

आज दिनांक 09.02..2012 को विश्वविद्यालय परिसर में निम्न विषय की पाठ्यक्रम समिति की एक आवश्यक बैठक हुई, जिसमें निम्न प्राध्यापकगण उपस्थित हुए :-

Date :- 09.02.2012

Subject :- Chemistry

Committee Place :- Committee Hall

1. Dr. K. A. Gupta
2. Dr. C. P. Singh
3. Dr. S. K. Pandey
4. Dr. S. K. Agarwal

M.J.P. ROHILKHAND UNIVERSITY
BAREILLY

Revised Syllabus
Of
Chemistry
For
Graduate &
Post Graduate Classes

Modified according to U.G.C. Model
Curriculum
to be enforced
w.e.f
ACADEMIC SESSION
2011-2012

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SYLLABU

S

B.Sc. Part - I
Paper I
Inorganic Chemistry

60 Hrs (2 Hrs/week),
Max. Marks: 50

I Atomic Structure 6 Hrs

Idea of de-Broglie matter waves, Heisenberg uncertainty principle, atomic orbitals, Schrodinger wave equation, significance of Ψ and Ψ^2 , quantum numbers, radial and angular wave functions and probability distribution curves, shapes of s, p, d orbitals. Aufbau and Pauli exclusion principles. Hund's multiplicity rule. Electronic configurations of the elements, effective nuclear charge.

II Periodic Properties 6 Hrs

Atomic and ionic, radii, ionization energy, electron affinity and electronegativity – definition, methods of determination or evaluation, trends in periodic table and applications in predicting and explaining the chemical behaviour.

III Chemical Bonding 20 Hrs

- (a) Covalent Bond – Valence bond theory and its limitations, directional characteristics of covalent bond, various types of hybridization and shapes of simple inorganic molecules and ions, Valence shell electron pair repulsion (VSEPR) theory to NH_3 , H_3O^+ , SF_4 , ClF_3 , ICl_2 and H_2O . MO theory, homonuclear and heteronuclear (CO and NO) diatomic molecules, multicentre bonding in electron deficient, molecules bond strength and bond energy, percentage ionic character from dipole moment and electronegativity difference.

(b) Ionic Solids – Ionic structures, radius ratio effect and coordination number, limitation of radius ratio rule, lattice defects, semiconductors, lattice energy and Born-Haber cycle, solvation energy and solubility of ionic solids, polarizing power and polarisability of ions, Fajan's rule. Metallic bond-free electron, valence bond and bond theories.

(c) Weak Interactions – Hydrogen bonding, van der Waals forces

IV s- Block Elements 6 Hrs

Comparative study, diagonal relationships, salient features of hydrides, solvation and complexation tendencies including their function in biosystems, an introduction to alkyls and aryls.

V p- Block Elements 20 Hrs

Comparative study (including diagonal relationship) of groups 13-17 elements. Compounds like hydrides, oxides, oxyacids and halides of groups 13-16, hydrides of boron-diborane and higher boranes, borazine, borohydrides, fullerenes, carbides, fluorocarbons, silicates (structural principle), tetrasulphur tetranitride, basic properties of halogens, interhalogens and polyhalides.

VI ChemiStry of Noble Gases 3 Hrs

Chemical properties of the noble gases. Chemistry of xenon, structure and bonding in xenon compounds.

Paper II

Organic Chemistry

60 Hrs (2 Hrs/week),
Max. Marks: 50

- I Structure and Bonding** **5 Hrs**
Hybridization, bond lengths and bond angles, bond energy, localized and delocalized chemical bond, van der Waals interactions, inclusion compounds, clathrates, charge transfer complexes, resonance, hyperconjugation, aromaticity, inductive and field effects, hydrogen bonding.
- II Mechanism of Organic Reactions** **8 Hrs**
Curved arrow notation, drawing electron movements with arrows, half-headed and double-headed arrows, homolytic and heterolytic bond breaking. Types of reagents-electrophiles and nucleophiles. Types of organic reactions. Energy considerations.
Reactive intermediates – carbocations, carbanions, free radicals, carbenes, arynes and nitrenes (with examples). Assigning formal charges on intermediates and other ionic species.
Methods of determination of reaction mechanism (product analysis, intermediates, isotope effects, kinetic and stereochemical studies).
- III Stereochemistry of Organic Compounds** **12 Hrs**
Concept of isomerism. Types of isomerism.
Optical isomerism – elements of symmetry. Molecular chirality, enantiomers. Stereogenic centre, optical activity, properties of enantiomers, chiral and achiral molecules with two stereogenic centres, diastereomers, threo and erythro diastereomers, meso compounds, resolution of enantiomers, inversion, retention and racemization.

Relative absolute configuration, sequence rules, D & L and R & S systems of nomenclature.

Geometric isomerism – determination of configuration of geometric isomers. E & Z system of nomenclature, geometric isomerism in oximes and alicyclic compounds.

Conformational isomerism – conformational analysis of ethane and n-butane; conformations of cyclohexane, axial and equatorial bonds, conformation of mono substituted cyclohexane derivatives. Newman projection and Sawhorse formulae, Fischer and flying wedge formulae.

Difference between configuration and conformation.

IV Alkanes and Cycloalkanes 7 Hrs

IUPAC nomenclature of branched and unbranched alkanes, the alkyl group, classification of carbon atoms in alkanes. Isomerism in alkanes, sources, methods of formation (with special reference to Wurtz reaction, Kolbe reaction, Corey-House reaction and decarboxylation of carboxylic acids), physical and chemical reactions of alkanes.

Mechanism of free radical halogenation of alkanes: orientation, reactivity and selectivity. Cycloalkanes – nomenclature, methods of formation, chemical, Baeyer's strain theory and its limitations. Ring strain in small rings (cyclopropane and cyclobutane), theory of strainless rings, The case of cyclopropane ring: banana bonds.

V Alkenes, Cycloalkenes, Dienes and Alkynes 12 Hrs

Nomenclature of alkenes, methods of formation, mechanisms of dehydration of alcohols and dehydrohalogenation of alkyl halides, regioselectivity in alcohol dehydration. The Saytzeff rule, Hofmann elimination, physical properties and relative stabilities of alkenes. Chemical reactions of alkenes – mechanisms involved in

hydrogenation, electrophilic and free radical additions, Markownikoff's rule, hydroboration – oxidation, oxymercuration-reduction. Epoxidation, ozonolysis, hydration, hydroxylation and oxidation with KMnO_4 Polymerization of alkenes. Substitution at the allylic and vinylic positions of alkenes. Industrial applications of ethylene and propene.

Methods of formation, conformation and chemical reactions of cycloalkenes.

Nomenclature and classification of dienes: isolated, conjugated and cumulated dienes. Structure of allenes and butadiene, methods of formation, polymerization. Chemical reaction – 1, 2 and 1, 4 additions, Diels-Alder reaction.

Nomenclature, structure and bonding in alkynes. Methods of formation. Chemical reactions of alkynes, acidity of alkynes. Mechanism of electrophilic and nucleophilic addition reactions, hydroboration-oxidation, metal-ammonia reductions, oxidation and polymerization.

VI Arenes and Aromaticity 12 Hrs

Nomenclature of benzene derivatives. The aryl group. Aromatic nucleus and side chain. Structure of benzene: molecular formula and Kekule structure. Stability and carbon-carbon bond lengths of benzene, resonance structure, MO picture. Aromaticity: the Huckel rule, aromatic ions. Aromatic electrophilic substitution – general pattern of the mechanism, role σ - and π - complexes. Mechanism of nitration, halogenation, sulphonation, mercuration and Friedel-Crafts reaction. Energy profile diagrams. Activating and deactivating substituents, orientation and ortho/para ratio. Side chain reactions of benzene derivatives. Birch reduction. Methods of

formation and chemical reactions of alkylbenzenes, alkynylbenzenes and biphenyl.

VII Alkyl and Aryl Halides

8 Hrs

Nomenclature and classes of alkyl halides, methods of formation, chemical reactions. Mechanisms of nucleophilic substitution reactions of alkyl halides, S_N2 and S_N1 reactions with energy profile diagrams. Polyhalogen compounds: chloroform, carbon tetrachloride. Methods of formation of aryl halides, nuclear and side chain reaction. The addition-elimination and the elimination-addition mechanisms of nucleophilic aromatic substitution reactions. Relative reactivities of alkyl, vinyl and aryl halides and halides. Synthesis and uses of DDT and BHC.

Paper III

Organic Chemistry

60 Hrs (2 Hrs/week),
Max. Marks: 50

I Mathematical Concepts and Computers 16 Hrs

(A) Mathematical Concepts

Logarithmic relations, curve sketching, linear graphs and calculation of slopes. Differentiation of functions like k_x , e^x , x^n , $\sin x$, $\log x$, maxima and minima, partial differentiation and reciprocity relations. Integration of some useful/relevant functions; permutations and combinations. Factorials. Probability.

(B) Computers

General introduction to computer, different components of a computer, hardware and software, input-output devices; binary numbers and arithmetic: introduction to computer languages. Programming, operation systems.

II Gaseous States 8 Hrs

Postulates of kinetic theory of gases, deviation from ideal behavior, vander Waals equation of state. Critical Phenomena: PV isotherms of real gases, continuity of states, the isotherms of van der Waals equation, relationship between critical constants and van der Waals equation, relationship between critical constants and van der Waals constants. The law of corresponding states. Reduced equation of state. Molecular velocities: Root mean square, average and most probable velocities, Qualitative discussion of the Maxwell's distribution of molecular velocities, collision number, mean free path and collision diameter. Liquification of gases (based on Joule-Thomson effect).

- III Liquid State** **6 Hrs**
Intermolecular forces, structure of liquids (a qualitative description). Structural differences between solids, liquids and gases. Liquid crystals: Difference between liquid crystal, solid and liquid. Classification, structure of nematic and cholestric phases. Thermography and seven segment cell.
- IV Solid State** **11 Hrs**
Definition of space lattice, unit cell. Laws of crystallography – (i) Law of constancy of interfacial angles (ii) Law of rationality of indices (iii) Law of symmetry. Symmetry elements in crystals. X-ray diffraction by crystals. Derivation of Bragg equation. Determination of crystal structure of NaCl, and CsCl (Laue's method and powder method).
- V Colloidal State** **6 Hrs**
Definition of colloids, classification of colloids. Solids in liquids (sols): properties – kinetic, optical and electrical; stability of colloids, protective action, Hardy-Schulze law, gold number. Liquids in liquids (emulsions): types of emulsions, preparation. Emulsifier. Liquids in solids (gels): classification. Preparation and properties, inhibition general applications of colloids.
- VI Chemical Kinetics and Catalysis** **13 Hrs**
Chemical kinetics and its scope, rate of a reaction, factors influencing the rate of a reaction – concentration, temperature, pressure, solvent, light catalyst. Concentration dependence of rates, mathematical characteristics of simple chemical reactions – zero order, first order, second order, pseudo order, half life and mean life. Determination of the order of reaction – differential method, method of integration, method of half life period and isolation

method. Radioactive decay as a first order phenomenon. Experimental methods of chemical kinetics: conductometric, potentiometric, optical methods, polarimetry and spectrophotometer. Theories of chemical kinetics: effect of temperature on rate of reaction, Arrhenius equation, concept of activation energy, Simple collision theory based on hard sphere model. Transition state theory (equilibrium hypothesis). Expression for the rate constant based on equilibrium constant and thermodynamic aspects. Catalysis, characteristics of catalysed reactions, classification of catalysis, miscellaneous examples.

LABORATORY COURSE

**60 Hrs (2 Hrs/week),
Max. Marks: 50**

I Inorganic qualitative analysis (preferably semi-micro):

Inorganic mixtures containing cations, anions and combination of anions, and interfering anions. Total number of cations and anions in a mixture shall be six.

II Inorganic quantitative analysis-volumetric exercises:

- (i) Acidimetry-alkalimetry and redox titrations including iodometry.
- (ii) Hardness of water by EDTA methods.
- (iii) Available chlorine in bleaching powder.

III Physical experiments based on surface tension and viscosity.

IV Pre-lab study and demonstrative exercises:

- (i) General awareness of laboratory items, hazardous chemicals, and safety measures.
- (ii) Errors, significant figures and lab-report writing.
- (iii) Demonstrative exercise viz. shapes of molecules three-dimensional representation, R&S, E&Z configurations, configurational and conformational study with the help of models.

Students are expected to perform all the above exercises. One exercise each out of mixture analysis volumetric analysis and physical experiments shall be given in the examination.

Distribution of marks will be as follows:

* (i) Mixture of analysis (six radicals)	15
(ii) Volumetric analysis	12
(iii) Physical experiment	10

** (iv) Viva-voice 05

(v) Annual record 08

* Full credit of marks shall be given upto 0.5% error after which for each 0.1 error, two marks shall be deducted.

** Viva-voice for ex-student shall carry 13 marks

Note:

1. The annual work of the candidate evaluated periodically should be carefully assessed. A total of minimum 16 exercises are expected to be carried out during the session to get full credit of marks in the annual record. If however, the total number of experiments done is less than 16, each experiment done shall be evaluated for half mark. A record of the same should be maintained in the department/college as an official record.

2. Less than zero mark should not be awarded.

3. The total number of candidates to be examined per batch in the practical shall not be more than 60.

B.Sc. Part - II
Paper I
Inorganic Chemistry

60 Hrs (2 Hrs/week),
Max. Marks: 50

- I Chemistry of Elements of First Transition Series 10 Hrs**
Characteristic properties of d-block elements. Properties of the elements of the first transition series, their binary compounds and complexes illustrating relative stability of their oxidation states, coordination number and geometry.
- II Chemistry of Elements of Second and Third Transition Series 10 Hrs**
General characteristics, comparative treatment with their 3d-analogues in respect of ionic radii. Oxidation states, magnetic behaviour, spectral properties and stereochemistry
- III Oxidation and Reduction 10 Hrs**
Use of redox potential data- analysis of redox cycle, redox stability stability in water – Frost, Latimer and Pourbaix diagrams. Principles involved in the extraction of the elements.
- IV Coordination Compounds 10 Hrs**
Werner's coordination theory and its experimental verification, effective atomic number concept, chelates, nomenclature of coordination compounds, isomerism in coordination compounds, valence bond theory of transition metal complexes
- V Chemistry of Lanthanide Elements 6 Hrs**
Electronic structure, oxidation states and ionic radii and lanthanide contraction, complex formation, occurrence and isolation, lanthanide compounds.

- VI Chemistry of Actinides** **4 Hrs**
General features and chemistry of actinides, chemistry of separation of Np, Pu and Am from U, similarities between the later actinides and the later lanthanides.
- VII Acids and Bases** **6 Hrs**
Arrhenius, Bronsted-Lowry, the Lux-Flood, solvent system and Lewis concepts of acids and bases.
- VIII Non-aqueous Solvents** **6 Hrs**
Physical properties of a solvent, types of solvent and their general characteristics, reactions in non-aqueous solvents with reference to liquid NH_3 and liquid SO_2 .

Paper - II

Organic Chemistry

60 Hrs (2 Hrs/week),
Max. Marks: 50

- I Electromagnetic Spectrum: Absorption Spectra 10 Hrs**
- Ultraviolet (UV) absorption spectroscopy – absorption laws (Beer-Lambert law). Molar absorptivity, presentation and analysis of UV spectra, types of electronic transitions, effect of conjugation. Concept of chromophore and auxochrome. Bathochromic, hypsochromic hyperchromic and hypochromic shifts UV spectra of conjugated enes and enones. Infrared (IR) absorption spectroscopy – molecular vibrations, Hooke's law, selection rules, intensity and position of IR bands, measurement of IR spectrum, fingerprint region characteristic absorptions of various functional groups and interpretation of IR spectra of simple organic compounds.
- II. Alcohols 6 Hrs**
- Classification and nomenclature.
- Monohydric alcohols – nomenclature, methods of formation by reduction of aldehydes, ketones, carboxylic acids and esters. Hydrogen bonding. Acidic nature, Reactions of alcohols. Dihydric alcohols – nomenclature, methods of formation, chemical reactions of vicinal glycols, oxidative cleavage $[\text{Pb}(\text{OAc})_4]$ and pinacol-pinacolone rearrangement. Trihydric alcohols-nomenclature and methods of formation, chemical reactions of glycerol.

