistance. Stereochemistry of SN^1 and SN^2 reactions.

(b) Aromatic electrophilic substitution (nitration, halogenation, sulfonation, Friedel-Craft's alkylation and Friedel-Craft's acylation). Reactivity and orientation in electrophilic aromatic substitution. Hammett equation (sigma and rho). The effects of multiple substitutions. Nucleophilic aromatic substitution (The addition- elimination and Elimination - addition mechanisms).

4. Addition Reactions

(a) Addition of halogens and halogen acids to alkenes. 1,2-Bishydroxylation, epoxidation and hydroboration-oxidation reactions to alkenes. Mechanism and stereochemistry of electrophilic addition reactions. Sharpless asymmetric epoxidation. Nucleophilic addition to alkenes.
(b) Addition to carbon-oxygen double (C=O) bonds, Cram's rule, Mechanisms of Aldol, Perkin, Knoevenagel, Claisen and Cannizzaro reactions.

5. Elimination Reactions

Mechanism and orientation of E1, E2, $E1_{CB}$ reactions. Factors affecting E1, E2, $E1_{CB}$ reactions. E1-E2-$E1_{CB}$ spectrum. Factors affecting substitution versus elimination. Hofmann and Saytzeff like eliminations. Stereochemistry of elimination reactions. Pyrolytic eliminations.

6. Stereochemistry

Elements of symmetry, chirality, molecules with more than one chiral center, threo and erythro isomers, Interconversion of Fischer, Newmann and Saw-Horse projections, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces. Asymmetric synthesis. Advance treatment of C=C geometrical isomerism (cis-trans and E - Z).

7. Aromaticity

Concept of aromaticity and Huckel's rule, antiaromaticity, non-aromaticity and homoaromaticity. Alternant and non-alternant hydrocarbons. Aromaticity in non-benzenoid compounds (troplone, Azulene, syndone, Ferrocene, Fullerenes and annulenes). Polycyclic aromatic compounds.

M. Sc. (Previous)

Paper–IV, Physical Chemistry–II

(Thermodynamics, Chemical Kinetics and Electrochemistry)

1. Thermodynamics

(a) Equilibrium Thermodynamics :

Joule–Thomson's effect, thermodynamic reversibility, entropy changes in reversible and irreversible processes, Maxwell's relations, thermodynamic equations of state, variation of entropy with temperature and pressure, Gibbs–Helmholtz equation.

Criterion of equilibrium, temperature and pressure dependence of equilibrium constant, Vant Hoff equation, Clausius–Clapeyron equation.

Partial molar quantities and their determination, chemical potential and its variation with temperature and pressure, Gibbs–Duhem equation, activity and fugacity, activity coefficients and their determination, thermodynamic treatment of solutions, elevation of boiling point, depression in freezing point, Nernst heat theorem, third law of thermodynamics, calorimetric and statistical methods of determination of absolute entropy, residual entropy, free energy and entropy of mixing, excess–functions.

(b) Non-Equilibrium Thermodynamics :

Postulates and methodology, Linear laws, Onsager reciprocal theory.

2. Chemical Kinetics

Reactions in solutions : Factors affecting the rate of reactions, (i) internal pressure of the solvent (ii) solvation of reactants and activated complexes, (iii) pressure.

The study of fast reactions : Flow systems, relaxation methods and shock tubes. Flash photolysis, autocatalysis and oscillatory chemical reactions, the Lotka–Volterra mechanism, the Brusselator, the Oregonator, Bistability, Chemical chaos, Dynamics of Molecular Collisions–Reactive collisions and Potential energy surfaces.

3. Electrochemistry

Brief description of ionic association, Wein effect and Debye–Falkenhagen effect. Effect of ionic strength on the rate of ionic reactions, Primary and secondary salt effects.

4. Electrical phenomena at interfaces

The electrical double layer, electro kinetic phenomena. Electrode Processes : concentration polarization, deposition and decomposition potentials, overvoltage, limiting current density and dropping mercury electrode. The Butler-Volmer equation and brief description of cyclic voltammetry.

Books

1. Chemical Thermodynamics by R.P. Rastogi and R.R. Mishra
2. Physical Chemistry by Atkins

M. Sc. (Previous)
Paper-V : Inorganic Chemistry-II
(Transition Elements)

1. Structures of 2 to 8 Coordinate metal complexes

Cation-anion ratio in various polyhedra, 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 (Ma_3bcd, Ma_2bcde, Mabcdef and complexes containing bi-and terdentate 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. **(a).** Kinetics and mechanism of substitution reactions in octahedral Co (III) and square planar Pt (II) Complexes.

(b). 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.

4. 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 spectrophotometric methods.

5. Metal-ligand Bonding

Limitations of CFT, Nephelauxetic series, Molecular orbital, energy level diagram of octahedral, tetrahedral and square planner complexes.

6. Metal Clusters : Conditions of formation of metal-metal bond. Halide and carbonyl type metal clusters (Di - to hexa - nuclear clusters). Electron count in metal clusters.

M.Sc. (Previous)
Paper – VI : Organic Chemistry – II
(Natural Products, Heterocycles and Alicyclics)

1. Alkaloids

General methods for determination of structure

Chemistry of nicotine, Coniine and Atropine

2. Heterocycles

General Introduction

Nomenclature of heterocyclic compounds containing two and three hetero atoms.