III. Phenols**6 Hrs**

Nomenclature, structure and bonding. Preparation of phenols, physical properties and acidic character. Comparative acidic strengths of alcohols and phenols, resonance stabilization of phenoxide ion. Reactions of phenols – electrophilic aromatic substitution acylation and carboxylation. Mechanisms of Fries rearrangement, Claisen rearrangement Gatterman synthesis, Hauben-Hoesch reaction, Lederer-Manasse reaction and Reimer-Tiemann reaction.

IV Ethers and Epoxides**3 Hrs**

Nomenclature of ethers and methods of their formation, physical properties. Chemical reactions – cleavage and autoxidation, Ziesel's method. Synthesis of epoxides. Acid and base-catalyzed ring opening of epoxides, orientation of epoxide ring opening, reactions of Grignard and organolithium reagents with epoxides.

V Aldehydes and Ketones**14 Hrs**

Nomenclature and structure of the carbonyl group. Synthesis of aldehydes and ketones with particular reference to the synthesis of aldehydes from acid chlorides, synthesis of aldehydes and ketones using 1,3-dithiaes, synthesis of ketones from nitriles and from carboxylic acids. Physical properties. Mechanism of nucleophilic additions to carbonyl group with particular emphasis on benzoin, aldol, Perkin and Knoevenagel condensations. Condensation with ammonia and its derivatives. Wittig reaction. Mannich reaction. Use of acetals as protecting group. Oxidation of aldehydes, Baeyer-Villiger oxidation of ketones, Cannizzaro reaction, MPV, Clemmensen, Wolff-Kishner, LiAlH_4 and NaBH_4 reductions. Halogenation of enolizable ketones.

An introduction to α,β unsaturated aldehydes and ketones.

- VI Carboxylic Acids** **6 Hrs**
Nomenclature, structure and bonding, physical properties, acidity of carboxylic acids, effects of substituents on acid strength. Preparation of carboxylic acids. Reactions of carboxylic acids. Hell-volhard-Zelinsky reaction. Synthesis of acid chlorides, esters and amides. Reduction of carboxylic acids. Mechanism of decarboxylation. Methods of formation and chemical reactions of halo acids. Hydroxy acids; malic, tartaric and citric acids. Methods of formation and chemical reactions of unsaturated monocarboxylic acids. Dicarboxylic acids: methods of formation and effect of heat and dehydrating agents.
- VII Carboxylic Acid Derivatives** **3 Hrs**
Structure and nomenclature of acid chlorides, esters, amides (urea) and acid anhydrides. Relative stability of acyl derivatives. Physical properties, interconversion of acid derivatives by nucleophilic acyl substitution. Preparation of carboxylic acid derivatives, chemical reactions. Mechanisms of esterification and hydrolysis (acidic and basic).
- VIII Organic Compounds of Nitrogen** **12 Hrs**
Preparation of nitroalkanes and nitroarenes. Chemical reactions of nitroalkanes. Mechanisms of nucleophilic substitution in nitroarenes and their reductions in acidic neutral and alkaline media. Picric acid. Halonitroarenes; reactivity, Structure and nomenclature of amines, physical properties stereochemistry of amines. Separation of a mixture of primary, secondary and tertiary amines. Structural features effecting basicity of amines. Amine salts as phase-transfer catalysts. Preparation of alkyl and aryl amines (reduction of nitro compounds, nitriles) reductive amination of aldehydic and ketonic compounds. Gabriel-

phthalimide reaction. Hofmann bromamide reaction. Reactions of amines, electrophilic aromatic substitution in aryl amines, reactions of amines with nitrous acid. Synthetic transformations of aryl diazonium salts, azo coupling.

Paper - III

Physical Chemistry

60 Hrs (2 Hrs/week),
Max. Marks: 50

- I Thermodynamics-I 12 Hrs**
- Definition of thermodynamic terms: system, surroundings etc. Types of systems, intensive and extensive properties. State and path functions and their differentials. Thermodynamic process. Concept of heat and work. First Law of Thermodynamics statement, definition of internal energy and enthalpy. Heat capacity, heat capacities at constant volume and pressure and their relationship. Joule's law-Joule-Thomson coefficient and inversion temperature. Calculation of w.q. dU & dH for the expansion of ideal gases under isothermal and adiabatic conditions for reversible process. Thermochemistry: standard state, standard enthalpy of formation. Hess's Law of heat summation and its applications. Heat of reaction at constant pressure and at constant volume. Enthalpy of neutralization. Bond dissociation energy and its calculation from thermo-chemical data, temperature dependence of enthalpy. Kirchhoff's equation.
- II Thermodynamics-II 13 Hrs**
- Second law of thermodynamics: need for the law, different statements of the law, Carnot cycle and its efficiency, Carnot theorem. Thermodynamic scale of temperature. Concept of entropy, entropy as a state function, entropy as a function of V & T , entropy as a function of P & T , entropy change in physical change. Clausius inequality. Entropy as a criteria of spontaneity and equilibrium. Entropy change in ideal gases and mixing of gases.

Third law of thermodynamics: Nernst heat theorem, statement and concept of residual entropy, evaluation of absolute entropy from heat capacity data Gibbs and Helmholtz functions: Gibbs function (G) and Helmholtz function (A) as thermodynamic quantities A & G as criteria for thermodynamic equilibrium and spontaneity, their advantage over entropy change. Variation of G and A with P, V and T

III. Chemical Equilibrium **5 Hrs**

Equilibrium constant and free energy. Thermodynamic derivation of law of mass action Le-chatelier's principle. Reaction isotherm and reaction isochore-Clapeyron equation and Clausius-Clapeyron equation, applications.

IV Phase Equilibrium **10 Hrs**

Statement and meaning of the terms – phase, component and degree of freedom, derivation of Gibbs phase rule, phase equilibria of one component system – water CO₂ and S Systems. Phase equilibria of two component system-solid-liquid equilibria, simple eutectic-Bi-Cd, Pb-Ag systems, desilverisation of lead.

Solid solutions- compound formation with congruent melting point (Mg-Zn) and incongruent melting point, (NaCl-H₂O), (FeCl₃-H₂O) and CuSO₄-H₂O) system, Freezing mixtures, acetone-dry ice

Liquid-liquid mixtures-ideal liquid mixtures, Raoult's and Henry's law non-ideal system-azeotropes-HCl-H₂O and ethanol-water systems. Partially miscible liquids – Phenol-water, trimethylamine-water, nicotine-water systems Lower and upper consolute temperature. Effect of impurity on consolute temperature. Immiscible liquids, steam distillation.

Nernst distribution law-thermodynamic derivation, applications.

V Electrochemistry-I**10 Hrs**

Electrical transport – conduction in metals and in electrolyte solutions, specific conductance and equivalent conductance, measurement of equivalent conductance, variation of equivalent and specific conductance with dilution. Migration of ions and Kohlrausch law, Arrhenius theory of electrolyte dissociation and its limitations, weak and strong electrolytes, Ostwald's dilution law its uses and limitations Debye-Huckel-Onsager's equation for strong electrolytes (elementary treatment only) Transport number, definition and determination by Hittorf method and moving boundary method. Applications of conductivity measurements: determination of degree of dissociation, determination of K_a of acids, determination of solubility product of a sparingly soluble salt, conductometric titrations.

VI Electrochemistry-II**10 Hrs.**

Types of reversible electrodes – gas-metal ion, metal-metal ion, metal-insoluble salt-anion and redox electrodes. Electrode reactions, Nernst equation, derivation of cell E.M.F. and single electrode potential, standard hydrogen electrode-reference electrodes-standard electrode potential, sign conventions, electrochemical series and its significance. Electrolytic and Galvanic cells – reversible and irreversible cells, conventional representation of electrochemical cells. EMF of a cell and its measurements. Computation of cell EMF. Calculation of thermodynamic quantities of cell reactions (ΔG , ΔH and K). polarization, over potential and hydrogen overvoltage. Concentration cell with and without transport, liquid junction potential, application of concentration cells, valency of ions, solubility product and activity coefficient potentiometric titrations.

Definition of pH and pK_a determination of pH using hydrogen, quinhydrone and glass electrodes, by potentiometric methods.

Buffers – mechanism of buffer action, Henderson-Hasselbalch equation.

Hydrolysis of salts Corrosion-types, theories and methods of combating it.

Laboratory Course

60 Hrs (2 Hrs/week),
Max. Marks: 50

- I Inorganic quantitative analysis : gravimetric estimation of Ba^{2+} , Zn^{++} , Fe^{3+} , Ni^{2+} and Cu^{2+} .
- II Inorganic synthesis cuprous chloride, potash alum, chrome alum, ferrous oxalate, ferrous ammonium sulphate, tetramine copper (II) sulphate and hexamine nickel (II) chloride.
- III Organic qualitative analysis: identification of organic compounds including calibration of thermometer, determination of mixed melting point, crystallization and decolourization.

Students are expected to perform all the above exercises. One exercise each out of gravimetric estimation, inorganic synthesis and identification of organic compound shall be given in the examination.

Distribution of marks will be as follows:

(i)	*Gravimetric estimation	15
(ii)	Inorganic synthesis	08
(iii)	Identification of organic compounds	14
(iv)	**Viva-voce	05
(v)	Annual record	08

* Full credit of marks shall be given upto 0.5% error after which for each 0.1% error, 02 marks should be deducted.

** Viva-voce for ex-students shall carry 13 marks.

Note:

1. The annual work of the candidate evaluated periodically should be carefully assessed. A total of minimum 16 exercises are expected be carried out during the session to get full credit of marks in the

annual record if, however, the total number of experiments done is less than 16 each experiment done shall be evaluated for half mark. A record of the same should be maintained in the department/college, as an official record.

2. Less than zero mark should not be awarded.
3. The total number of candidates to be examined per batch in the practical shall not be more than 60.

B.Sc. Part - III
Paper I
Inorganic Chemistry

60 Hrs (2 Hrs/week),
Max. Marks: 50

- I Hard and Soft Acids and Bases (HSAB) 7 Hrs**
Classification of acids and bases as hard and soft. Pearson's HSAB concept, acid-base strength and hardness and softness. Symbiosis, theoretical basis of hardness and softness, electronegativity and hardness and softness.
- II Metal-ligand Bonding in Transition Metal Complexes 10 Hrs.**
Limitations of valence bond theory, an elementary idea of crystal-field theory, crystal field splitting in octahedral, tetrahedral and square planar complexes, factors affecting the crystal-field parameters.
- III Magnetic Properties of Transition Metal Complexes 7 Hrs**
Types of magnetic behaviour, methods of determining magnetic susceptibility, spin-only formula. L-S coupling, correlation of μ_s and μ_{eff} values, orbital contribution to magnetic moments, application of magnetic moment data for 3d-metal complexes.
- IV Electron Spectra of Transition Metal Complexes 7 Hrs**
Types of electronic transitions, selection rules for d-d transitions, spectroscopic ground states, spectrochemical series, Orgel-energy level diagram for d^1 and d^9 states, discussion of the electronic spectrum of $[\text{Ti}(\text{H}_2\text{O})_6]^{3+}$ complex ion.

V Thermodynamic and Kinetic Aspect of Metal Complexes 5Hrs

A brief outline of thermodynamic stability of metal complexes and factors affecting the stability, substitution reactions of square planar complexes.

VI Organometallic Chemistry 10 Hrs

Definition, nomenclature and classification of organometallic compounds, Preparation, properties, bonding and applications of alkyls and aryls of Li, Al, Hg, Sn and Ti, a brief account of metal-ethylenic complexes and homogeneous hydrogenation, mononuclear carbonyl is and the nature of bonding in metal carbonyls.

VII Bioinorganic Chemistry 10 Hrs

Essential and trace elements in biological processes, metalloporphyrins with special reference to haemoglobin and myoglobin. Biological role of alkali and alkaline earth metal ions with special reference to Ca^{2+} . Nitrogen fixation.

VII Silicones and Phosphazenes 4 Hrs

Silicones and phosphazenes as examples of inorganic polymers, nature of bonding in triphosphazenes.

Paper II

Organic Chemistry

60 Hrs (2 Hrs/week),
Max. Marks: 50

- I Spectroscopy 10 Hrs**
Nuclear magnetic resonance (NMR) spectroscopy
Proton magnetic resonance (¹H NMR) spectroscopy, nuclear shielding and deshielding, chemical shift and molecular structure, spin-spin splitting and coupling constants, areas of signals, interpretation of PMR spectra of simple organic molecules such as ethyl bromide, ethanol, acetaldehyde, 1,1,2-tribromoethane, ethyl acetate, toluene and acetophenone. Problems pertaining to the structure elucidation of simple organic compounds using UV, IR and PMR spectroscopic techniques.
- II Organometallic Compounds 4 Hrs**
Organomagnesium compounds; the Grignard reagents-formation, structure and chemical reactions. Organozinc compound: formation and chemical reactions. Organolithium compounds: formation and chemical reactions.
- III Organosulphur Compounds 4 Hrs**
Nomenclature, structural features, Methods of formation and chemical reactions of thiols, thioethers, sulphonic acids, sulphonamides and sulphaguanidine.
- IV Heterocyclic Compounds 8 Hrs**
Introduction: Molecular orbital picture and aromatic characteristics of pyrrole, furan, thiophene and pyridine. Methods of synthesis and chemical reactions with particular emphasis on the mechanism of electrophilic substitution. Mechanism of nucleophilic

substitution reactions in pyridine derivatives. Comparison of basicity of pyridine, piperidine and pyrrole. Introduction to condensed five and six- membered heterocycles. Preparation and reactions of indole, quinoline and isoquinoline with special reference to Fisher indole synthesis, Skraup synthesis and Bischler-Napieralski synthesis. Mechanism of electrophilic substitution reactions of indole, quinoline and isoquinoline.

V Organic Synthesis Via Enolates 6Hrs

Acidity of α -hydrogens, alkylation of diethyl malonate and ethyl acetoacetate. Synthesis of ethyl acetoacetate: the Claisen condensation. Keto-enol tautomerism of ethyl acetoacetate. Alkylation of 1,3-dithianes. Alkylation and acylation of enamines

VI Carbohydrates 8 Hrs.

Classification and nomenclature. Monosaccharides, mechanism of osazone formation, interconversion of glucose and fructose, chain lengthening and chain shortening of aldoses. Configuration of monosaccharides. Erythro and threo diastereomers. Conversion of glucose into mannose. Formation of glycosides, ethers and esters, Determination of ring size of monosaccharides. Cyclic structure of D(+)-glucose. Mechanism of Mutarotation. Structures of ribose and deoxyribose. An introduction to disaccharides (maltose, sucrose and lactose) and polysaccharides (starch and cellulose) without involving structure determination.

VII Amino Acids, Peptides, Proteins and Nucleic Acids 6 Hrs

Classification, structure and stereochemistry of amino acids. Acid-base behavior, isoelectric point and electrophoresis. Preparation and reactions of α -amino acids. Structure and nomenclature of peptides and proteins. Classification of proteins. Peptide structure determination, end group analysis, selective hydrolysis of peptides.

Classical peptide synthesis, solid-phase peptide synthesis. Structures of peptides and proteins. Levels of protein structure. Protein denaturation/renaturation. Nucleic acids: introduction. Constituents of nucleic acids. Ribonucleosides and ribonucleotides. The double helical structure of DNA.

VIII Fats, Oils and Detergents

2 Hrs

Natural fats, edible and industrial oils of vegetable origin, common fatty acids, glycerides, hydrogenation of unsaturated oils. Saponification value, iodine value, acid value. Soaps, synthetic detergents, alkyl and aryl sulphonates.

IX Synthetic Polymes

4 Hrs.

Addition or chain-growth polymerization, Free radical vinyl polymerization, ionic inyl polymenzation Ziegler-Natta polymerization and vinyl polymers. Condensation or step growth polymerization. Polyesters, polyamides, phenol formaldehyde resins, urea formaldehyde resins, epoxy resins and polyurethanes. Natural and synthetic rubbers.