3. Chemistry of :

Five membered : Pyrazoles, Imidazoles and Oxazoles.

Six Membered : Pyrimidines, Pyridazines and Pyrazines

4. Terpenoids

(a) Introduction and classification

(b) General methods of structure determination

(c) Acyclic monoterpenoids: Citral and Geraniol

(d) Monocyclic monoterpenoid: alpha-Terpineol, Menthol and Limonene

(e) Bicyclic monoterpeniod: α-Pinene and Camphor

5. Vitamins and Hormones

Isolation, Structure and physiological function of Vitamin A & C.

Structure and function of Thyroxin and Adrenaline.

6. Ureides and Purines

Chemistry and structure of Pyrimidine and Purine bases present in nucleic acids.

Structure of Uric acid, Synthesis of Theobromine , Caffeine and Theophylline.

7. Dyes

General introduction and classification, chemistry of Alizarin and Indigo.

8. Alicyclic compounds.

General methods for preparation of medium and large ring alicyclic compounds. Stability of ring systems. Baeyer strain theory, theory of strainless rings.

Conformation of simple cycloalkanes. Basic principles of conformational analysis of mono- and disubstituted cyclohexanes. Configuration of *cis* and *trans* decalins and decalols.

M.Sc.(Previous)

Practical

Total duration of the examination will be 14 hours spread over two days. Experiments will be given as follows:

Section A (Inorganic Chemistry) - One experiment is to be given from each exercise.

Section B (Organic Chemistry) - Two different experiments of different categories, and

Section C (Physical Chemistry) - One experiment is to be given

Section A (Inorganic Chemistry)

Exercise No. 1

Qualitative analysis of an inorganic mixture of seven radicals including Tl, W, Mo, 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.

Exercise No. 2

Either both gravimetric or one gravimetric and one volumetric estimations of the following metal ions from a mixture of the solution.

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

Exercise No. 3

Volumetric determination of any one of the following:

i. Chloride and iodide in admixture.

ii. Bromide and iodide in admixture.

iii. Nitrite by Ce (IV) or MnO_4^- oxidation.

iv. Arsenic (III) by BrO_3^- oxidation.

v. Ammonia in an ammonium salt by OBr^- oxidation.

OR

Exercise 4

Chromatographic separation of metal ions given in any one of the following combination:

i. Pb^{2+}, Ag^{+}, Hg_2^{2+}

ii. Co^{2+}, Ni^{2+}, Cu^{2+}

iii. Fe^{3+}, Cr^{3+}, Al^{3+}

iv. Ba^{2+}, Sr^{2+}, Ca^{2+}

Section B (Organic Chemistry)

1. Separation of binary organic mixtures (liquid-liquid, liquid-solid and solid-solid) and characterization of the component.

2. Simple preparation involving two stages. Emphasis should be laid on the following processes : Purification of the organic compounds, distillation under reduced pressure, steam distillation and fractional crystallization.
3. Determination of equivalent weight of an acid by direct titration method.
4. Determination of saponification and iodine number of an oil.

Section C (Physical Chemistry)

1. Relative strength of acids by acid hydrolysis of ester.
2. Kinetics of alkali hydrolysis of ester.
3. Partition coefficient of I_2 in two immiscible solvents.
4. Solubility curve of water-acetic acid-chloroform system.
5. Adsorption isotherm of acetic acid on activated charcoal.
6. Adsorption isotherm of oxalic acid on activated charcoal.
7. Determination of heat of solution of a salt by solubility method.
8. Conductometric titration.
9. Preparation of Buffer solution and measurement of pH by pH meter.
10. Setting time of cement in presence of salts with the help of Vicat apparatus.

Distribution of marks

Section A (Inorganic Chemistry)		
	Exercise 1	21
	Exercise 2	14+10
	Exercise 3 or 4	5
Section B (Organic Chemistry)		30
Section C (Physical Chemistry)		30
Viva		30
Record		10
	Total	150

M. Sc. Final

Paper - I: Structure of molecules

1. **Nuclear Magnetic Resonance Spectroscopy :** Molecular spectroscopy, Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurements, factors influencing chemical shift, deshielding, spin-spin interactions, factors influencing coupling constant 'J', classification of splitting pattern, spin - de coupling, chemical exchange, effect of deuteration, complex spin - spin interaction between two, three, four and five interacting nuclei (first order spectra) virtual coupling stereo chemistry, hindered rotation, Karplus curve, nuclear magnetic double resonance, shift reagent, Nuclear Overhauser Effect (NOE),

   Basic ideas about instrument, NMR studies of nuclei other than proton-^{19}F and ^{31}P, FT NMR, advantages of FT NMR.

2. **Carbon - ^{13}NMR Spectroscopy :**
   General Introduction, peak assignments, chemical classes and chemical shifts, ^{13}C-^{1}H spin coupling (J Values), DEPT, correlation spectrometry.