X Synthetic Dyes

8 Hrs

Colour and constitution (electronic concept). Classification of dyes. Chemistry and synthesis of Methyl orange, Congo red, Malachite green, Crystal Violet, phenolphthalein, Fluorescein, Alizarin and Indigo.

Paper III

Physical Chemistry

60 Hrs (2 Hrs/week),
Max. Marks: 50

I Elementary Quantum Mechanics

20 Hrs

Black-body radiation, Planck's radiation law, photoelectric effect, heat capacity of solids, Bohr's model of hydrogen atom (no derivation) and its defects, Compton effect. De Broglie hypothesis, the Heisenberg's uncertainty principle, Sinusoidal wave equation, Hamiltonian operator, Schrodinger wave equation and its importance, physical interpretation of the wave function, postulates of quantum mechanics, particle in a one dimensional box.

Schrodinger wave equation for H-atom, separation into three equations (without derivation), quantum numbers and their importance, hydrogen like wave functions, radial wave functions, angular wave functions.

Molecular orbital theory, basic ideas – criteria for forming M.O. from A.O. construction of M.O's by LCAO – H_2^* ion, calculation of energy levels from wave functions, physical picture of bonding and antibonding wave functions, concept of $\sigma, \sigma^*, \pi, \pi^*$ orbitals and their characteristics. Hybrid orbitals – sp, sp^2 sp^3 , calculation of coefficients of A.O.'s used in these hybrid orbitals.

Introduction to valence bond model of H_2 , comparison of M.O. and V.B. models.

II Spectroscopy

20Hrs

Introduction: electromagnetic radiation, regions of the spectrum, basic features of different spectrometers, statement of the Born-oppenheimer approximation, degrees of freedom.

Rotational Spectrum

Diatomic molecules. Energy levels of a rigid rotor (semi-classical principles), selection rules, spectral intensity, distribution using population distribution (Maxwell-Boltzmann distribution) determination of bond length, qualitative description of non-rigid rotor, isotope effect.

Vibrational Spectrum

Infrared spectrum: Energy levels of simple harmonic oscillator, selection rules, pure vibrational spectrum, intensity, determination of force constant and qualitative relation of force constant and bond energies, effect of anharmonic motion and isotope on the spectrum, idea of vibrational frequencies of different functional groups. Raman Spectrum: Concept of polarizability, pure vibrational and pure vibrational - Raman spectra of diatomic molecules, selection rules.

Electronic Spectrum

Concept of potential energy curves for bonding and antibonding molecular orbitals, qualitative description of selection rules and Franck-Condon principle. Qualitative description of σ , π - and n M.O., their energy levels and the respective transitions.

III Photochemistry

8 Hrs.

Interaction of radiation with matter, difference between thermal and photochemical processes. Laws of photochemistry: Grothus – Drapper law, Stark – Einstein law, Jablonski diagram depicting various processes occurring in the excited state, qualitative description of fluorescence, phosphorescence, non-radiative processes (internal conversion, intersystem crossing), quantum yield, photosensitized reactions – energy transfer processes (simple examples).

IV Physical Properties and Molecular Structure 5 Hrs

Optical activity, polarization – (Clausius- Mossotti equation), orientation of dipoles in an electric field, dipole moment, induced dipole moment, measurement of dipole moment-temperature method and refractivity method, dipole moment and structure of molecules, magnetic properties-paramagnetism, diamagnetism and ferromagnetics.

V Solutions, Dilute Solutions and Colligative Properties 7 Hrs

Ideal and non-ideal solutions, methods of expressing concentrations of solutions, activity and activity coefficient.

Dilute solution, colligative properties, Raoult's law, relative lowering of vapour pressure molecular weight determination.

Osmosis, law of osmotic pressure and its measurement, determination of molecular weight from osmotic pressure.

Elevation of boiling point and depression of freezing point,

Thermodynamic derivation of relation between molecular weight and elevation in boiling point and depression in freezing point.

Experimental methods for determining various colligative properties. Abnormal molar mass, degree of dissociation and association of solutes.

Laboratory Course

60 Hrs (2 Hrs/week),
Max. Marks: 50

- I Organic qualitative : Organic binary mixture
(separable by $\text{H}_2\text{O}/\text{NaHCO}_3$)
- II. Organic synthesis involving nitration halogenation, acetylation, sulphonation, oxidation etc.
- III. Physical experiments: Transition temperature, phase equilibria, thermochemistry and electrochemistry.
- IV. Demonstrative chromatographic experiments:
Paper and thin-layer chromatography and analytical separation of amino acids/carbohydrates/fatty acids (may be performed in groups).

Students are expected to perform all the above exercises. One exercise each out of organic binary mixture analysis organic synthesis and physical experiments shall be given in the examination.

Distribution of marks shall be as follows:

i) Organic qualitative analysis (Binary mixture)	17
ii) Organic synthesis	10
iii) Physical experiment	10
iv) * Viva-Voce	05
v) Annual record	08

* Viva-voce for ex-students shall carry 13 marks.

Note:

1. The annual work of the candidate evaluated periodically should be carefully assessed. A total of minimum 16 exercises are

expected to be carried out during the session to get full credit of marks in the annual record. If, however, the total number of experiments done is less than 16, each experiment done shall be evaluated for half mark. A record of the same should be maintained in the department/college as an official record.

2. Less than zero mark should not be awarded.
3. The total number of candidates to be examined per batch in the practical shall not be more than 60.

Books Suggested (Theory Courses)

1. Basic inorganic chemistry, F.A. Cotton, G. Wilkinson and P.L. Gaus, Wiley.
2. Concise Inorganic Chemistry, J.D. Lee, ELBS
3. Concepts of Models of Inorganic Chemistry B. Douglas, D. McDaniel and J. Alexander, John Wiley.
4. Inorganic Chemistry, D.E. Shrive, P.W. Atkins and C.H. Langford, Oxford
5. Inorganic Chemistry, W.W. Porterfield Addison-Wesley
6. Inorganic Chemistry, A.G. Sharpe, ELBS
7. Inorganic Chemistry, Morrison and Boyd, Prentice-Hall.
8. Organic Chemistry, Morrison and Boyd, Prentice-Hall.
9. Organic Chemistry, L.G. Wade Jr. Prentice-Hall.
10. Fundamentals of Organic Chemistry, Solomons, John Wiley
11. Organic Chemistry vol. I, II & III. S.M. Mukherji, S.P. Singh and R.P. Kapoor wiley Eastern Ltd. (New Age International).
12. Organic Chemistry F.A. Carey, McGraw-Hill, Inc.
13. Introduction to Organic Chemistry Streitwieser, Headcock and Kosover, Macmillan.
14. Physical Chemistry G.M. Barrow International Student Edition, McGraw Hill.
15. Basic Programming with Application, V.K. Jain, Tata McGraw Hill.
16. Computers and Common Sense, R. Hunt and Shelly, Prentice Hall.
17. University General Chemistry, C.N.R. Rao Macmillan.
18. Physical Chemistry, R.A. Alberty Wiley Eastern Ltd.
19. The Elements of Physical Chemistry, P.W. Atkins, Oxford.

20. Physical Chemistry through problems, S.K. Dogra and S. Dogra, Wiley Eastern Ltd.

Books Suggested (Laboratory Courses)

1. Vogel's qualitative inorganic analysis, revised, Svehla, Orient Longman.
2. Vogel's Textbook of quantitative inorganic analysis (revised), J. Bassett, R.C. Denney, G.H. Jeffery and J.
3. Standard Methods of Chemical Analysis, W.W. Scott. The Technical Press.
4. Experimental inorganic Chemistry. W.G. Palmer, Cambridge.
5. Handbook of Preparative Inorganic Chemistry. Vol I&II, Brauer, Academic Press.
6. Inorganic Synthesis, McGraw Hill.
7. Experimental Organic Chemistry Vol I&II, P.R. Singh, D.S. Gupta and K.S. Bajpai, Tata McGraw Hill.
8. Laboratory Manual in Organic Chemistry, R.K. Bansal, Wiley Eastern.
9. Vogel's Textbook of Practical Organic Chemistry, B.S. Furniss, A.J. Hannaford, V. Rogers, P.W.G. Smith and A.R. Tatchell. ELBS
10. Experiments in General Chemistry, C.N.R. Rao and U.C. Agarwal, East-West Press.
11. Experiments in Physical Chemistry, R.C. Das and B. Behra, Tata McGraw Hill.

12. Advanced Practical Physical Chemistry J.B. Yadav, Goel Publishing House.
13. Advanced Experimental Chemistry, Vol-I Physical, J.N. Guru and R.Kapoor, S. Chand & Co.
14. Selected Experiments in Physical Chemistry, N.G. Mukherjee. J.N. Ghose & Sons.
15. Experiments in Physical Chemistry, J.C. Ghosh. Bharati Bhavan

M.Sc Ist Year
Paper. I
Inorganic Chemistry

120 Hrs (4 Hrs/week)

Max. Marks = 100

I Stereochemistry and Bonding in Main Group Compounds. 12Hrs

VSEPR, Walsh diagrams (tri- and penta- atomic molecules) $d_{\pi} - p_{\pi}$ bonds, bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules.

II Metal- Ligand Equilibria in Solution 8 Hrs

Stepwise and overall formation constants and their interaction, trends in stepwise constants, factors affecting the stability of metal complexes with references to the nature of metal ion and ligand, chelate effect and its thermodynamic origin, determination of binary formation constants by pH- metry and spectrophotometry.

III Reaction Mechanism of Transition Metal Complexes 24 Hrs

Energy profile of a reaction, reactivity of metal complexes, inert and labile complexes, kinetic application of valence bond and crystal field theories, kinetics of octahedral substitution, acid hydrolysis factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidences in favour of conjugate mechanism, anation reactions, reactions without metal lig and bond cleavage. Substitution reactions in square planer complexes, the trans effect, mechanism of the substitution reaction. Redox reaction, electron transfer reactions, outer-sphere type reactions, cross reactions and Marcus- Hush theory, inner sphere type reactions

- IV Metal- Ligand Bonding** **15 Hrs**
Limitation of crystal field theory, molecular orbital theory, octahedral, tetrahedral and square planer complexes, π -bonding and molecular orbital theory.
- V Electronic Spectra and Magnetic Properties of Transition Metal Complexes** **24 Hrs**
Spectroscopic ground states, correlation, Orgel and Tanabe- Sugano diagrams for transition metal complexes (d^1 - d^9 states), calculation of Dq , B and β parameters, charge transfer spectra, spectroscopic method of assignment of absolute configuration in optically active metal chelates and their stereochemical information, anomalous magnetic moments, magnetic exchange coupling and spin crossover.
- VI Metal π - Complexes** **18 Hrs**
Metal carbonyls, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls; preparation, bonding structure and important reactions of transition metal nitrosyl, dinitrogen and dioxygen complexes; tertiary phosphine as ligand.
- VII Metal Clusters** **15Hrs**
Higher boranes, carboranes, metalloboranes and metallocarboranes. Metal carbonyl and halide clusters, compounds with metal- metal multiple bonds.
- VII Isopoly and Heteropoly Acids and Salts** **4 Hrs**

Books Suggested

1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
2. Inorganic chemistry, J.E. Huhey, Harpes & Row.
3. chemistry of the Elements N.N. Greenwood and A. Earnshow, Pergamon

4. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
5. Magnetochemistry, R.L.Carlin, Springer Verlag.
6. Comprehensive Coordination Chemistry eds, G. Wilkinson, R.D.Gillers and J.A. McCleverty, Pergamon.

Paper- II

Organic Chemistry

120 Hrs (4 Hrs/week)

Max. Marks = 100

- I Nature of Bonding in Organic Molecules 10 Hrs**
- Delocalized chemical bonding - conjugation, cross conjugation, resonance, hyperconjugation, bonding in fullerenes tautomerism.
- Aromaticity in benzenoid and non-benzenoid compounds alternant and non-alternant hydrocarbons. Huckel's rule, homo-aromaticity, energy level of π - molecular orbitals, annulences, anti-aromaticity, Ψ -aromaticity, home-aromaticity PMO approach Bonds weaker than covalent-addition compounds, crown ether complexes and cryptands, inclusion compounds, cyclodextrins, catenanes and rotaxanes.
- II Stereochemistry 15 Hrs**
- Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity, conformation of sugars, steric strain due to unavoidable crowding . Elements of symmetry, chirality, molecules with more than one chiral center, threo and erythro isomers, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis. Asymmetric synthesis. Optical activity in the absence of chiral carbon (biphenyls, allens and spiranes), chirality due to helical shape.
- Stereochemistry of the compounds containing nitrogen, sulphur and phosphorus.
- III Reaction Mechanism: Structure and Reactivity 12 Hrs**
- Types of mechanism, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle. Potential energy diagrams, transition states

and intermediates, methods of determining mechanism, isotope effects. Hard and soft acids and bases.

Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes. Effect of structure on reactivity-resonance and field effects, steric effect, quantitative treatment. The Hammett equation and linear free energy relationship, substituent and reaction constants. Taft equation.

IV Aliphatic Nucleophilic Substitution 15 Hrs

The S_N2 , S_N1 , mixed S_N1 and S_N2 and SET mechanisms.

The neighbouring group mechanism, neighbouring group participation by π and σ bonds, anchimeric assistance. Classical and nonclassical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements. Application of NMR spectroscopy in the detection of carbocations. The S_N1 mechanism. Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon.

Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis and ultrasound, ambident nucleophile, regioselectivity.

V Aliphatic Electrophilic Substitution 5 Hrs

Bimolecular mechanisms- S_E2 and S_{Ei} . The S_{E1} mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity.

VI Aromatic Electrophilic Substitution 6 Hrs

The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles. Diazonium coupling, Vilsmeier reaction, Gattermann-Koch reaction.

- VII Aromatic Nucleophilic Substitution 5 Hrs**
The S_{NAr} , S_N1 benzyne and $S_{RN}1$ mechanisms. Reactivity- effect of substrate structure, leaving group and attacking nucleophile. The von Richer, sommelet- Hauser and Smiles rearrangements.
- VIII Free Radical Reactions 8 Hrs**
Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. Reactivity in the attacking radicals. The effect of solvents on reactivity.
Allylic halogenation (NBS) oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction. Free radical rearrangement. Hunsdiecker reaction.
- IX Addition to Carbon- Carbon Multiple Bonds 7 Hrs**
Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemoselectivity, orientation and reactivity. Addition to cyclopropane ring. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration, Michael reaction. Sharpless asymmetric epoxidation.
- X Addition to Carbon- Hetero Multiple Bonds 12 Hrs**
Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds. Wittig reaction.
Mechanism of condensation reactions involving enolates- Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions, Hydrolysis of esters and amides, ammonolysis of esters.
- XI Elimination Reactions 5 Hrs**

The E2, E1 and E1_cB mechanisms and their spectrum. Orientation of the double bond. Reactivity- effects of substrate structures, attacking base, the leaving group and the medium . Mechanism and orientation in pyrolytic elimination.

XII Pericyclic Reactions

20 Hrs

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward- Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions- conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems. Cycloadditions- antarafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3 dipolar cycloadditions and cheletropic reactions. Sigmatropic rearrangements- suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 3,3- and 5,5 – sigmatropic rearrangements, Claisen, Cope and aza-Cope rearrangements. Fluxional tautomerism, Ene reaction.

Books Suggested

1. Advanced Organic Chemistry- Reactions, Mechanism and Structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Plenum.
3. A Guide Book to Mechanism in Organic chemistry, Peter Sykes, Longman.
4. Structure and Mechanism in Organic Chemistry. C.K. Ingold, Cornell University Press
5. Organic Chemistry, R.T. Morrison and R.N. Boyd, Prentice- Hall
6. Modern Organic Reactions, H.O. House, Benjamin.