3. **Electron Spin Resonance Spectroscopy :** Basic principles, zero field splitting and Kramer's degeneracy, factors affecting 'g' value, Isotropic and anisotropic hyperfine coupling constants, spin polarization for atoms and transition metal ions, application to transition metal complex (having one unpaired electrons) and to inorganic free radicals such as PH_4, F_2, $[BH_3]$. Applications to organic free radicals - methyl free radical, naphthalene and benzene free radicals, CID NP,

4. **Raman Spectroscopy :** Theories of Raman effect, condition for Raman active vibrations, selection rules, polarised and depolarised Raman lines, study of (i) Simple molecules - SO_2, CO_2, N_2O and C_2H_2 (ii) Hydrogen bonding (iii) Metal ions in solution, mutual exclusion principle.

5. **Infrared Spectroscopy :** Vibrational spectroscopy **:** Review of **:** Linear harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constant and bond strengths, anharmonicity, Morse potential energy diagram, vibration - rotation spectroscopy, P, Q, R branches. Breakdown of Born - Oppenheimer approximation, selection rules, group frequencies, overtones, hot bands, factors affecting the band positions and intensities, far I.R. regions, brief description of I.R. and F.T.I.R. instruments.

   Application of I.R. spectroscopy:

   (1) In the determination of structure of organic compounds
   (2) In inorganic chemistry

   (a) vibrations of diatomic, linear and bent triatomic, pyramidal and planar four atom molecules.
   (b) Metal-ligand vibrations (M-C, M-N, M-halogen, M-P and M-S), shifting of frequencies upon donation. Applications in identification of geometrical isomers.

6. **U-V- Visble Spectroscopy :** Different type of electronic transitions. Lambert's-Beer's law, chromophores, auxochromes, solvent effect, red shift, blue shift, absorption in dyes. Woodward's rule

for conjugated cyclic and acyclic dienes, absorption in aromatic compounds. Woodwards rule for unsaturated ketones, charge-transfer complexes.

7. **Mass Spectrometry :** Measurement technique (El, Cl, FD, FAB), Resolution, exact masses of nucleides, molecular ions, isotope ions, fragment ions of odd and even electron types, rearrangement ions, factors affecting cleavage patterns, simple cleavage, cleavage at a hetero atom, multi centre-fragmentation-Mclafferty rearrangements, retro Diels-Alder fragmentation. Structure elucidation of organic compounds employing mass-spectroscopy. Special methods of GC-MS, High resolution MS, introduction to radical-anion mass spectroscopy.

8. **Mössbauer spectroscopy:** Theory, Instrumentation, Applications - isomer shift, nuclear quadrupole coupling and magnetic hyperfine interaction.

9. **Photoelectron spectroscopy:** Theory, Instrumentation and Applications-Ionisation potentials, nature of molecular orbitals and chemical analysis.

Books

1. Spectroscopic Methods in Organic Chemistry by D.H. Williams and I. Fleming, 4th edition, Tata Mc Graw-Hill Publishing company Ltd., New Delhi.
2. Basic Principles of Spectroscopy by Raymond Chang Mc Graw Hill, New Delhi.
3. Physical Methods in Inorganic Chemistry by R. S. Drago, Affiliated East-West Press Pvt. Ltd., New Delhi.
4. Spectroscopy of Organic Compounds by P.S. Kalsi, New Age International Publisher, New Delhi.
5. Physical Chemistry by Atkins.

M.Sc.(Final)
Paper II (A)
Organic reactions and rearrangements

1. Selective organic name reactions and their synthetic applications

Reformatsky reaction, Robinson's annulation, Shapiro reaction, Michael addition, Mannich reaction, ene reaction, Barton reaction, Baylis-Hillman reaction, Hofmann-Loffler-Freytag reaction, Stork-enamine reaction, Peterson's reaction and Woodward-Prevost hydroxylation.

2. Pericyclic reactions

i. Introduction, classification and characteristics of pericyclic reactions.

ii. Conservation of Molecular orbital symmetry. Woodward-Hoffmann correlation diagrams

iii. Use of correlation diagrams: FMO and PMO approaches to study of:

(a) Electrocyclic reactions of linear conjugated diene, triene and allyl systems.

(b) Cycloaddition reactions involving [2+2] and [4+2] systems.

(c) Sigmatropic rearrangements ([1,3], [1,5] and [3,3]). Claisen, cope, aza and oxo-cope rearrangements. Conrotatory and disrotatory motions. Antarafacial and supratacial additions.

3. Molecular rearrangements

(a) Rearrangements involving carbanions:

i. Favorskii rearrangement

ii. Sommelet-Hauser rearrangement

iii. Stevens rearrangement

(b) Rearrangement involving carbocations:

i. Baeyer-Villiger oxidation

ii. Demjanov rearrangement

iii. Wagner-Meerwein rearrangement

(c) Rearrangements involving electron-deficient nitrogen:

i. Hoffman rearrangement

ii. Curtius rearrangement

iii. Wolff rearrangement

iv. Schmidt rearrangement

v. Lossen rearrangement

(d) Miscellaneous molecular rearrangements:

i. Benzidine rearrangement

ii. Dienone-phenol rearrangement

iii. Grovenstein-Zimmerman rearrangement

M. Sc. Final

PAPER II (B) :Molecular Symmetry and Group theory

1. Meaning and examples of different symmetry elements and generated operations. Derivation of matrices for rotation, reflection, rotation - reflection and inversion operations. Symmetry operations of all the molecular point groups (C_n , D_n, C_{nh} , D_{nb} C_{nv}, D_{nd}, S_n, T, T_d, T_h, O, O_h, I and I_h). Determination of the classes of operations by similarity transform method (only C_{2v}, C_{2h}, C_{3v} , S_4) and general rules (rest others), conversions of Schoenflies point group symbols into Hermann-Mauguin symbols.

2. The defining properties of 'group' . Meaning and examples of different types of groups (Isomorphic , Cyclic and Abelion). Subgroups, reducible and irreducible representations. Properties of irreducible representations. Construction of character tables for C_{2v}, C_{3v} and C_{4v} point groups. Direct products of representations.

3. Normal modes of vibrations :

Cartesian coordinate and internal coordinate methods of normal mode analysis applied to C_{2v} (symmetric XY_2, ZXY_2, T–shaped XY_3 , cis – N_2F_2 , oct cis – MX_4Y_2 and mer – MX_3Y_3), C_{3v} (XY_3 , fac – MX_3Y_3) T_d (XY_4) and O_h (XY_6) systems.

4. Valence bond treatment :

Formation of hybrid orbitals of XY_3 (planar), XY_4 (tetrahedral and square planar), XY_5 (square pyramidal and trigonal bipyramidal), XY_6 (octahedral and trigonal prismatic) and XY_7 (pentagonal bipyramid and monocapped trigonal prism with capping on tetragonal face).

5. Crystal fields:

Derivation of 'd' orbital splitting patterns of central atom (M) in ML_2, ML_3, ML_5, and ML_7 system (energy calculations are not required). The effect of weak crystal field on S, P, D, F and G spectroscopic terms in O_h and T_d point groups.

6. Molecular orbitals :

A_2 and AB_n (n = 1 to 3) type molecules.

BOOKS:

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.

M. Sc. Final

Paper II(C) : Thermodynamics and Intermolecular Forces

Axiomatic Approach

Caratheodory's principle. Thermodynamics in the presence of external fields : electrical field, magnetic field and gravitational field.

Intermolecular forces :

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

Thermodynamics of mixtures :

Excess thermodynamic functions. Activity coefficients : **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.

Solutions of macromolecules, Regular Solutions. Elementary ideas of lattice. Cell model and average potential model of liquid mixtures.

Phase Equilibria :

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

Liquid State :

Radial distribution function. Configurational entropy and free energy. Cell theory of liquid state, Hole theory, Gas like and solid like, Molecular theory of liquid viscosity, Mesomorphism.

Thermodynamics of Surfaces :

Gibbs adsorption equation. Thin films. Thermodynamic theory of stability of equilibrium.

Thermodynamics of Irreversible processes :

Thermodynamic criteria for non-equilibrium states ; Entropy production and entropy flow in irreversible processes, Entropy balance equation for heat flow, relation between fluxes and forces. Non-equilibrium stationary states, Linear phenomenological equations, Onsager's reciprocity relation. Curie Prigogine priniciple. Linear thermodynamic theory of thermosmosis. Electro kinetic phenomena and Reverse Osmosis. Far from equilibrium phenomena : Membrane Oscillations.

Books :

1. Pitzer : Thermodynamics
2. Guggenheim : Chemical Thermodynamics
3. Mac Glashan : Chemical Thermodynamics
4. Rowlinson : Liquids and liquid Mixtures
5. Buckingham : Thermodynamics
6. Haase : Irreversible Thermodynamics
7. Prigogine : Molecular Theory of
8. Eyring : Significant liquid Structures 9.Ion–Exchange Vol. I edited by J. A. Mannsky

M. Sc. Final

Paper III (A) - Biomolecules and Organic Spectroscopy

1. Vitamins :

A study of isolation, structure and physiological behaviour of the following:

I. Thiamine : Riboflavin, Pyridoxin and Pantothenic acid

II. Vitamin D : Calciferol

III. Vitamin E : Tocoferol

IV. Vitamin K : Vitamin K_1

2. Sex Hormones :

I. A general introduction to estrogens and androgens

II. Estrone : Structure and synthesis, relationship to estradiol

III. Progesterone : Preparation from steroid and physiological functions

3. Carbohydrates :

I. Disaccharides : Sucrose, Lactose, Maltose and Cellobiose

II. Polysaccharides : Starch and Cellulose.

4. Nucleic acids : General structure of RNA and DNA

5.Bioregulators:

(a) Lipids:

I. Introduction and classification

II. Chemistry of phospholipids, lecithin, cephalin and their biological importance

III. Estimation of fatty acids content in lipids.

(b) Prostaglandins:

Nomenclature,classification and chemistry of E_2 and $E_{2\alpha}$

6. Spectral characterisation of organic compounds :

Application of UV, IR, NMR, (^1H and ^{13}C) and Mass spectrometry in solving simple structural problems in organic chemistry.