7. Principles of Organic Synthesis, R.O.C Norman and J.M.Coxon, Blackie Academic & Professional .
8. Pericyclic Reactions, S.M. Mukherji, Mecomilan, India.
9. Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh, Macmillan.
10. Stereochemistry of Organic compounds, D. Nasipuri, New Age International.
11. Stereochemistry of Organic Compounds, P.S.Kalsi, New Age International.

Paper - III

Physical Chemistry

120 Hrs (4 Hrs/week)

Max. Marks = 100

- I Quantum Chemistry** **30 Hrs**
- A Introduction to Exact Quantum Mechanical Results**
The Schrodinger equation and the postulates of quantum mechanics. Discussion of solutions of the Schrodinger equation to some model systems viz, particle in a box the harmonic oscillator, the rigid rotor, the hydrogen atom.
- B Approximate Methods**
The variation theorem, linear variation principle, perturbation theory (first order and non-degenerate). Applications of variation method and perturbation theory to the Helium atom.
- C Angular Momentum**
Ordinary angular momentum, generalized angular momentum, eigenfunctions for angular momentum, eigenvalues of angular momentum, operator using ladder operators, addition of angular momenta, spin, antisymmetry and pauli exclusion principle.
- D Electronic Structure of Atoms**
Electronic configuration, Russell- Saunders terms and coupling schemes, Slater- Condon parameters, term separation energies of the p^n configuration, term separation energies for the d^n configurations, magnetic effects: spin- Orbit coupling and Zeeman splitting. Introduction to the methods of self-consistent field, the virial theorem.

E Molecular Orbital Theory

Huckel theory of conjugated systems, bond order and charge density calculations. Applications to ethylene, butadiene, cyclopropenyl radical, cyclobutadiene etc. Introduction to extended Huckel theory

II Thermodynamics 30 Hrs.

A Classical Thermodynamics

Brief resume of concepts of laws of thermodynamics, free energy, chemical potential and entropies. Partial molar properties; partial molar free energy, partial molar volume and partial molar heat content and their significances. Determinations of these quantities. Concept of fugacity and determination of fugacity.

Non-ideal systems: Excess functions for non-ideal solutions. Activity coefficient, Debye-Huckel theory for activity coefficient of electrolytic solutions; determination of activity and activity coefficients; ionic strength. Application of phase rule to three component systems; second order phase transitions.

B Statistical Thermodynamics

Concept of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging Canonical, grand canonical and microcanonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers).

Partition functions- translational, rotational, vibrational and electronic partition functions, calculations of thermodynamic properties in terms of partition functions. Application of partition functions. Heat capacity behaviour of solids- chemical equilibria and equilibrium constant in terms of partition functions, Fermi-Dirac statistics, distribution law and applications to metal Bose-Einstein statistics- distribution law and application to helium.

C Non Equilibrium Thermodynamics

Thermodynamic criteria for non-equilibrium states, entropy production and entropy flow, entropy balance equations for different irreversible processes (e.g., heat flow, chemical reaction etc) transformations of the generalized fluxes and forces, non equilibrium stationary states, phenomenological equations, microscopic reversibility and Onsager's reciprocity relations, electrokinetic phenomena, diffusion, electric conduction, irreversible thermodynamics for biological systems, coupled reactions.

III Chemical Dynamics

20 Hrs

Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation and the activated complex theory; ionic reactions, kinetic salt effects, steady state kinetics, kinetic and thermodynamic control of reactions, treatment of unimolecular reactions.

Dynamic chain (hydrogen-bromine reaction, prolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogen-bromine and hydrogen-chlorine reactions) and oscillatory reactions (Belousav-Zhabotinsky reaction), homogeneous catalysis kinetics of enzyme reactions, general features of fast reactions, study of fast reactions by flow method, relaxations method, flash photolysis and the nuclear magnetic resonance method. Dynamic of molecular motions, probing the transition state, dynamics of barrierless chemical reactions in solution, dynamics of unimolecular reactions (Lindemann- Hinshelwood and Rice-Ramsperger- Kassel- Marcus (RRKM) theories of unimolecular reactions)

IV Surface Chemistry

20 Hrs

A. Adsorption

Surface tension, capillary action, pressure differences across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, estimation of surface area (BET equation) Surface films on liquids (Electro- kinetic phenomenon), catalytic activity at surfaces.

B Micelles

Surface active agents, classification of surface active agents, micellization, hydrophobic, interaction, critical miceller concentration (CMC), factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization- phase separation and mass action models, solubilization, micro emulsion, reverse micelles.

C Macromolecules

Polymer- definition, types of polymers, electrically conducting, fire resistant, liquid crystal polymers, kinetics of polymerization, mechanism of polymerization. Molecular mass, number and mass average molecular mass, molecular mass determination (osmometry, viscometry, diffusion and light scattering methods), sedimentation, chain configuration of macromolecules, calculation of average dimensions of various chain structures.

V Electrochemistry

20 Hrs

Electrochemistry of solutions, Debye-Huckel- Onsager treatment and its extension, ion solvent interactions. Debye-Huckel-Jerum mode. Thermodynamics of electrified interface equations. Derivation of electro-capillarity, Lippmann equations (surface excess), methods of determination. Structure of electrified interfaces. Guoy- Chapman, Stern, Graham-Devenathan- Mottwatts, Tobin, Bockris, Devanathan models.

Over potentials, exchange current density, derivation of Butler- Volmer equation, Tafel plot. Quantum aspects of charge transfer at electrodes- solution interfaces, quantization of charge transfer, tunneling. Semiconductor interfaces- theory of double layer at semiconductor, electrolyte solution interfaces, structure of double layer interfaces. Effect of light at semiconductor solution interface.

Electrocatalysis- influence of various parameters, Hydrogen electrode.

Bioelectrochemistry, threshold membrane phenomena, Nernst- Planck equation, Hodges- Huxley equations, core conductor models electrocardiography. Polarography theory, Ilkovic equation; half wave potential and its significance. Introduction to corrosion, homogenous theory, forms of corrosion, corrosion monitoring and prevention methods.

Books Suggested

1. Physical Chemistry, P.W . Atkins, ELBS.
2. Introduction to Quantum Chemistry, A.K. Chandra. Tata McGraw Hill.
3. Quantum Chemistry, Ira N. Levine, Perntice Hall.
4. Coulson's Valence, R. McWeeny, ELBS
5. Chemical Kinetics, K.L. Laidier, Mcgraw- Hill.
6. Kinetics and Mechanism of Chemical Transformation, J. Rajaraman and J.Kuriacose, McMillian.
7. Micelies, Theoretical and Applied Aspects, V. Morol, Plenum.
8. Modern Electrochemistry Vol. I and II. J.O.M Bockris and A.K.N. Reddy, Plenum.
9. Introduction to Polymer Science, V.R. Gowarikar, N.V.Vishwanthan and J. Sridhar, Wiley Eastern.

Paper - IV

120 Hrs (4 Hrs/week)

Max. Marks = 100

a. Group Theory, spectroscopy and Diffraction Methods. MM. = 75

I Symmetry and Group Theory in Chemistry 12 Hrs

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

II Unifying Principles 10 Hrs

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

III Microwave Spectroscopy 3 Hrs

Classification of molecules, rigid rotor model, effect of isotopic substitution on the transition frequencies, intensities, non-rigid rotor. Stark effect, nuclear and electron spin interaction and effect of external field. Applications.

IV Vibrational Spectroscopy 12 Hrs

A Infrared 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 Oppenheimer approximation; vibrations of polyatomic molecules. Selection rules, normal modes of vibration, group frequencies, overtones, hot bands, factors affecting the band positions and intensities, far IR region, metal-ligand vibrations, normal co-ordinate analysis.

B Raman Spectroscopy

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

V Electronic Spectroscopy

12 Hrs

A. Atomic Spectroscopy

Energies of atomic orbitals, vector representation of moments and vector coupling spectra of hydrogen atom and alkali metal atoms.

B. Molecular Spectroscopy

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

C Photoelectron Spectroscopy

Basic principles; photo-electronic effect, ionization process, Koopmans's theorem. Photoelectron Spectra of simple molecules, ESCA, chemical information from ESCA.

Auger electron spectroscopy- basis idea.

- VI Magnetic Resonance Spectroscopy** **20 Hrs**
- A Nuclear Magnetic Resonance Spectroscopy**
- Nuclear spin, nuclear resonance, shielding of magnetic nuclei, chemical shift and its measurements, factors influencing chemical shift, deshielding spin-spin interactions, factors influencing coupling constant 'J' Classification (ABX, AMX, ABC, A₂B₂ etc.) spin decoupling basic ideas about instrument, NMR studies of nuclei other than proton- ¹³C, ¹⁹F and ³¹P. FT NMR advantage of FT NMR use of NMR in medical diagnostics.
- B Electron Spin Resonance Spectroscopy**
- Basic principles, Zero field splitting and kramer's degeneracy, factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densities and McConnell relationship, measurement techniques, applications.
- C Nuclear Quadrupole Resonance Spectroscopy**
- Quadrupole nuclei, quadrupole moments, electric field gradient, coupling constant, splittings. Applications.
- VII Photoacoustic Spectroscopy** **3 Hrs**
- Basic principles of photoacoustic spectroscopy (PAS). PAS-gases and condensed systems, chemical and surface application.
- VIII X-ray Diffraction** **12 Hrs**
- Bragg condition, Miller indices, Laue method, Bragg method, Debye-Scherrer method of X-ray structural analysis of crystals, index reflections, identifications of unit cells from systematic absence in diffraction pattern, Structure of simple lattices and x-ray intensities, structure factor its relation to intensity and electron density, phase problem, Description of the procedure for an X-ray structure analysis, absolute configuration of molecules, Ramchandran diagram.

- IX Electron Diffraction** **3 Hrs**
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.
- X Neutron Diffraction** **3 Hrs**
Scattering of neutrons by solids and liquids, magnetic scattering, measurements techniques . Elucidation of structure of magnetically ordered unit cell.

Books suggested

1. Modern Spectroscopy, J.M.Hollas, John Wiley.
2. Applied Electron Spectroscopy for Chemical Analysis Ed. H.Windalwl and F.L.Ho.Wiley Insterscience.
3. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V.Parish, Ellis Harwood.;
4. Physical Methods in Chemistry, R.S. Drago, Saunders College.
5. Chemical Applications of Group Theory, F.A.Cotton.
6. Introduction to Molecular Spectroscopy, G.M. Barrow. McGraw Hill.
7. Basic principles of spectroscopy, R.Chang. McGarw Hill.
8. Theory and Applications of UV Spectroscopy, H.H. Jaffe and M.Orchin, IBH-Oxford.
9. Introduction to Photoelectron Spectroscopy, P.K.Ghosh, John Wiley.
- 10.Introduction to Magnetic Resonance, A, Carrington and A.D. Maclachalan, Harper & Row.

(b) Mathematics for Chemists

30 Hrs(1 Hrs/week)

M.M. = 25

For Students without mathematics in B.Sc

I	Vectors and Matrix Algebra	10 Hrs
A	Vectors	
	Vectors, dot, cross and triple products etc. The gradient, divergence and curl. Vector calculus, Gauss' theorem, divergence theorem etc.	
B	Matrix Algebra	
	Addition and multiplication, inverse, adjoint and transpose of matrices, special matrices (Symmetric, Skew-symmetric, Hermitian, Skew-Hermitian, unit, diagonal, unitary etc.) and their properties. Matrix equation : Homogeneous, non-homogeneous linear equations and conditions for the solution, linear dependence and independence.	
	Introduction to vector spaces matrix eigenvalues and eigenvectors, diagonalization, determinants (examples from Huckel theory).	
	Introduction to tensors; polarizability and magnetic susceptibility as examples.	
II	Differential Calculus	10 Hrs
	Functions, continuity and differentiability, rules for differentiation application of differential calculus including maxima and minima (examples related to maximally populated rotational energy levels, Bohr's radius and most probable velocity from Maxwell's distribution etc.) exact and inexact differentials with their applications to thermodynamic properties.	
	Integral calculus, basic rules for integration, integration by parts, partial fraction and substitution, Reduction formulae, applications of integral calculus.	

Functions of several variables, partial differentiation, co- ordinate transformations (e.g. Cartesian to spherical polar), curve sketching.

III Elementary Differential Equations 7 Hrs

Variables-separable and exact first-order differential equations, homogeneous, exact and linear equations. Applications to chemical kinetics, Secular equilibria, Quantum chemistry etc. Solutions of differential equations by the power series method, Fourier Series, solutions of harmonic oscillator and Legendre equation etc. spherical harmonics, second order differential equations and their solutions.

IV Permutation and probability 3 Hrs

Permutation and combinations, probability and probability theorems, probability curves, average, root mean square and most probable errors, examples form the kinetic theory of gases etc.) with a general polynomial fit.

Books Suggested

1. The chemistry Mathematics Book, E. Steiner, Oxford University press.
2. Mathematics for Chemistry, Doggett and Sucliffe, Longman.
3. Mathematical Preparation for Physical Chemistry, F, Daniels, McGraw Hill.
4. Chemical Mathematics, D.M. Hirst, Longman.
5. Applied Mathematics for Physical Chemistry, J.R. Barrante, Prentice Hall.
6. Basic Mathematics for Chemists , Tebbutt, Wiley.

(b) Biology for Chemists

30 Hrs(1 Hrs/week)

M.M. = 25

For Students without biology in B.Sc

- I Cell structure and Functions 10 Hrs**
Structure of prokaryotic and eukaryotic cells, intracellular organelles and their functions, comparison of plant and animal cells. Overview of metabolic processes – catabolism and anabolism. ATP – the biological energy currency. Origin of life – unique properties of carbon, chemical evolution and rise of living systems. Introduction to biomolecules, building blocks of bio-macromolecules.
- II Carbohydrate 8 Hrs**
Conformation of monosaccharides, structure and functions of important derivatives of monosaccharides like glycosides, deoxy sugars, myoinositol, amino sugars. N-acetylmuramic acid, sialic acid, disaccharides and polysaccharides. Structural polysaccharides – cellulose and chitin. Storage polysaccharides – starch and glycogen.
Structure and biological functions of glycosaminoglycans or mucopolysaccharides. Carbohydrates of glycoproteins and glycolipids. Role of sugars in biological recognition. Carbohydrate metabolism. Ascorbic acid.
Carbohydrate metabolism – Kreb's cycle, glycolysis, glycogenesis and glycogenolysis, gluconeogenesis, pentose phosphate pathway.
- III Lipids 6 Hrs**
Fatty acids, essential fatty acids, structure and function of triacylglycerols, glycerophospholipids, sphingolipids, cholesterol, bile acids, prostaglandins. Lipoproteins – composition and function, role in atherosclerosis.

Properties of lipid aggregates-micelles, bilayers, liposomes and their possible biological membranes, Fluid mosaic model of membrane structure, Lipid metabolism - β - oxidation of fatty acids.

IV Amino-acids, Peptides and Proteins 6 Hrs

Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing. Secondary structure of proteins, forces responsible for holding of secondary structures. α - helix, β - sheets, super secondary structure, triple helix structure of collagen. Tertiary structure of protein-folding and domain structure. Quaternary structure.

Amino acid metabolism – degradation and biosynthesis of amino acids, sequence determination: chemical/enzymatic/mass spectral, racemization. detection. Chemistry of oxytocin and tryptophan releasing hormone (TRH).

V Nucleic Acids 5 Hrs

Purine and pyrimidine bases of nucleic acids, base pairing via H-bonding. Structure of ribonucleic acids (RNA) and deoxyribonucleic acids (DNA), double helix model DNA and forces responsible for holding it. Chemical and enzymatic hydrolysis of nucleic acids. The chemical basis for heredity, an overview of replication of DNA, transcription, translation and genetic code. Chemical synthesis of mono and trinucleoside.

Books Suggested

1. Principles of Biochemistry, A.L. Lehninger, Worth Publishers.
2. Biochemistry, L.Stryer, W.H.Freeman.
3. Biochemistry, J.David Rawn, Neil Ratterson.
4. Biochemistry, Voet and Voet, John Wiley.

Laboratory course

200 Hrs (18 Hrs/week)

Max. Marks = 200

Practical Examinations will be of 18 Hrs. spread in 3 days. Students should be familiar with elementary operations in laboratory such as cleaning drying and uses of glassware, weighing volume measurement, heating, refluxing, extraction, distillation (simple, steam, vacuum) and crystallization.

Inorganic Chemistry

Qualitative and Quantitative Analysis

- (a) Qualitative analysis of mixtures containing not more than six radicals including (i) Rare-earth elements (ii) Anions, which have not been done in under graduate practical (iii) Insoluble.
- (b) Qualitative Analysis of mixtures of metal ion involving Volumetric (by complexometric titration using masking and demasking agents) and gravimetric analysis.

Chromatography

Separation of cations and anions by

- (a) Paper Chromatography
- (b) Column Chromatography – ion exchange.

Preparations

Preparation of selected inorganic compounds and their studies by I.R. electronic spectra, Mossbauer, E.S.R. and magnetic susceptibility measurements.

Handling of air and moisture sensitive compounds

- (1) $\text{VO}(\text{acac})_2$
- (2) $\text{TiO}(\text{C}_9\text{H}_8\text{NO})_2 \cdot \text{H}_2\text{O}$
- (3) $\text{cis-K}[\text{Cr}(\text{C}_2\text{O}_4)_2(\text{H}_2\text{O})_2]$
- (4) $\text{Na}[\text{Cr}(\text{NH}_3)_2(\text{SCN})_4]$
- (5) $\text{Mn}(\text{acac})_3$

- (6) $K_3[Fe(C_2O_4)_3]$
(7) Prussian Blue, Turnbull's Blue.
(8) $[Co(NH_3)_6][Co(NO_2)_6]$
(9) cis- $[Co(trine)(NO_2)_2]Cl \cdot H_2O$
(10) $Hg[Co(SCN)_4]$
(11) $[Co(Py)_2Cl_2]$
(12) $[Ni(NH_3)_6]Cl_2$
(13) $Ni(dmgl)_2$
(14) $[Cu(NH_3)_4]SO_4 \cdot H_2O$
(15)

Organic Chemistry

Qualitative Analysis

Separation, purification and identification of compounds of binary mixture (one liquid and one solid) using tlc and column chromatography, chemical tests. IR spectra to be used for functional group identification.

Organic Synthesis

Acetylation: Acetylation of cholesterol and separation of cholesteryl acetate by column chromatography

Oxidation: Adipic acid by chromic acid oxidation of cyclohexanol

Grignard reaction: Synthesis of triphenylmethanol from benzoic acid

Aldol condensation: Dibenzal acetone from benzaldehyde

Sandmeyer reaction: p-Chlorotoluence from p-toludine

Acetoacetic ester Condensation: Synthesis of ethyl-n-butylacetoacetate by A.E.E. condensation.

Cannizzaro reaction: 4-Chlorobenzaldehyde as substrate

Friedel Crafts Reaction: β - Benzoyl propionic acid from succinic anhydride and benzene

Aromatic electrophilic substitutions: Synthesis of p-nitroaniline and p-bromoaniline

The Products may be Characterized by Spectral Techniques

Quantitative Analysis

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

Estimation of amines/phenols using bromate bromide solution/or acetylation method.

Determination of Iodine and Saponification values of an oil sample.

Determination of DO, COD and BOD of water sample

Physical Chemistry

Number of hours for each experiment: 3-4 hours

A list of experiments under different heading is given below. Typical experiments are to be selected from each type.

Error Analysis and Statistical Data Analysis

Errors, types of errors, minimization of errors, error distribution curves, precision, accuracy and combination; statistical treatment for error analysis, student 't' test, null hypothesis, rejection criteria, F & Q test; linear regression analysis, curve fitting.

Calibration of volumetric apparatus, burette, pipette and standard flask.

Adsorption

To study surface tension – concentration relationship for solution (Gibbs equation).

Phase Equilibria

(i) Determination of congruent composition and temperature of a binary system (e.g., diphenylamine-benzophenone system).

- (ii) Determination of glass transition temperature of a given salt (e.g. CaCl_2) conductometrically.
- (iii) To construct the phase diagram for three component system (e.g. chloroform-acetic acid-water).

Chemical Kinetics

- (i) Determination of the effect of (a) Change of temperature (b) Change of concentration of reactants and catalyst and (c) Ionic strength of the media on the velocity constant of hydrolysis of an ester/ionic reactions.
- (ii) Determination of the velocity constant of hydrolysis of an ester/ionic reaction in micellar media.
- (iii) Determination of the rate constant for the oxidation of iodide ions by hydrogen peroxide studying the kinetics as an iodine clock reaction.
- (iv) Flowing clock reaction (Ref: Experiments in Physical Chemistry by Showmaker)
- (v) Determination of the primary salt effect on the kinetics of ionic reactions and testing of the Bronsted relationship (iodide ion is oxidized by persulphate ion)
- (vi) Oscillatory reaction.

Solutions

- (i) Determination of molecular weight of non-volatile and non-electrolyte/electrolyte by cryoscopic method and to determine the activity coefficient of an electrolyte.
- (ii) Determination of the degree of dissociation of weak electrolyte and to study the deviation from ideal behaviour that occurs with a strong electrolyte.

Electrochemistry

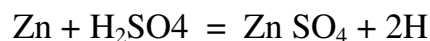
A. Conductometry

- (i) Determination of the velocity constant, order of the reaction and energy of activation for saponification of ethyl acetate by sodium hydroxide conductometrically.
- (ii) Determination of solubility and solubility product of sparingly soluble salts (e.g., PbSO_4), BaSO_4) Conductometrically
- (iii) Determination of the strength of strong and weak acids in a given mixture conductometrically.
- (iv) To study the effect of solvent on the conductance of AgNO_3 /acetic acid and to determine the degree of dissociation and equilibrium constant in different solvents and in their mixtures (DMSO, DMF, dioxane, acetone, water) and to test the validity of Debye-Huckel-Onsager theory.
- (v) Determination of the activity coefficient of zinc ions in the solution of 0.002 M zinc sulphate using Debye Huckel's limiting law.

B. Potentiometry/pH metry

- (i) Determination of strengths of halides in a mixture potentiometrically.
- (ii) Determination of the valency of mercurous ions potentiometrically.
- (iii) Determination of the strength of strong and weak acids in a given mixture using a potentiometer/pH meter.
- (iv) Determination of temperature dependence of EMF of a cell.
- (v) Determination of the formation constant of silver-ammonia complex and stoichiometry of the complex potentiometrically.
- (vi) Acid-base titration in a non-aqueous media using a pH meter.
- (vii) Determination of activity and activity coefficient of electrolytes.
- (viii) Determination of the dissociation constant of acetic acid in DMSO, DMF, acetone and dioxane by titrating it with KOH.

- (xi) Determination of the dissociation constants of monobasic/dibasic acid by Albert-Serjeant method.
- (xii) Determination of thermodynamic constants, G S and H for the reaction by e.m.f. method.



Polarimetry

- (i) Determination of rate constant for hydrolysis/inversion of sugar using a polarimeter.
- (ii) Enzyme kinetics-inversion of sucrose.

Marks distribution for lab. course for M.Sc. Previous as

(a)	Inorganic qualitative analysis (Mixture six radicals)	18 Marks.
	Quantitative analysis (estimation)	20 Marks
	Inorganic preparation	10 Marks
	Chromatorgraphy	10 Marks
(b)	Organic Chemistry : Separation and identification	22 Marks
	Quantitative analysis (estimation)	18 Marks
	Organic Synthesis	12 Marks
(c)	Physical : One Exercise	25 Marks
(d)	Viva :	15 Marks
(e)	Internal assessment (Attendance + Seminar + Record)	50 Marks

Note :

1. **Interanl Assessment** : The students will be assessed three times in an academic year for 10 marks each. It will be based on punctuality, sincerity, attendance, performance in the class and record. The students should deliver at least one seminar and the performance of the seminar will be assessed by department. Over all marks will be based on all the above criteria. The marks obtained by the candidate must be displayed to the students after each assessment and copy must be sent to the registrar

(Exam). The marks of Internal assessment should be informed to the student before the commencement of the examination. In case of Ex-students, marks of internal assessment will remain same as he got as a regular student.

2. Deduct one mark for each wrongly reported ion and deduct 50% marks for not giving confirmatory test for each ion reported.
3. For volumetric/gravimetric exercises full marks up to 0.5% error and deduct one mark for every additional 0.1% error after 0.5% error.
4. Manipulation : Five marks should be deducted.

SYLLABUS STRUCTURE

There should be four papers in all branches i.e., Inorganic, Organic and Physical. The Paper I and II will be compulsory for all branches the additional paper III and IV for respective Branches will be as follows:-

A. Compulsory papers for all the branches

Spectroscopy, Photochemistry and

Solid State Chemistry Paper - I MM-100

Bioinorganic, Bioorganic, Biophysical Chemistry

& Environmental Chemistry Paper-II MM-100

B. Additional Paper for Respective Branches

1. Inorganic Chemistry

Organotransition Metal Chemistry Paper-III MM-50

Bioinorganic and supramolecular Chemistry Paper-III MM-50

Photoinorganic Chemistry Paper-IV MM-50

Analytical Chemistry Paper-IV MM-50

2. Organic Chemistry

Synthesis – I Paper-III MM-50

Synthesis- II Paper-III MM-50

Heterocyclic Chemistry Paper-IV MM-50

Chemistry of Natural Products Paper-IV MM-50

3. Physical Chemistry

Chemistry of Materials Paper-III MM-50

Advance Quantum Chemistry Paper-III MM-50

Liquid State Paper-IV MM-50

Polymers Paper-IV MM-50

M.Sc Final Year

PAPER – I

Max.Marks = 100

(a) Application of spectroscopy

60 Hrs (2 Hrs/week)

Max.Marks= 50

Inorganic Chemistry

I Vibrational Spectroscopy

5 Hrs

Symmetry and shapes of AB₂, AB₃, AB₅, and AB₆, mode of bonding of ambidentate ligands, ethylenediamine and diketronato complexes. Application of resonance Raman spectroscopy particularly for the study of active sites of metalloproteins.

II Electron Spin Resonance Spectroscopy

8 Hrs

Hyperfine coupling, spin polarization for atoms and transition metal ions, spin-orbit coupling and significance of g-tensors, application to transition metal complexes (having one unpaired electron) including biological systems and to inorganic free radicals such as PH₄, F₂ and [BH₃].

III Nuclear Magnetic Resonance of Paramagnetic Substances in Solution

7 Hrs

The contact and pseudo contact shifts, factors affecting nuclear relaxation, some application including biochemical system, an overview of NMR of metal nuclides with emphasis on ¹⁹⁵Pt and ¹¹⁹Sn NMR.

IV Mossbauer Spectroscopy

6 Hrs

Basic principles, spectral parameters and spectrum display. Application of the technique to the studies of (1) bonding and structures of Fe^{+2} and Fe^{-3}

Compounds including those of intermediate spin, (2) Sn^{+2} and Sn^{+4} compounds — nature of M-L bond, coordination number, structure and (3) detection of oxidation state and inequivalent MB atoms.

Organic Chemistry

I Ultraviolet and Visible Spectroscopy

3 Hrs

Various electronic transitions (185-800nm), Beer-Lambert law, effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes, Fieser-Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds. Steric effect in biphenyls.

II Infrared Spectroscopy

5 Hrs

Instrumentation and sample handling. Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance. FT IR. IR of gaseous, solids and polymeric materials.

- III Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD) 3 Hrs**
Definition, deduction of absolute configuration, octant rule for ketones.
- IV Nuclear Magnetic Resonance Spectroscopy 10 Hrs**
General introduction and definition, chemical shift, spin-spin interaction, shielding mechanism, mechanism of measurement, chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides & mercapto). Chemical exchange, effect of deuteration, complex spin-spin interaction between two, three, four and five nuclei (first order spectra), virtual coupling. Stereochemistry, hindered rotation, Karplus curve-variation of coupling constant with dihedral angle. Simplification of complex spectra nuclear magnetic double resonance, contact shift reagents, solvent effects. Fourier transform technique, nuclear Overhauser effect (NOE). Resonance of other nuclei-F, P.
- V Carbon-13 NMR Spectroscopy 5 Hrs**
General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants. Two dimension NMR spectroscopy – COSY, NOESY, DEPT, INEPT, APT and INADEQUATE techniques.
- VI Mass Spectrometry 8 Hrs**
Introduction, ion production – EI, CI, FD and FAB, factors affecting fragmentation, ion analysis ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement, Nitrogen rule. High

resolution mass spectrometry. Examples of mass spectral fragmentation of organic compounds with respect of their structure determination.

Books Suggested

1. Physical Methods for Chemistry, R.S. Drago, Saunders Company.
2. Structural Methods in inorganic Chemistry, E.A.V. Ebsworth, D.W.H. Rankin and S. Cradock, ELBS.
3. Infrared and raman Spectra: Inorganic and Coordination Compounds, K. Nakamoto, Wiley.
4. Progress in inorganic Chemistry vol., 8 ed., F.A. Cotton, vol., 15, ed. S.J. Lippard, Wiley.
5. Transition Metal Chemistry ed. R.L. Carlin vol. 3. Dekker.
6. Inorganic Electronic Spectroscopy, A.P.B. Lever, Elsevier.
7. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Horwood.
8. Practical NMR Spectroscopy, M.L., J.J. Delpuch and G.J. Sassler and T.C. Morrill, John Wiley.
9. Spectrometric Identification of Organic Compounds, R.M. Silverstein, G.C. Bassler and T.C. Morrill, John Wiley.
10. Introduction to NMR Spectroscopy, R.J. Abraham, J. Fisher and P. Loftus. Wiley.
11. Application of Spectroscopy of Organic compounds, J.R. Dyer, Prentice Hall.
12. Spectroscopic Methods in Organic Chemistry, D.H. Williams, I. Fleming. Tata McGraw-Hi

(b) Photochemistry

30 Hrs(1Hrs/week)

Max.Marks=25

I Photochemical Reactions

4 Hrs

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

II Determination of Reaction Mechanism

4 Hrs

Classification, rate constants and life times of reactive energy states – determination of rate constants of reactions. Effect of light intensity on the rate of photochemical reactions. Types of photochemical reactions – photo-dissociation, gas-phase photolysis.

III Photochemistry of Alkenes

6 Hrs

Intramolecular reactions of the olefinic bond – geometrical isomerism, cyclisation reactions, rearrangement of 1, 4- and 1, 5-dienes.

IV Photochemistry of Carbonyl Compounds

8 Hrs

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

Intermolecular cycloaddition reaction – dimerisations and oxetane formation.

V Photochemistry of Aromatic Compounds

4 Hrs

Isomerisations, additions and substitutions.

VI Miscellaneous Photochemical Reactions

4 Hrs

Photo-Fries reaction of anilides. Photo-Fries rearrangement.

Barton reaction. Singlet molecular oxygen reactions, Photochemistry formation of smog. Photodegradation of polymers. Photochemistry of vision.

Books Suggested

1. Fundamentals of Photochemistry, K.K. Rohtagi-Mukherji, Wiley-Eastern
2. Essentials of Molecular Photochemistry, A.Gilbert and J.Baggott, Blackwell Scientific Publication.
3. Molecular Photochemistry, N.J. Turro, W.A. Benjamin.
4. Introductory Photochemistry, A. Cox and T.Camp. McGraw-Hill.
5. Photochemistry, R.P. Kundall and A.Gilbert, Thomson Nelson.
6. Organic Photochemistry, J.Coxon and B.Halton, Cambridge University Press.

(c) Solid State Chemistry

30 Hrs (1 Hrs/week)

Max. Marks = 25

I Solid State Reactions

4 Hrs

General principles, experimental procedures, co-precipitation as a precursor to solid state reactions, kinetics of solid state reactions.

II Crystal Defects and Non-Stoichiometry

6 Hrs

Perfect and imperfect crystals, intrinsic and extrinsic defects – line and plane defects, vacancies-Schottky defects and Frenkel defects. Thermodynamics of Schottky and Frenkel defect formation, colour centres, non-stoichiometry and defects.