M. Sc. Final

Paper-III (b) :Coordination Chemistry

1. Energy levels in an atom :

Relation between electronic configuration and energy terms, Hole formalism, 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, Definition of D_q and factors affecting its magnitude, Medium and strong field approximation in O_h 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 $M[H_2O]_6^{n+}$, calculation of Dq, B and β parameters, Spectra of spin free and spin paired MA_6. Jahn Teller distortion and its effect on electronic spectra, Charge transfer spectra

4. Magnetic properties of Complexes :

Dia, para, ferro and antiferromagnetism, spin cross over, correlation of magnetic susceptibility with effective magnetic moment, spin only formula, μ_{S+L} formula. Temperature independent k, paramagnetic behaviour. Quenching of orbital angular momentum by ligand fields. The magnetic properties of A, E and T terms. Electron delocalization and the magnetic properties of complexes with A,E and T ground terms.

5. Photochemical Reactions

(a) Basics of photochemistry : Absorption, excitation, Frank-condon principle, Energy dissipation by radiative and non - radiative processes, quantum yield.

I. Photosubstitution reactions in chromium (III) complexes

II. Photoredox reactions in cobalt complexes

III. Ligand photoreactions

IV. Solar energy conversion

M. Sc. Final

Paper III(C) : Statistical Mechanics, Transport Phenomena and Reactions Dynamics

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, the 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 and the ideal gas equation.

5. **Imperfect Gases :**

   The configurational partition function and the derivation of second virial coefficient for a hard sphere gas.

6. **Applications :**

   Equilibrium Constants from partition function for: Isomerisation equilibrium,

   Ionisation– equilibrium ($H \rightleftharpoons H^+ + e$),

   Dissociation equilibrium ($Na_2 \rightleftharpoons 2Na$) and

   Isotopic exchange equilibrium ($H_2 + D_2 \rightleftharpoons 2HD$)

   Heat capacity of Solids, ortho and para hydrogen, Negative temperatures, Laser.

7. **Transport Phenomena :**

   Boltzmann distribution of velocities from partition–function, Average velocity and average kinetic energy of the molecules.

8. **Non–eqilibrium velocity distribution functions :**

   Elementary discussion of Boltzmann–H–theorem and irreversibility. Elementary theory of non–equilibrium fluctuation and principle of onsager reciprocal relation.

9. **Statistical Treatment of kinetics :**

   Limitation of Lindemann theory, Hinshel-wood treatment, RRK theory, RRKM theory, Slater's theory based on non-equilibrium statistical mechanics-stochastic theory, Treatment of reaction rate in terms of random walk.

10. **Reaction Dynamics :**

    Molecular Collisions - Collision cross-section & inter-molecular potentials. Potential energy surfaces and their calculations, Elastic molecular collisions, Reaction cross-section methods in molecular reaction dynamics. Photo fragment spectroscopy, Crossed-molecular beam, a case study of $F + H_2$ and $H + D_2$ reactions.

Books :

1. Norman Davidson – Statistical Mechanics
2. T. L. Hill – Statistical Mechanics
3. L. K. Nash – Statistical Mechanics
4. J. H. Knox – Molecular Thermodynamics
5. Mayer & Mayer – Statistical Mechanics
6. R. C. Tolman – The principles of Statistical Mechanics
7. Entropy and Energy Levels – Oxford Chemistry Series, R. P. H., Gasser and W. G. Richards.
8. W. J. Moore – Physical Chemistry
9. Laidler – Chemical Kinetics
10. Theory of Non–Uniform Gases –Chapman & Cowling
11. Kauzmann – Kinetic Theory of Gases
12. B. K. Agarwal & M. Eiser – Statistical Mechanics

M. Sc. Final

Paper IV (A): Select Topics in organic chemistry

1. Optical isomerism, principles of assymetry, optical isomerism of compounds containing no asymmetric carbon atom,(Biphenyls, Allenes, Spiranes)Optical activity due to intra molecular overcrowding, absolute configuration.

2. Stereochemistry of tri and tetra covalent nitrogen compounds, geometrical isomerism of compounds containing carbon nitrogen (C=N) and nitrogen nitrogen (N=N) double bonds. Stereochemistry of compounds containing sulfur and phosphorus.

3. **Reagents in organic synthesis**: Preparation and use of following reagents in organic synthesis and functional group transformations. Lithium aluminium hydride (LAH), Dicyclohexylcarbodiimide (DCC), Diazomethane, Wittig reagent, Lithium diisopropylamide (LDA), Lithium dimethyl cuperate, DDQ, Trimethylsilyl Iodide, 1,3-dithiane, Wilkinson's catalyst, Baker yeast and Phase transfer catalyst.

4. **Stereo selective synthesis**:

   Chiral synthesis, newer method of asymmetric synthesis (enzymatic and catalytic nexus), enantio and diastereoselective synthesis.

5. **Protective groups**: Principles of protection and deprotection of alcohols, thiols, 1,2- and 1,3-diols, amines, carbonyl and carboxyl groups in organic synthesis.

6. **Photochemistry:** Electronically excited states, physical properties, time-dependent phenomenon and energy transfer photochemical elimination, redox reaction, photochemistry of alkenes, Norrish type-I and Norrish type-II reactions, Patterno-Buchii reaction, Photo-Fries rearrangement, singlet molecular oxygen reactions, Di- pi methane and related rearrangements. Photochemistry of aromatic compounds (Isomerizations, additions and substitutions).