III. Electronic Properties and Band Theory

15 Hrs

Metals, insulators and semiconductors, electronic structure of solids-band theory, band structure of metals, insulators and semiconductors. Intrinsic and extrinsic semiconductors, doping semiconductors, p-n junctions, super conductors.

Optical properties – Optical reflectance, photoconduction-photoelectric effects.

Magnetic Properties – Classification of materials: Quantum theory of paramagnetics-cooperative phenomena-magnetic domains, hysteresis.

IV Organic Solids

5 Hrs

Electrically conducting solids, organic charge transfer complex, organic metals, new superconductors.

Book Suggested

1. Solid State Chemistry and its Applications, A.R. West, Plenum.
2. Principles of the Solid State, H.V. Keer, Willey Eastern.
3. Solid State Chemistry, N.B. Hannay.
4. Solid State Chemistry, D.K. Chakrabarty, New Age International.

PAPER- II

120 Hrs (4Hrs/week)
Max. Marks = 100

(a) Bioinorganic Chemistry

30 Hrs (1 Hrs/week)

Max. Marks = 25

I. Metal ions in Biological Systems

Essential and trace metals.

II Na⁺/K⁺ Pump

Role of metals ions in biological processes.

III. Bioenergetics and ATP Cycle

DNA polymerization, glucose storage, metal complexes in transmission of energy; chlorophylls, photosystem I and photosystem II in cleavage of water. Model systems.

IV. Transport and Storage of Dioxygen

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

V. Electron Transfer in Biology

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

VI. Nitrogenase

Biological nitrogen fixation, molybdenum nitrogenase, spectroscopic and other evidence, other nitrogenases model systems.

Books Suggested

1. Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.
2. Bioinorganic Chemistry, I. Berthini, H.B. Gray, S.J. Lippard and J.S. Valentine, University Science Books.
3. Inorganic Biochemistry vols I and II. Ed. G.L. Eichhorn, Elsevier.
4. Progress in Inorganic Chemistry, Vols. 18 and 38 ed. J.J. Lippard, Wiley.

(b) Bioorganic Chemistry

30 Hrs (1 Hrs/week)

Max. Marks = 25

I	Introduction	2 Hrs
	Basic considerations. Proximity effects and molecular adaptation.	
II	Enzymes	6 Hrs
	Introduction and historical perspective, chemical and biological catalysis. Remarkable properties of enzymes like catalytic power, specificity and regulation. Nomenclature and classification, extraction and purification. Fischer's lock and key and Koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site-directed mutagenesis. Enzyme kinetics, Michaelis-Menten and Lineweaver-Burk plots, reversible and irreversible inhibition.	
III	Mechanism of Enzyme Action	3 Hrs
	Transition-state theory, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortion, Example of some typical enzyme mechanisms for chymotrypsin, ribonuclease, lysozyme and carboxypeptidase A.	
IV	Kinds of Reaction Catalysed by Enzymes	6 Hrs
	Nucleophilic displacement on a phosphorus atom. Multiple displacement reaction and the coupling of ATP cleavage to endergonic processes. Transfer of sulphate, Addition and elimination reactions, enolic intermediates in isomerization reaction, β -cleavage and condensation, some isomerization and rearrangement reaction. Enzyme catalyzed carboxylation and decarboxylation.	

V Co-Enzyme Chemistry**4 Hrs**

Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD^+ , NADP^+ , FMN, FAD, lipoic acid, vitamin B_{12} . Mechanisms of reactions catalyzed by the above cofactors.

VI. Enzme Models**4 Hrs**

Host-guest chemistry, chiral recognition and catalysis, molecular recognition, molecular asymmetry and prochirality, Biomimetic chemistry, crown ethers, cryptates. Cyclodextrins, cyclodextrin-based enzyme models, calixarenes, ionophores, micelles, synthetic enzymes or synzymes.

VII Biotechnological Applications of Enzymes**5 Hrs**

Large-scale production and purification of enzymes, techniques and methods of immobilization of enzymes, effect of immobilization on enzyme activity, application of immobilized enzymes, use of enzymes in food and drink industry-brewing and cheese-making, syrups from corn starch, enzymes as targets for drug design. Clinical uses of enzymes, enzyme therapy, enzymes and recombinant DNA technology.

Books Suggested

1. Bioorganic Chemistry: A Chemical Approach to Enzyme Action. Hermann Dugas and C. Penny, Springer Verlag.
2. Understanding Enzymes, Trevor Palmer, Prentice Hall.

3. Enzyme Chemistry: Impact And Applications, Ed. Collin J Suckling. Chapman and Hall.
4. Enzyme Mechanisms Ed, M.I. Page and A. Williams, Royal Society of Chemistry.
5. Fundamentals of Enzymology, N.C. Price and L. Stevens, Oxford University Press.
6. Immobilized Enzymes: An Introduction and Applications in Biotechnology, Michael D. Trevan, John Wiley.
7. Enzymatic Reaction Mechanisms. C. Walsh. W.H. Freeman.
8. Enzyme Structure and Mechanism, A. Fersht, W.H. Freeman.
9. Biochemistry: The Chemical Reaction of Living Cells, D.E. Metzler, Academic Press.

(c) Biophysical Chemistry

30 Hrs (1 Hrs/week)

Max.Marks = 25

- I Biological Cell and its Constituents** **2 Hrs**
Biological cell, structure and functions of proteins, enzymes, DNA and RNA in living systems. Helix coil transition.
- II Bioenergetics** **3 Hrs**
Standard free energy change in biochemical reactions, exergonic, endergonic. Hydrolysis of ATP, synthesis of ATP from ADP.
- III. Statistical Mechanics in Biopolymers** **5 Hrs**
Chain configuration of macromolecules, statistical distribution end to end dimensions, calculation of average dimension for various chain structures. Polypeptide and protein structures, introduction to protein folding problem.
- IV. Biopolymer Interactions** **5 Hrs**
Forces involved in biopolymer interactions. Electrostatic charges and molecular expansion, hydrophobic forces, dispersion force interactions. Multiple equilibria and various types of binding processes in biological systems. Hydrogen ion titration curves.

- V Thermodynamics of Biopolymer Solutions 4 Hrs**
Thermodynamics of biopolymer solutions, osmotic pressure, membrane equilibrium, muscular contraction and energy generation in mechanochemical system.
- VI Cell Membrane and Transport of Ions 3 Hrs**
Structure and function of cell membrane, ion transport through cell membrane, irreversible thermodynamic treatment of membrane transport. Nerve conduction.
- VII Biopolymers and their Molecular Weights 5 Hrs**
Evaluation of size, shape, molecular weight and extent of hydration of biopolymers by various experimental techniques. Sedimentation equilibrium, hydrodynamic methods, diffusion, sedimentation velocity, viscosity, electrophoresis and rotational motions.
- VIII Diffraction Methods 3 Hrs**
Light scattering, low angle X-ray scattering, X-ray diffraction and photo correlation spectroscopy. ORD.

Books Suggested

1. Principles of Biochemistry, A.L.L Lehninger, Worth Publishers.
2. Biochemistry, L.Stryer, W.H.Freeman.
3. Biochemistry, J David Rawn, Neil Patterson.
4. Biochemistry, Voet and Voet, John Wiley.
5. Outlines of Biochemistry, E.E. Conn and P.K. Stumpf, John Wiley.
6. Bioorganic Chemistry: A Chemical Approach to Enzyme Action, H. Dugas and C. Penny, Springer-Verlag.
7. Macromolecules: Structure and Function. F.Wold, Prentice Hall.

(d) Environment Chemistry

30 Hrs (1 Hrs/week)

Max. Marks= 25

I	Environment	8 Hrs
	Introduction. Composition of atmosphere, vertical temperature, heat budget of the earth atmospheric system, vertical stability atmosphere. Biogeochemical cycles of C, N, P, S and O Biodistribution of elements.	
II	Hydrosphere	12 Hrs
	Chemical composition of water bodies-lakes, streams. Rivers and wet lands etc. Hydrological cycle. Aquatic pollution – inorganic, organic pesticide, agricultural industrial and sewage, detergents, oil spills and oil pollutants. Water quality parameters – dissolved oxygen, biochemical oxygen demand, solids, metals, content of chloride, sulphate, phosphate, nitrate and micro-organisms Analytical methods for measuring BOD, DO, COD, F, Oils, metals (As, Cd, Cr, Hg, Pb, Se etc.), residual chloride and chlorine demand. Purification and treatment of water.	
III	Industrial Pollution	10 Hrs
	Cement, sugar, distillery, drug, paper and pulp, thermal power plants, nuclear power plants, metallurgy. Polymers, drugs etc. Radionuclide analysis. Disposal of wastes and their management.	

Books Suggested

Environmental Chemistry, S.E. Manahan, Lewis Publishers.

Environmental Chemistry, Sharma & Kaur, Krishna Publishers.

Environmental Chemistry, A.K.De. Wiley Eastem.

Environmental Chemistry, S.M.Khopka, Wiley Eastern

Standard Method of Chemical Analysis, F.J. Welcher Vol. III. Van Nostrand
Reinhold Co.

Environmental Toxicology, Ed. J. Rose, Gordon and Breach Science
Publication.

Elemental Analysis of Airbone Particles, Ed. S. Landsberger and M.
Creatchman, Gordon and Breach Science Publication.

Environmental Chemistry, C. Baird, W.H. Freeman.

Additional papers
For Inorganic Chemistry Branch
PAPER-III

120 Hrs (4 Hrs/week)
Max. Marks= 100

(a) Organotransition Metal Chemistry **60 Hrs(2 Hrs/week)**

Max. Marks= 50

I Alkyls and Aryls of Transition Metals **5 Hrs**

Types, routes of synthesis, stability and decomposition pathways, organocopper in organic synthesis.

II Compounds of Transition Metal-Carbon Multiple Bonds **12 Hrs**

Alkylidenes, alkylidynes, low valent carbenes and carbynes- synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions on the ligands, role in organic synthesis

III Transition Metal π - Complexes **18 Hrs**

Transition metal π - complexes with unsaturated organic molecules, alkenes, alkynes, allyl, diene, dienyl, arene and trienyl complexes, preparations, properties, natures, nature of bonding and structural features. Important reactions, relations to nucleophilic and electrophilic attack on ligands and to organic synthesis.

IV Transition Metal Compounds with Bonds to Hydrogen **3 Hrs**

Transition metal compounds with bonds to hydrogen.

V Homogeneous Catalysis**14 Hrs**

Stoichiometric reactions for catalysis, homogeneous catalytic hydrogenation, Zeigler-Natta polymerization of olefins, catalytic reactions involving carbon monoxide such as hydrocarbonylation of olefins (oxo reaction), oxopalladation reaction, activation of C-H bond.

VI Fluxional Organometallic Compounds**8 Hrs**

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

Books Suggested

1. Principles and Application of Organotransition Metal Chemistry, J.P. Collman, L.S. Hegsdus, J.R. Norton and R.G. Finke, University Science Books.
2. The Organometallic Chemistry of the Transition Metals, R.H. Crabtree. John Wiley.
3. Metallo-organic Chemistry, A.J. Pearson, Wiley.
4. Organometallic Chemistry, R.C. Mehrotra and A. Singh, New Age International.

(b) Bioinorganic and Supramolecular Chemistry

**60 Hrs(2 Hrs/week)
Max. Marks= 50**

- | | | |
|------------|---|---------------|
| I | Metal Storage Transport and Biomineralization | 5 Hrs |
| | Ferritin, transferrin, and siderophores | |
| II | Calcium in Biology | 6 Hrs |
| | Calcium in living cells, transport and regulation, molecular aspects of intramolecular processes, extracellular binding proteins. | |
| III | Metalloenzymes | 20 Hrs |
| | Zinc enzymes – carboxypeptidase and carbonic anhydrase. Iron enzymes – catalase, peroxidase and cytochrome P-450. Copper enzymes – superoxide dismutase. Molybdenum oxotransferase enzymes – xanthine oxidase. Cofactor vitamin B ₁₂ . | |
| IV | Metal – Nucleic Acid Interactions | 6 Hrs |
| | Metal ions and metal complex interactions. Metal complexes – nucleic acids | |
| V | Metals in Medicine | 5 Hrs |
| | Metal deficiency and disease, toxic effects of metals, metals used for diagnosis and chemotherapy with particular reference to anticancer drugs. | |

VI Supramolecular Chemistry

18 Hrs

Concepts and language.

- (A) Molecular recognition : Molecular receptors for different types of molecules including arisonic substrates, design and synthesis of coreceptor and multiple recognition.
 - (B) Supramolecular reactivity and catalysis.
 - (C) Transport processes and carrier design.
 - (D) Supramolecular devices. Supramolecular photochemistry, supramolecular electronic, ionic and switching devices.
- Some example of self-assembly in supramolecular chemistry.

Books Suggested

1. Principles of Bioinorgainc Chemistry, S.J.Lippard and J.M. Berg, University Books.
2. Bioinorganic Chemistry, I.Bertini, H.B. Gray, S.J.Lippard and J.S. Valentine, University Science Books.
3. Inorganic Biochemistry vols I and II. Ed. G.L. Eichhorn, Elsevier.
4. Progress in Inorganic Chemistry, Vols 18 and 38 ed. J.J. Lippard, Wiley
5. Supramolecular Chemistry, J.M. Lehn, VCH.

PAPER-IV

120 Hrs (4 Hrs/week)

Max. Marks = 100

(a) Photoinorganic chemistry

60 Hrs. (2 Hrs/Week)

Max.Marks = 50

- I Basics of Photochemistry** **10 Hrs**
Absorption, excitation, photochemical laws, quantum yield, electronically excited states life times-measurements of the times. Flash photolysis, stopped flow techniques. Energy dissipation by radiative and non-radiative processes, absorption spectra, Franck-Condon principle, photochemical stages-primary and secondary processes.
- II Properties of Excited States** **10 Hrs**
Structure, dipole moment, acid-base strengths, reactivity. Photochemical kinetics-calculation of rates of radiative processes. Bimolecular deactivation – quenching.
- III Excited States of Metal Complexes** **8 Hrs**
Excited states of metal complexes: comparison with organic compounds, electronically excited states of metal complexes, charge-transfer spectra, charge transfer excitations methods for obtaining charge-transfer spectra.

- IV Ligand Field Photochemistry 8 Hrs**
Photosubstitution, photooxidation and photoreduction, lability and selectivity, zero vibrational levels of ground state and excited state, energy content of excited state, zero-zero spectroscopic energy, development of the equations for redox potentials of the excited states.
- V Redox Reactions by Excited Metal Complexes 16 Hrs**
Energy transfer under conditions of weak interaction and strong interaction-exciplex formation; conditions of the excited states to be useful as redox reactants, excited electron transfer, metal complexes as attractive candidates (2,2'-bipyridine and 1, 10-phenanthroline complexes), illustration of reducing and oxidizing character of Ruthenium²⁺ (bipyridal complex, comparison with Fe(bipy)₃; role of orbit coupling-life time of these complexes. Application of redox processes of electronically excited states for catalytic purposes, transformation of low energy reactants into high energy products, chemical energy into light.
- VI Metal Complex Sensitizers 8 Hrs**
Metal complex sensitizer, electron relay, metal colloid systems, semiconductor supported metal or oxide systems, water photolysis, nitrogen fixation and carbon dioxide reduction.

Books Suggested

1. Concepts of Inorganic Photochemistry, A.W.Adamson and P.D. Fleischauer, Wiley.
2. Inorganic Photochemistry. J. Chem. Educ., vol. 60, no. 10, 1983.
3. Progress in Inorganic Chemistry, vol. 30 ed. S.J.Lippard. Wiley.
4. Coordination Chem. Revs., vol. 39, 121, 131; 1975, 15, 321; 1990, 97, 313.

5. Photochemistry of Coordination Compounds, V. Balzari and V. Carassiti, Academic Press.
6. Elements of Inorganic Photochemistry, G.J.Ferraudi, Wiley.

(b) ANALYTICAL CHEMISTRY

60 Hrs (2 Hrs/week)
Max. Marks. 50

- I Introduction 10 Hrs**
- Role of analytical chemistry. Classification of analytical methods-classical and instrumental. Types of instrumental analysis. Selecting an analytical method. Neatness and cleanliness. Laboratory operations and practices. Analytical balance. Techniques of weighing, errors. Volumetric glassware-cleaning and calibration of glassware. Sample preparations – dissolution and decompositions. Gravimetric techniques. Selecting and handling of reagents. Laboratory notebooks. Safety in the analytical laboratory.
- II Errors and Evaluation 7 Hrs**
- Definition of terms in mean and median. Precision-standard deviation, relative standard deviation. Accuracy-absolute error, relative error. Types of error in experimental data-determinate (systematic), indeterminate (or random) and gross. Sources of errors and the effects upon the analytical results. Methods for reporting analytical data. Statistical evaluation of data-indeterminate errors. The uses of statistics.
- III Food Analysis 12 Hrs**
- Moisture, ash, crude protein, fat, crude fibre, carbonhydrates, calcium, potassium, sodium and phosphate. Food adulteration-common adulterants in food, contamination of food stuffs. Microscopic examination of foods for adulterants. Pesticide analysis in food products. Extraction and purification of sample. HPLC. Gas chromatography for

organophosphates. Thin-layer chromatography for identification of chlorinated pesticides in food products.

IV Analysis of Water Pollution 12 Hrs

Origin of waste water, pollutants and their effects. Sources of water pollution domestic, industrial, agricultural soil and radioactive wastes as sources of pollution. Objectives of analysis-parameter for analysis-colour, turbidity, total solids, conductivity, acidity, alkalinity, hardness, chloride, sulphate, fluoride, silica, phosphates and different forms of nitrogen. Heavy metal pollution-public health significance of cadmium, chromium, copper, lead, zinc, manganese. Mercury and arsenic. General survey of instrumental technique for the analysis of heavy metals in aqueous systems. Measurements of DO, BOD and COD. Pesticides as water pollutants and analysis. Water laws and standards.

V Analysis of Soil, Fuel, Body Fluids and Drugs 17 Hrs

- (a) Analysis of soil: moisture, pH, total nitrogen, phosphorus, silica, lime, magnesia, manganese, sulphur and alkali salts.
- (b) Fuel analysis: solid, liquid and gas. Ultimate and proximate analysis-heating values- grading of coal. Liquid fuels-flash point, aniline point, octane number and carbon residue. Gaseous fuels-producer gas and water gas-calorific value.
- (c) Clinical chemistry: Composition of blood-collection and preservation of samples. Clinical analysis. Serum electrolytes, blood glucose, blood urea nitrogen, uric acid, albumin, globulins, barbiturates, acid and alkaline phosphatases. Immunoassay:

principles of radio immunoassay (RIA) and applications. The blood gas analysis trace elements in the body.

(d) Drug analysis: Narcotics and dangerous drugs. Classification of drugs. Screening by gas and thin-layer chromatography and spectrophotometric measurements.

Books Suggested

1. Analytical Chemistry, G.D. Christian, J. Wiley.
2. Fundamentals of Analytical Chemistry, D.A. Skoog, D.M. West and F.J. Holler, W.B. Saunders.
3. Analytical Chemistry-Principles, J.H. Kennedy, W.B. Saunders.
4. Analytical Chemistry-Principles and Techniques, L.G. Hargis, Prentice Hall.
5. Principles of Instrumental Analysis, D.A. Skoog and J.L. Loary, W.B. Saunders.
6. Principles of Instrumental Analysis, D.A. Skoog, W.B. Saunders.
7. Quantitative Analysis, R.A. Day, Jr. and A.L. Underwood, Prentice Hall.
8. Environmental Solution Analysis, S.M. Khopkar, Wiley Eastern.
9. Basic Concepts of Analytical Chemistry, S.M. Khopkar, Wiley Eastern.
10. Handbook of Instrumental Techniques for Analytical Chemistry, F. Settle, Prentice Hall.

Laboratory Course

Max. Marks = 200

Note:- The allotted time for the practical examination will be 15 Hrs. which is to be split in three days.

1. Preparation

60 Marks

Any two Preparations should be given in examination- 30 marks each.

Synthesis of selected inorganic compounds/complexes and their characterization by IR, electronic spectra (UV and visible), NMR, Mossbauer, ESR and magnetic susceptibility etc. measurement. Selection can be made from the following or any other from the existed literature.

- (i) Cis and Trans isomers of $[\text{o}(\text{en})_2\text{Cl}_2]\text{Cl}$.
- (j) Chem. Soc., 1960, 4369
- (ii) Metal acetylacetonates: $\text{Cr}(\text{acac})_3$; Vanadyl acetylacetonate, $\text{Cu}(\text{acac})_2$, H_2O etc.
Inorg. Synth., 1957, 5, 130; 1, 183
- (iii) Ferrocene
J. Chem. Edu. 1966, 43, 73; 1976, 53, 730
- (iv) Cr(III) complexes; $[\text{Cr}(\text{H}_2\text{O})_6] (\text{NO}_3)_3 \cdot 3\text{H}_3\text{H}_{22}\text{O} \cdot 4\text{Cl}_2 \cdot \text{Cl} \cdot 2\text{H}_2\text{O}$
 $[\text{Cr}(\text{en})_3]\text{Cl}_3$
Inorg. Synth., 1972, 13 184
- (v) Tin (IV) IODINE, tin (iv) CHLORIDE, tin (ii) IODIDE
Inorg. Synth. 1953, 4, 19
- (vi) Mixed valence d⁸nuclear complexes of manganese (III, IV).
- (vii) Preparation of triphenyl phosphine and its transition metal complexes.

(viii) Reaction of Cr (III) with multidentate ligand, a kinetic experiment
(visible spectra of Complex)

J. Am. Chem. Soc. 1953, 75. 5670

(ix) Other new synthesis reported in literature

(ix) Bromination of Cr (acac)³

J. Chem. Edu., 1986, 63, 90

(xii) Creative stability of Tin (IV) and Pb (IV), preparation of ammonium hexachlorostannate, (NH₄)₂SnCl₆ and ammonium hexachloro plumbate; (NH₄)₂PbCl₆.

II. Analysis of ores, alloys and inorganic substances by various chemical methods. 60 marks

Any two of the following should be given in examination- 30 marks each

I. Spectrophotometric Determinations

- (a) Manganese/Chromium/vanadium in steel sample
- (b) Nickel/molybdenum/tungsten/vanadium/uranium by extractive spectro photometric method.
- (c) Fluoride/nitrite/phosphate
- (d) Iron-phenanthroline complex: Job's Method of continuous variation
- (e) Zirconium-alizarin Red-S complex: Mole-ratio method.
- (f) Copper-ethylene diamine complex : Slope-ratio method.

II. Flame photometric Determinations

- (a) Sodium and Potassium when present together
- (b) Lithium/Calcium/Barium/Strontium
- (c) Cadmium and magnesium in tap water

III. Nephelometric

- (a) Sulphate
- (b) Phosphate
- (c) Silver

IV. Chromatographic separations: Paper or TLC and determination of R_f values:

- (a) Cadmium and Zinc
- (b) Silver, Lead and mercury
- (c) Nickel, Magnesium, Vanadium and Zinc

Viva **30 Marks**

**Internal Assessment (Attendance
+ Seminar + Record)** **50 Marks**

Note:-

Internal Assessment:- The students will be assessed three times in an academic year for 10 marks each. It will be based on punctuality, sincerity, attendance, performance in the class and record. The students should deliver at least one seminar and the performance of the seminar will be assessed by department. Over all marks will be based on all the above criteria. The marks obtained by the candidate must be displayed to the students after each assessment and copy must be sent to the registrar (Exam.) The marks of Internal assessment should be informed to the student before the commencement of the examination. In case of ex-students marks of internal assessment will remain same as he got as a regular student.

Additional Papers

For Organic Chemistry Branch Paper-III

**120 Hrs (4 Hrs/week)
Max. Marks = 100**

(a) Organic Synthesis- I

60 Hrs. (2 Hrs./week)

M.M. 50

I Organometallic Reagents

25 Hrs

Principle, preparations, properties and application of the following in organic synthesis with mechanistic details

Group I and II metal organic compounds

Li, Mg, Hg, Cd, Zn and Ce compounds

Transition metals

Cu, Pd, Ni, Fe, Co, Rh, Cr and Ti Compounds

Other elements

S, Si, B and I compounds.

II Oxidation

7 Hrs

Introduction. Different oxidative processes.

Hydrocarbons-alkenes, aromatic rings, saturated C-H groups (activated and unactivated). Alcohols, diols, aldehydes, and sulphides.

Amines, hydrazines, and sulphides.

Oxidations with ruthenium tetroxide, iodobenzene diacetate and thallium (III) nitrate.

III Reduction 7 Hrs

Introduction. Different reductive processes.

Hydrocarbons-alkanes, alkenes, alkynes and aromatic rings.

Carbonyl compounds-aldehydes, ketones, acids and their derivatives, Epoxides.

Nitro, nitroso, azo and oxime groups.

Hydrogenolysis.

IV Rearrangements 12 Hrs

General mechanistic considerations – nature of migration, migratory aptitude, memory effects.

A detailed study of the following rearrangements

Pinacol-pinacolone, Wagner-Meerwein-Meerwein, Demjanov, Benzil-Benzilic acid, Favorskii, Arndt-Emmerich synthesis, Neber, Beckmann, Hofmann, Curtius, Schmidt, Baeyer-Villiger, Shapiro reaction.

V Metallocenes, Nonbenzenoid Aromatics and Polycyclic Aromatic Compounds 9 Hrs

General considerations, synthesis and reactions of some representative compounds

Books Suggested

1. Modern Synthetic Reactions, H.O. House, W.A. Benjamin.

2. Some modern Methods of Organic Synthesis, W. Carruthers Univ. Press
3. Advanced Organic Chemistry, Reactions Mechanisms and Structure, J. March, John Wiley.
4. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic & Professional.
5. Advanced Organic Chemistry Part B, F.A. Carey and R.J. Sundberg. Plenum Press.
6. Rodd's Chemistry of Carbon Compounds Ed. S. Coffey, Elsevier.

(b) ORGANIC SYNTHESIS II

60 Hrs (2 Hrs/week)

M.M. = 50

- I Disconnection Approach** **18 Hrs**
An introduction to synthons and synthetic equivalents, disconnection approach, functional group inter-conversions, the importance of the order of events in organic synthesis, one group C-X and two group C-X disconnections, chemoselectivity, reversal of polarity, cyclisation reactions, amine synthesis.
- II Protecting Groups** **5 Hrs**
Principle of protection of alcohol, amine, carbonyl and carboxyl groups.
- III One Group C-C Disconnection** **7 Hrs**
Alcohols and carbonyl compounds, regioselectivity. Alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis.
- IV Two Group C-C Disconnections** **10 Hrs**
Diels-Alder reaction, 1,3-difunctionalised compounds, α, β -unsaturated carbonyl compounds, control in carbonyl condensations, 1,5-difunctionalised compounds. Michael addition and Robinson annelation.
- V Ring Synthesis** **8 Hrs**
Saturated heterocycles, synthesis of 3-, 4-, 5- and 6-membered rings, aromatic heterocycles in organic synthesis.

VI Synthesis of Some Complex Molecules

12 Hrs

Application of the above in the synthesis of following compounds.

Comphor, Longifoline, Cortisone, Reserpine, Vitamin D, Juvabione, Aphidicolin and Fredericamycin A.

Books Suggested

1. Designing Organic Synthesis, S. Warren, Wiley.
2. Organic Synthesis-Concept, Methods and Starting Materials, J.Fuhrhop and G.Penzilin, Verlage VCH.
3. Some Modern Methods of Organic Synthesis. W. Carruthers, Cambridge Univ. Press.
4. Modern Synthetic Reactions, H.O. House, W.A. Benjamin,
5. Advanced Organic Chemistry:Reactions, Mechanisms and Structure, J. March, Wiley.
6. Principles of Organic Synthesis, R.Norman and J.M.Coxon, Blackie Academic & Professional.
7. Advanced Organic Chemistry Part B, F.A. Carey and R.J.Sundberg, Plenum Press.

Paper-IV

120 Hrs (4 Hrs/week)

Max. Marks = 100

(a) Heterocyclic Chemistry

60 Hrs(2 Hrs/Week)

M.M. 50

- I Nomenclature of Heterocycles** **4 Hrs**
Replacement and systematic nomenclature (Hantzsch-Widman system) for monocyclic, fused and bridged heterocycles.
- II Aromatic Heterocycles** **5 Hrs**
General chemical behavior of aromatic heterocycles. Classification (structural type), criteria of aromaticity (bond lengths, ring current and chemical shifts in ^1H NMR-spectra, empirical resonance energy, delocalization energy and Dewar resonance energy, diamagnetic susceptibility exaltations.)
- III Non-aromatic Heterocycles** **6 Hrs**
Strain-bond angle and torsional strains and their consequences in small ring heterocycles
Conformation of six-membered heterocycles with reference to molecular geometry, barrier to ring inversion, pyramidal inversion and 1,3-diaxial interaction.

Stereo-electronic effects – anomeric and related effects. Attractive interactions – hydrogen bonding and intermolecular nucleophilic – electrophilic interactions.

- IV Heterocyclic Synthesis 4 Hrs**
Principles of heterocyclic synthesis involving cyclization reaction and cycloaddition reaction.
- V Small Ring Heterocycles 5 Hrs**
Three-membered and four-membered heterocycles-synthesis and reactions of aziridines, oxiranes, thiranes, azetidines, oxetanes and thietanes.
- VI Benzo-Fused Five-Membered Heterocycles 5 Hrs**
Synthesis and reaction including medicinal applications of benzopyrroles. Benzofurans and benzothiophenes.
- VII Meso-ionic Heterocycles 5 Hrs**
General classification, chemistry of some important meso-ionic heterocycles of type-A and B and their applications.
- VIII Six-Membered Heterocycles with One Heteroatom 6 Hrs**
Synthesis and reaction of pyrylium salts and pyrones and their comparison with pyridinium & thiopyrylium salts and pyridones.

Synthesis and reaction of quinolizinium and benzopyrylium salts, coumarins and chromones.

IX Six-Membered Heterocycles with Two or More Heteroatoms

5 Hrs

Synthesis and reaction of diazines, triazines, tetrazines and thiazines.

X Seven- and Large-Membered Heterocycles

5 Hrs

Synthesis and reaction of azepines, oxepines, thiepinines, diazepines, thiazepines, azocines, diazocines, dioxocines and dithiocines.

XI Heterocyclic Systems Containing P, As Sb and B

10 Hrs

Heterocyclic rings containing phosphorus: introduction, nomenclature, synthesis and characteristics of 5- and 6- membered ring systems- phosphorinanes, phosphorines, phospholanes and phospholes.

Heterocyclic rings containing As and Sb: introduction, synthesis and characteristics of 5- and 6- membered ring systems.

Books Suggested

1. Heterocyclic Chemistry Vol.1-3, R.R. Gupta, M. Kumar and V.Gupta, Springer Verlag.
2. The chemistry of Heterocycles, T. Eicher And S. Hauptmann, Thieme.
3. Heterocyclic Chemistry, J.A. Joule, K. Mills and G.F. Smith, Chapman and Hall.
4. Heterocyclic Chemistry, T.L Gilchrist, Longman Scientific Technical.

5. Contemporary Heterocyclic Chemistry, G.R. Newkome and W.W. Paudler, Wiley-Inter Science.
6. An Introduction to the Heterocyclic Compounds, R.M. Acheson, John Wiley.
7. Comprehensive Heterocyclic Chemistry, A.R. Katritzky and C. W. Rees, eds, Pergamon Press.