M. Sc. Final

PAPER IV (b)- 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 photosystem 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 :

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.

M. Sc. Final

Paper IV(C) : Quantum Chemistry

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. **Molecular Orbital Theory of Inorganic Compounds :**

   Molecular orbitals for □-bonding in AB_n molecules : The tetrahedral AB_4 and octahedral AB_6 cases,

   Molecular orbitals for □-bonding in AB_n molecules : The tetrahedral AB_4 and octahedral AB_6 cases.

4. **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, use of Gaussian orbitals in non–empirical methods with special reference to Gaussian Software of Pople et.al.

5. **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.

6. **Quantum Mechanical Treatment of Weak Molecular Interactions :** Charge transfer, hydrogen bond, van der waal's forces.

Books

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. Quantum Chemistry by Ira N. Levine Prentice Hall of India New Delhi 1995.
7. Coulson's volume by R. McWeeny ELBS 1978.

M. Sc. Final

Paper V(A) - Natural Products

1. **Biosynthesis of natural products** :
   - (i) The acetate hypothesis, poly β-keto acid and their aldol type condensation, meta-orientation of –OH group in naturally occurring phenols.
   - (ii) Isoprene rule, mevolonic acid from acetyl co-enzyme – A, biogenesis of terpenoids.
   - (iii) Shikimic acid pathway of biogenesis of aromatic ring.
   - (iv) General biogenesis of alkaloids.
2. **Acetogenenins** : Classification, general method of structure determination of
   - (i) Cyanin and cyanidin chlorides
   - (ii) Chrysin and quercetin
   - (iii) Coumarins
3. **Terpenoids** : Chemistry of
   - (i) Sesquiterpenoids : Cadenin and Eudesmol.
   - (ii) Diterpenoids : Abietic acid Phytol.
   - (iii) Triterpenoids : Squalene.
4. **Alkaloids** : Chemistry of
   - (i) Opium alkaloids : Papaverine and Morphine
   - (ii) Rauwolfia alkaloids : Reserpine
   - (iii) Chincona alkaloids : Quinine
5. **Steroids** : General method for determination of ring system, position of hydroxyl group double bond angular methyl group, position and nature of side chain in steroids. Detail study of cholesterol and its relation to caprostanol.
6. **Corticoids :** Chemistry of Cortisone and therapeutic uses of Corticoids.

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PAPER V(B)

Organotransition Metal Chemistry

1. Organometallic compounds

Definition and classification of organometallic compounds on the basis of nature of M-C bond.

2. Alkyls and Aryls of Transition Metals

Types, General Synthetic Routes, Stability and decomposition pathways.

3. Compounds of Transition Metal - Carbon Multiple Bond

Carbenes and Carbynes ;

Synthesis, Structural Characteristics, Nucleophilic and Electrophilic reactions on the ligands.

4. 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.

5. Metal carbonyl compounds :

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, carbonylate anions and carbony1 hydrides, carbony1 carbide complexes of Fe, Ru, Os, Co and Rh, Arene and cyclopentadienyl metal carbonyls.

6. Catalysis involving organometallic compounds

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

7. Fluxional Organometallic Compounds

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

BOOKS

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.

M. Sc. Final

Paper V(C) : Electro Chemistry (Passed in the BOS Meeting held on 14-09-09)

1. **Conductance in non–aqueous media :**

   Ion association, its effect on conductance, diffusion of electrolytes, measurements of diffusion coefficient, diffusion in relation to conductance.

2. **Concentration Cells :**

   Cells with and without transference, concentration cells involving mixture of electrolyte, Amalgam cells, Centrifugal cell, Liquid junction Potential, Membrane Potential, T. M. S. Theory

3. **Photo electro chemical cells**

4. **Electro Kinetic Phenomena :**

   Quantitative treatment of electro–osmosis, electro phoresis and streaming potential, electrical double layer theories

5. **Electrodics :**

   The equilibrium exchange current density, Butler–Volmer Equation Tafel plot, over potential and activation energy.

6. **Electroanalytical Techniques :**

   Basic principles, techniques and applications of Polarography, Cyclicvoltametry, Coulometry, Chronopotentiometry and impedance measurements.

7. **Corrosion :**

   Electrochemical corrosion theory, estimation of corrosion rates, principles of electrochemical deposition and electropolymerization processes.

Books Recommended

1. S. Glasston : Electro Chemistry
2. Robinson & Stokes : Electrolytic Solutions
3. Bockris and Reddy, Modern Electrochemistry Vol I and II
4. Ilna Fried, The Chemistry of Electrode Processes, Academic Press, London.
5. Gouglas, A Skoog and Donald M West, Principles of Instrumental Analysis, Saunder's College, Philadelphia, 1980.
6. Donald T Sawyer and Julien Roberts, Jr., Experimental Electrochemistry for Chemists, John Wiley and sons, New York, 1974.
7. N.J. Selly, Experimental Approach to electrochemistry, Edward Arnold (Publishers) Ltd., London, 1977.

M. Sc. Final

PAPER VI (a) : 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 ionisation 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.

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Paper VI B

Analytical Chemistry

1. **Electroanalytical methods**

   (a). Principle, instrumentation and application of the following methods:

   I. Coulometry

   II. Ampereometry

   III. Voltametry and cyclicvoltametry

   (b). Conductometry: Discussion of the nature of curves in acid-base (including mixture of acids), precipitation and complexometric titrations.

   (c). Potentiometry: Different types of electrodes, discussion of the nature of curves for oxidation-reduction and acid-base titrations, comparison with the conductometric method.

   (d). Polarography: Dropping mercury electrode and its advantages, polarographically acive species, concept of residual, diffusion and limiting currents and half-wave potential, Ilkovic equation and factors affecting diffusion current.

2. **Thermochemical methods**

   (a). Thermogravimetric: Apparatus, factors affecting TGA, interpretation of TG curves of $CaC_2O_4.H_2O$ and $MgC_2O_4.2H_2O$ and in the analysis of their mixture.

   (b). Differential Thermal Analysis and Differential Scanning Calorimetrty: Apparatus, factors affecting DTA/DSC curves with special reference to heating rate, particle size and packing, measurements of heats of transition or heat of reaction and heat of hydration of metal salt hydrates.

3. **Radiochemical methods**

   Isotopic dilution, inverse isotopic dilution and neutron activation techniques

4. **Spectroscopic methods**

   Principle, instrumentation and application of the following methods

   (a). Flame photometry

   (b). Nephleometry and turbidimetry

   (c). Molecular luminescence and Fluorometry

Recommended Books:

1. Fundamentals of Analytical Chemistry, DA Skoog, DM West, FJ Holler and WB Saunders
2. Quantitative Inorganic Analysis, AI Vogel
3. Instrumental Methods of Chemical Analysis, BK Sharma
4. Instrumental Methods of Chemical Analysis, H Kaur
5. Analytical Chemistry, Gary D Christian

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Paper VI (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

Molecular Weight of Polymers: Concept of average molecular weights in polymers: Number, Weight and Viscosity average molecular weights, Monodispersity, Polydispersity and molecular weight distribution, Most probable and Poisson distributions, Measurement of molecular weights by light scattering and ultracentrifugation methods.

4. Polymer Solutions

Criteria of Polymer Solubility, Solubility Parameters, Size of the polymer molecules – The freely jointed chain model, Concept of theta temperature, theta solvent and unperturbed dimensions, Fractionation of polymers with special reference to Gel Permeation Chromatography technique.

5.. Degradation of Polymers

Significance of polymer degradation, Types of degradation – Random degradation and Chain depolymerization, A general idea of Thermal, Mechanical and Oxidative degradations, Antioxidants and stabilizers.

6.. Morphology, Structure and Rheology of Polymers

Configurations of polymer chains,,Crystallinity in polymers, Polymer Crystallization, factors affecting crystallinity and effect of crystallinity on the properties of the polymers.

Viscous flow, Rubber Elasticity (thermodynamics and entropy elasticity), Visco-elasticity, The Glassy state and the glass transition temperature (Tg), Effect of molecular weight, copolymerization, diluents and chemical structure on the glass transition temperature, Relationship between Tg and Tm.

7. Polymer Processing

Plastic Technology: A general idea of Moulding and Extrusion techniques, Thermoforming and Thermofoaming, Fibre Reinforced Plastics (FRP), Fillers and Plasticizers.

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

Elastomer Technology: Vulcanization of Rubbers, Chemistry of Vulcanization .

8.. Functional Polymers

A brief idea of Fire retarding and Electrically conducting Polymers. Biomedical Polymers – contact lens, dental polymers, artificial heart, kidney, skin and blood cells.

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PAPER VI (D)

SOLID STATE CHEMISTRY

1. Crystal Structures

Rock Salt, Zinc Blende, Wurtzite, Diamond, Graphite, Fluorite, Sesquoxide, Spinel (Normal/inverse), ReO_3, 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

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

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Paper VI (E)

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-transpost : 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

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.

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Paper VI (F)

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) Applications.
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

Ref. Books:

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

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Paper VI (G)

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. Glasses, Ceramics and Composites

Glasses - Glassy ptate, glass formers and glass modifiers, electrical conducting glasses.

Ceramics- Introduction, type of ceramics and their crystal structures, mechanical properties of ceramics - Brittle fracture, stress-strain behaviour, plastic deformation and non-crystalline ceramics.

Composites- Introduction, Particle reinforced composites, fiber reinforced composites, Polymer Based composites, Metal matrix composites, ceramics matrix composites, carbon - carbon composite, structural composites, ultra high performance concretes.

12. Binding materials

Portland cements - manufacture and hydration, Blended cements, Calcium sulphate based binding materials and their hydration.

13. Polymeric materials

Introduction, type and classification, molecular weight, polymer synthesis and processing, Thermoplastic and thermo set polymers, Mechanical and Rheological properties of polymers with special reference to viscoelasticity and glass transition temperature. Conducting, light emitting and Biodegradable polymers.

14. Nano materials

Introduction, preparation of nano materials, size property relationship, Carbon nanotubes, Discussion of some nano particles such as barium titarate, gold Applications of nano meterials.

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PAPER-VI (H)

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

M. Sc. FINAL

PRACTICALS

INORGANIC CHEMISTRY

1. Gravimetric estimation of the following involving not more than two separations:

   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.