(b) Chemistry of Natural Products

60 Hrs(2 Hrs/Week)

M.M. 50

- I Terpenoids and Carotenoids** **15 Hrs**
Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule,
Structure determination stereochemistry, biosynthesis and synthesis of the following representative molecules: Citral, Geraniol, α - Terperneol, Menthol, Farnesol, Zingiberene, Santonin, Phytol, Abietic acid and β - Carotene..
- II Alkaloids** **15 Hrs**
Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring. Role of alkaloids in plants.
- III Steroids** **15 Hrs**
Occurrence, nomenclature, basis skeleton, Diel's hydrocarbon and stereochemistry.
Testosterone, Estrone, Progesterone, Aldosterone.
Biosynthesis of steroids.
- IV Plant Pigments** **7 Hrs**
Occurrence, nomenclature and general methods of structure determination. Isolation and synthesis of Apigenin,

Luteolin, Quercetin, Myrcetin, Quercetin-3glucoside, Vitexin,
Biosynthesis of flavonoids: Acetate pathway and Shikimic acid
pathway.

V Porphyrins 3 Hrs

Structure and synthesis of Haemoglobin and Chlorophyll.

VI Prostaglandins 3 Hrs

Occurrence, nomenclature, Classification, biogenesis and
physiological effects.

VII Pyrethroids and Rotenones 2 Hrs

Synthesis and reaction of Pyrethroids and Rotenones.

(For structure elucidation, emphasis is to be placed on the use of
spectral parameters wherever possible)

Books Suggested

1. Natural Products: Chemistry and Biological Significance, J.Mann.
R.S.Davidson, J.B.Hobbs, D.V. Banthrope and J.B. Harborne.
Longman, Essex.
2. Organic Chemistry, Vol 2, I.L. Finar, EIBS
3. Stereoselective Synthesis: A Practical Approach, M. Nogradi, VCH.
4. Rodd's Chemistry of Carbon Compounds, Ed.S. Coffey, Elsevier.
5. Chemistry, Biological and Pharmacological Properties of Medicinal
Plants from the Americas, Ed.Kurt Hostettmann. M.P. Gupta and A.
Marston. Harwood Academic Publishers.
6. Introduction to Flavonoids, B.A. Bohm, Harwood Academic
Publishers.

7. New Trends in Natural Product: Chemistry, Atta-ur-Rahman and M.I. Choudhary, Harwood Academic Publishers.

Insecticides of Natural Origin, Sukh Dev, Harwood Academic Publishers.

Laboratory Course

Max. Marks = 200

Note : The allotted time for the practical examination will be 15 hrs which is to be split in three days.

1. Qualitative Analysis

40 Marks

Separation, purification and identification of the components of a mixture of three organic compounds (three solids or two liquids and one solid, two solid and one liquid), using TLC for checking and purity of the separated compounds.

2. Multi-Step synthesis or Organic Compounds

30 Marks

The exercise should illustrate the use of organic reagent and may involve purification of the products by chromatographic techniques.

Photochemical reaction

Benzophenon Benzpinacol Benzipinacolone

Backmann rearrangement : Benzanilide from benzene

Benzene Benzophenone benzophenone oxime Benzanilide

Benzilic acid rearrangement : Benzilic acid from benzoin

Benzioc Benzyl Benzilic acid

Synthesis of heterocyclic compounds

Skraup synthesis: Preparation of quinoline from aniline. Fisher-

Indole synthesis: Preparation of 2-phenyl indole from phenylhydrazine.

Enzymatic synthesis : Enzymatic reduction: Reduction of ethyl acetoacetate using Baker's yeast to yield enantiomeric excess of S (+) ethyl-3-hydroxybutanoate and determine its optical purity.

Biosynthesis of ethanol from sucrose.

Synthesis using microwaves

Alkylation of diethyl malonate with benzyl chloride.

Synthesis using phase transfer catalyst.

Alkylation of diethyl malonate or ethylacetoacetate with an alkyl halide.

Any two of the following experiments should be given in the examination – 25 marks each

A. Extraction of Organic Compounds from Natural Sources

1. Isolation of caffeine from tea leaves.
2. Isolation of casein from milk (the students are required to try some typical colour reaction of proteins). 343 U
3. Isolation of lactose from milk (purity of sugar should be checked and R_f value reported).
4. Isolation of nicotine dipicrate from tobacco.
5. Isolation of cinchonine from cinchona bark.
6. Isolation of Piperine from black pepper.
7. Isolation of lycopene from tomatoes
8. Isolation of β -carotene from carrots.
9. Isolation of oleic acid from olive oil (involving the preparation of complex with urea and separation of linoleic acid).
10. Isolation of eugenol from cloves.
11. Isolation of limonene from citrus fruits.

B. Paper Chromatography

Separation and identification of the sugar present in the given mixture of glucose, fructose and sucrose by paper chromatography and determination of R_f values.

C. Spectroscopy

Identification of organic compounds by analysis of their spectral data (UV, IR, PMR, CMR and MS)

D. Spectrophotometric (UV/VIS) Estimations

1. Amino acids
2. Proteins
3. Carbohydrates
4. Cholesterol
5. Ascorbic acid
6. Aspirin
7. Caffeine

Viva

30 Marks

Internal Assessment (Attendance

+ Seminar + Record)

50 Marks

Note:-

Internal Assessment:- The students will be assessed three times in an academic year for 10 marks each. It will be based on punctuality, sincerity, attendance, performance in the class and record. The students should deliver at least one seminar and the performance of the seminar will be assessed by department. Over all marks will be based on all the above criteria. The marks obtained by the candidate must be displayed to the students after each assessment and copy must be sent to the registrar (Exam.) The marks of Internal assessment should be informed to the student before the commencement of the examination. In case of ex-students marks of internal assessment will remain same as he got as a regular student.

ADDITIONAL PAPERS

For Physical Chemistry Branch

Paper III

120 Hrs (4 Hrs/week)

Max. Marks.= 100

(a) Chemistry of Material

60 Hrs. (2 Hrs/week)

M.M. = 50

I. Mulptiephase Materials

Ferrous alloys; Fe-C phase transformation in ferrous alloys; stainless steels, non-ferroys, properties of ferrous and non-ferrous alloys and their applications.

II. Glasses, Ceramics, composites and Nanomaterials

Glassy state, glass formers and glass modifiers, applications. Ceramic structures, mechanical properties, clay products. Refractories, characterization, properties and applications.

Microscopic composites; dispersion-strengthened and particle-reinforced fibre-reinforced composites, macroscopic compsites Nanocrystalline phase, preparation procedures, special properties, applications.

III. Thin Films and Langmuir-Blodgett Films

Preparation techniques; evaporation/sputtering, chemical process, MOCVD, solgel etc. Langmuir-Blodgett (LB) film, growth techniques, photolithography, properties and applications of thin and LB films.

IV. Liquid Crystals

Mesomorphic behaviour liquid crystals, positional order, bond orientational order, nematic and smectic mesophases; smectic-nematic transition and clearing temperature-homeotropic, planar and schlieren textures, twisted nematics, chiral nematics, molecular arrangement in smectic C phase, optical properties of liquid crystals. Dielectric susceptibility and dielectric constants. Lyotropic phase and their description of ordering in liquid crystals.

V. Polymeric materials

Molecular shape, structure and configuration. crystallinity, stress strain behaviour, thermal behaviour, polymer types and their applications conducting and ferro-electric polymers.

VI. Ionic Conductors

Types of ionic conductors, mechanism of ionic conductors, interstitial jumps (Frenkel); vacancy mechanism, diffusion, superionic conductors; phase transitions and mechanism of conduction of superionic conductors, examples and applications of ionic conductors.

VII. High Tc Materials

Defect perovskites, high Tc superconductivity in cuprates, preparation and characterization of 1-2-3 and 2-1-4 materials, normal state properties; anisotropy; temperature dependence of electrical resistance; optical phonon modes, superconducting state; heat capacity; coherence length, elastic constants, position lifetimes, microwave absorption-pairing and multigap structure in high Tc materials, applications of high Tc materials.

VIII. Materials for Solid State Devices

Rectifiers, transistors, capacitors –IV – V compounds low-dimensional quantum structures: optical properties.

IX. Organic Solids, Fullerenes, Molecular Devices

Conducting organics, organic superconductors, magnetism in organic materials. Fullerenes-doped, fullerenes as superconductors.

Memory and switches –sensors.

Nonlinear optical materials: nonlinear optical effects, second and third order-molecular hyperpolarisability and second order electric susceptibility-materials for second and third harmonic generation.

Books Suggested:

1. Solid State Physics, N.W. Ashcroft and N.D. Mermin, Saunders College.
2. Material Science and Engineering, An Introduction, W.D., Callister, Wiley.
3. Principles of the Solid State, H.V. Keer, Wiley Eastern
4. Materials Science, J.C. Anderson, K.D. Leaver, J.M. Alexander and R.D. Rawlings, ELBS.

5. Thermotropic Liquid Crystals, Ed., G.W. Gray, John Wiley.
6. Handbook of Liquid Crystals, Kelker and Hatz, Chemie Verla

(b) ADVANCED QUANTUM CHEMISTRY

60 Hrs (2 Hrs/week)

Max. Marks = 50

- I Theoretical and Computational Treatment of Atoms
And Molecules, Hartree-Fock Theory 12 Hrs**
- Review of the principles of quantum mechanics, Born-Oppenheimer approximation. Slater Condon rules, Hartree-Fock equation, Koopmans and Brillouin theories, Roothan equation, Gaussian basis sets.
- II Configuration Interaction and MC-SCF 12 Hrs**
- Introduction to CI; full and truncated CI theories, size consistency, Introductory treatment of coupled cluster and MC-SCF methods.
- III Semi-Empirical Theories 12 Hrs**
- A review of the Hückel, EHT and PPP treatments, ZDO approximation, detailed treatment of CNDO and INDO theories. A discussion of electronic energies and properties. An introduction to MOPAC and AMI with hands on experience on personal computers.
- IV Density Functional Theory 12 Hrs**
- Derivation of Hohenberg-Kohn theorem. Kohn-Shah formulation, N- and V- representabilities; review of the performance of the existing local (e.g. Slater X α and other method) and non-local functionals, treatment of chemical concepts with the density functional theory.

V Computer Experiments 12 Hrs

Computer experiments using quantum chemistry – software packages such as GAUSSIAN/GAMESS/MOPAC and modeling software e.g.MM2/AMBER/CHARM etc.

Book Suggested

1. Modern Quantum Chemistry, N.S. Ostlund and A. Szabo, McGraw Hill.
2. Methods of Molecular Quantum Mechanics, R. Mcweeny and B.T. Sutcliffe, Academic Press.
3. Density Functional Theory of Atoms and Molecules, R.G. Parr and W. Yang, Oxford.
4. Exploring Chemistry with Electron Structure Methods, J.B. Foresman and E. Frish. Goussian Inc.
5. Semi-empirical MO Theory, J.Pople and D.L.Beveridge.

PAPER –IV

120 Hrs (4Hrs/week)

Max. Marks = 100

(a) Liquid State

60 Hrs (2Hrs/week)

Max. Marks = 50

- I General Properties of Liquids** **13 Hrs**
- a) Liquids as dense gases, liquids as disordered solids, some thermodynamic relations internal pressure and its significance in liquids. Equations of state, critical constants. Different types of intermolecular force in liquids, different potential functions for liquids, additivity of pair potential approximation.
- b) A classical partition function for liquids, correspondence principle, configuration integral, configuration properties.
- II Theory of Liquids** **9 Hrs**
- Theory of liquids partition function method or model approach; single cell models, communal energy and entropy, LTD model, significant structure model.
- III Distribution Function and Related Equations** **14 Hrs**
- Radial distribution function method, equation of state in terms of RDF. Molecular distribution functions, pair distribution function. Relationship between pair distribution function and pair potential function. The IBG equation, the HNC equation, the PY equation, cluster expansion.

IV Methods for Structure Determination and Computational Techniques **12 Hrs**

Spectroscopic techniques for liquid dynamic structure studies.
Neutron and X-ray scattering spectroscopy.
Computation Techniques-Monte Carlo and molecular dynamics methods.

V Supercooled and Ionic Liquids **12 Hrs**

Supercooled and ionic liquids, theories of transport properties; non Arrhenius behaviour of transport properties. Cohen-Turnbull free volume model, configurational entropy model, Macedo-Litovitz hybrid model, glass transition in supercooled liquids.

Books Suggested

1. An Introduction to Liquid State P.A. Egelstaff, Academic Press.
2. The Dynamic Liquids State. A.F.M. Barton, Longman.
3. Introduction to Statistical Thermodynamics. T.L.Hill Addison Wiley.
4. Significant Liquid Structures, H.Eyring and M.S. John.

b) Polymers

60 Hrs (2Hrs/week)

Max. Marks = 50

MM. =

I Basics

8 Hrs

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

II Polymer Characterization

14 Hrs

Polydispersion-average molecular weight concept. Number, weight and viscosity average molecular weights. Polydispersity and molecular weight distribution. The practical significance of molecular weight. Measurement of molecular weight. End-group, viscosity. Light scattering, osmotic and ultracentrifugation methods. Analysis and testing of polymers chemical analysis of polymers. Spectroscopic methods. X-ray diffraction study. Microscopy. Thermal analysis and physical testing-tensile strength. Fatigue, impact. Tear resistance. Hardness and abrasion resistance.

III. Structure and Properties

14 Hrs

Morphology and order in crystalline polymers-configuration of polymer chains. Crystal structures of polymers. Morphology of crystalline polymers, strain-induced morphology, crystallization and melting. Polymer structure and physical properties-crystalline melting

point T_m – melting points of homogeneous series, effect of chain flexibility and other steric factors, entropy and heat of fusion. The glass transition temperature, T_g -Relationship between T_m and T_g . Effects of molecular weight. Diluents, chemical structure, chain topology, branching and cross linking. Property requirements and polymer utilization.

IV Polymer Processing 12 Hrs

Plastic, elastomers and fibres, compounding. Processing techniques: Calendering, die casting, rotational casting, film casting, Injection moulding, blow moulding, extrusion moulding, thermoforming, foaming, reinforcing and fibre spinning.

V Properties of Commercial Polymers 12 Hrs

Polyethylene, polyvinyl chloride. Polyesters, phenolic resins, epoxy resin and silicone polymers. Functional polymers – fire retarding polymers and electrically conducting polymers. Biomedical polymers – contact lens, dental polymers, artificial heart, kidney, skin and blood cells.

Books Suggested

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

Laboratory Course:

Max. Marks. = 200

Note: The allotted time for the practical examination will be 15 hrs, which is to be split in three days. Any three of the following experiments should be given in examination-40 marks each.

1. Verification of the law photochemical equivalence.
2. Order of reaction by
 - (a) Isolation method
 - (b) Half life period method
 - (c) Integration method
3. Temperature coefficient of a reaction
4. Energy of activation of a reaction.
5. Entropy of a reaction.
6. Determination of pH by following methods:
 - (a) Electrical conductivity, (b) E.M.F. (c) Polarography
7. Hydrolysis of the salts by following methods:
 - (a) Cryoscopic (b) Electrical Conductivity (c) E.M.F.
8. Study of complex formation by the following methods and determination of stability constant wherever practicable.
 - (a) Cryoscopic, (b) Electrical Methods, (c) E.M.F.
9. Determination of solubility of sparingly soluble salts by the following methods:
 - (a) Electrical Conductivity (b) E.M.F]
10. Dissociation contents of polybasic acids.
11. Determination of transport number.
12. Determination of liquid junction potential.
13. Determination of the charge on colloidal particle.
14. Polarography

15. Beer's law verification
16. Decomposition of potential determination
17. Validity of Freundlich's adsorption isotherm.
18. Validity of Langmuir's adsorption isotherm.
19. Determination of partial molar volume of solute.
20. Determination of CMC of surfactants.

Viva

30 Marks

Internal Assessment (Attendance

+ Seminar + Record)

50 Marks

Note:-

Internal Assessment:- The students will be assessed three times in an academic year for 10 marks each. It will be based on punctuality, sincerity, attendance, performance in the class and record. The students should deliver at least one seminar and the performance of the seminar will be assessed by department. Over all marks will be based on all the above criteria. The marks obtained by the candidate must be displayed to the students after each assessment and copy must be sent to the registrar (Exam.) The marks of Internal assessment should be informed to the student before the commencement of the examination. In case of ex-students marks of internal assessment will remain same as he got as a regular student.