4. Chromatographic Exercises:

   Separation of Cl^{-} and Br^{-}; Co^{++} and Ni^{++}; Zn^{++} and Mn^{++} by suitable ion exchangers.

5. Potentiometry :

   a. Acid-Base, redox and precipitation titrations.

   b. Determination of stability constants of suitable complex systems.

6. Conductometry

7. Colorimetry and Spectrophotometry:

   Estimation of the following metals in solution V, Cr, Mo, Fe and Ni.

8. Flame Photometry:

   Estimation of sodium and potassium in admixture.

   a. Estimation of magnesium and calcium in tap water.

   b. Estimation of calcium in calcium salt solution.

Books Recommended:

1. Text Book of Quantitative Inorganic Analysis : A. I. Vogel, Longmans. 1978
2. Synthesis and Techniques in Inorganic chemistry. R.J. Angelici. W.B. Saunders Company 1969.

M. Sc. FINAL

PRACTICALS

ORGANIC CHEMISTRY

1. Multi step synthesis of organic compounds preferably involving the use of organic reagents and purification using chromatographic technique.
2. Estimation of amino acid (formal titration) molecular weight determination of simple organic acids.
3. Estimation of sulphur and halogens in organic compounds.
4. Preparation, molecular weight determination and characterization (IR. NMR) of the following polymers : Polystyrene, Nylon 66, Polyester and thikol.
5. Separation and purification of the components of a ternary mixture. (Liquid-liquid-liquid, liquid-liquid-solid, solid-solid-solid). Each component should not contain more than two functional groups The student should check the purity by TLC.
6. Estimation of C. H. and N in organic compounds.
7. Estimation of $-NH_2$ and -OH (both alcoholic and phenolic) and - NO_2
8. Estimation of glucose and sucrose (Fehling solution method).
9. Following experiments on chromatography.
    a. Separation of mixtures of fluorene. anthracene and diglyme (diethylene-glucxoldimethyl ether) by TLC.
    b. Separation of anthracene from anthracene picrate by column chromatography.
    c. Separation of a mixture of methy1 orange and methylene blue by column chromatography.
10. Interpretation of IR and PMR spectra of simple organic compounds hydrocarbons, carbonyl compounds, hydroxy compounds, amines, acids and their derivatives.

Books Recommended:

1. Experimental organic chemistry by M.P. Dayal and U.S. Mungall, John-Wiley and Sons, 1988.
2. Utilized Experiments in Organic Chemistry by Ray O. Brewester, A. Vanderware and William E. MC. Even (D. Van Nestrands & Co).
3. Vogel's text book of practical organic chemistry.
4. Experimental Organic Chemistry Vol. I by P.R. Singh. D.D. Gupta and K.S. Bajpai (Tata McGraw. Delhi)

M. Sc.

FINAL PRACTICALS

PHYSICAL CHEMISTRY

Experiments should be set to give an insight into the following techniques:

(i). Vacuum technique

(ii). Measurement of Pressure and temperature

(iii). Optical measurements

(iv). Electroanalytical techniques and Polarography.

GROUP A

ELECTROCHEMISTRY

1. Conductometry:

   Measurements of conductance of solutions. Hydrolysis constants of weak acids and base. Solubility of sparingly soluble salts. basicity of acids. Determination of Onsager constant. Conductometric titrations.

2. Potentiometry

   Ssetting up of electrodes. Measurement of E. M. F. of a concentration cell, preparation of buffer solutions, Measurement of pH. First, second and third dissociation constants of polybasic acids. Valency of ions. Compositions of complex ions. Solubility of sparingly soluble salts potentiometrically, oxidation-reduction potentials, potentiometric titrations.

3. Determination of transport number by moving boundary method.

CHEMICALKINETICS

HOMOGENEOUS REACTIONS :

Use of different techniques for the study of reaction rates. Mechanism and determination of temperature coefficient of typical reactions such as decomposition of diacetone diazonium chloride. Inversion of sucrose, decomposition of diacetone alcohol and bromination of acetone Time period of oscillation in a typical Oscillatory reaction

HETEROGENEOUS REACTIONS

Ion exchange reactions. photochemical reaction. Hydrolysis of monochloroaetic acid, bromination of cinnamic acid and reaction between thionene and ferrous sulphate.

GROUP B

Programing and computational exercises involving use of calculators and computer.

COLLIGATIVE PROPERTIES

Measurement of osmotic pressure, freezing point depression and boiling point elevation.

NEW EXPERIMENTS

1. Estimation of transport numbers by liquid junction potential and membrane potential measurements.

2. Verification of Henderson's equation
3. Determination of diffusion coefficient
4. Determination of zeta potential from electrophoretic mobility
5. Determination of activity coefficient of an electrolyte
6. Determination of hydrolysis of tertiary amyl iodide
7. Determination of energy of activation
8. Determination of dipole moment and verification of additivity of molar refraction
9. Determination of vapour pressure by dew point method
10. Calorimetric study of reaction kinetics
11. Reaction kinetics by turbidity measurements.

Duration of practical examination will be 14 hours in each branch, spread over two days. The marks will be allocated as follows:

Practical exercises:	110
Viva-Voce:	25
Record:	15
Total	150