

M.Sc. Semester - I
Chemistry Paper - II
(Reaction Mechanism-I)

1. Carbocyclic compound - Aromatically in benzenoid and non-benzenoid compounds, alternat and non-alternat hydrocarbons, Huckel's rule, energy level of π -molecular orbitals, annulenes, anti-aromaticity, aromaticity, homo-aromaticity. PMO approach. Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity.

2. Stereochemistry - 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, allenes and spiranes).

3. Reaction Mechanism : Structure and Reactivity- carbenes and nitrenes. Effect of structure on reactivity - resonance and field effects, steric, quantitative treatment, The Hammett equation and linear free energy relationship, substituent and reaction constants, Taft equation.

4. Aliphatic Nucleophilic Substitution- The S_N2 , S_N1 , mixed S_N2 and SET mechanism. S_N1' and S_N2' .

The neighbouring group mechanism, neighbouring group participation by π and σ bonds, anchimeric assistance.

Classical and non-classical carbocations. phenonium ions, norbornyl system, common carbocation rearrangements.

The S_N1 mechanism.

Nucleophilic substitution at an allylic, Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium.

5. Aromatic Electrophilic substitution - The arenium ion mechanism, orientation and reactivity, energy profile diagram, ortho-para, ratio, ipso attack, orientation in other ring system. Vilsmeier, reaction Gattermann Koch reaction.

6. Aromatic nucleophilic substitution - The S_NAr , S_N1 , benzene and SRN_1 mechanism, reactivity, effect of substrate structure, leaving group and attacking nucleophile, The Von-Richter, Sommelet-Hauser and.

M.Sc. Semester - I
Chemistry Paper - II
(Quantum, Thermodynamics,)

I. Quantum Chemistry

(a) **Introduction to Exact Quantum Mechanical Results** : The Schrodinger equation and the postulates of quantum mechanics. Discussion of solution of the Schrodinger equation to some model system viz... particle in a three dimension box, one dimensional 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.

II. Thermodynamics :

(a) **Classical Thermodynamics** : Partial molar properties; partial molar free energy, partial molar volume and partial molar heat content and their significance. Determinations of these quantities. Concept of fugacity and determination of fugacity. Application of phase rule to three component systems, second order phase transition.

(b) **Solutions** : Thermodynamics properties of solution, chemical potential of pure substance, Chemical potential of real gases & fugacity, Chemical potential of ideal gas mixture, Thermodynamic functions of mixing, properties of liquid solutions, chemical potential of non-ideal solution, Excess function of non-ideal

(c) **Non Equilibrium Thermodynamics** : Thermodynamics 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 reactions.

III. Cell Membrane & Transport of ions :

(a) Structure and functions of cell membrane, ion transport through cell membrane, irreversible thermodynamic treatment of membrane transport, Nerve conduction.

M.Sc. Semester - II
Chemistry Paper - I
(Molecular Symmetry & Bioinorganic chemistry)

1. Basics - Symmetry elements and symmetry operations; Point symmetry group, Classification of molecules in point groups.

2. 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 system.

3. Transport and Storage of Dioxygen

I-iron proteins and oxygen uptake, structure and functions of haemoglobin, myoglobin, haemocyanins, hemerythrin, model synthetic complexes of iron, cobalt and copper.

4. Nitrogenase

Biological nitrogen fixation, molybdenum nitrogenase, spectroscopic and other evidences, other nitrogenases model system.

5. Metalloenzymes

Zinc enzyme-carboxypeptidase and carbonic anhydrase. Iron enzymes-catalase, peroxidase and cytochrome P-450. Copper enzyme-superoxide dismutase. Molybdenum oxotransferase and oxidase Co enzyme vitamin B₁₂

6. Electron Transfer in Biology

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

7. Metals in Medicines :

Metal deficiency and disease toxic effects of metals, metals used for diagnosis and chemotherapy with particular reference to anti cancer drugs.

M.Sc. Semester - II
Chemistry Paper - III
(Dynamics, Surface, Electro, Biophysical-II)

1. Chemical Dynamics :

Method 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.

Dynamic chain (hydrogen-bromine reaction, pyrolysis of acetadehyde, decomposition of ethane). photochemical (hydrogen-bromine and hydrogen-chlorine reactions) and oscillatory reactions (Belousov-Zhabotinsky reaction).

II. Surface Chemistry :

(a) Adsorption : Surface tension, capillary action. pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, estimation of surfaces (By BET Equation only) surface films on liquids (Electro-kinetic phenomenon).

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

III. Electrochemistry :

Electrochemistry of solutions. Debye-Huckel-Onsager treatment and its extension. ion solvent interactions. Structure of electrified interface. Guoy-Champman, Stern-theories of electrified surfaces. Electrocatalysis influence of various parameters, Hydrogen electrode. Polarography theory, Ilkovic reaction; half wave potential and its significance, introduction to corrosion, homogenous theory, forms of corrosion, corrosion monitoring and prevention methods.

M.Sc. Semester - III
Chemistry Compulsory Paper - I
(Spectroscopy-II)

1. Magnetic Resonance Spectroscopy :

Nuclear Magnetic Resonance Spectroscopy

Nuclear spin, Nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurements, factors influencing chemical shift deshielding. spin-spin interactions, factors influencing coupling constant J. Classification (ABX, AMX, ABC, A₂B₂ etc.) spin decoupling FT NMR, advantages of FT NMR. Chemical exchange, effect of deuteration, complex spin-spin interaction between two, three, four and five nuclei (first order spectra), virtual coupling. Simplification of complex spectra-magnetic double resonance, contact shift reagents, solvent effects. Fourier transform technique nuclear Overhauser effect (NOE). Stereochemistry Hindered rotation, Karplus curve-variation of coupling constant with Dihedral angle.

II. Carbon -13 NMR Spectroscopy :

General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants.

III. Mass Spectrometry :

Introduction, ion production -EI, CI, FD and FAB factors affecting fragmentation, ion analysis, ion abundance, Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement. Nitrogen rule. High resolution mass spectrometry, Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

IV. Electron Spin Resonance Spectroscopy :

Basic principles, zero field splitting and Kramer's degeneracy, factors affecting the value, isotropic and anisotropic hyperfine coupling constant, spin Hamiltonian, spin densities and McConnell relationship, measurement techniques, applications.

V. Photo Electron Spectroscopy :

Basic principle, photo electric effect, ionization process, Koopman's theorem, Photoelectron Spectra of simple molecule, ESCA, Chemical information from ESCA Auger electron spectroscopy-basic idea.

M.Sc. Semester - III
Chemistry Compulsory Paper - III
(Organic Synthesis-I and Photochemistry)

1. Oxidation :

Introduction, Different oxidative process.

Hydrocarbons-alkenes, aromatic rings, saturated C-H groups (activated and unactivated). Alcohols, diols, aldehydes, ketones, ketals and carboxylic acids.

Anines, hydrazines, and sulphides.

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

II. Reduction :

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.

III. Rearrangements :

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

A detailed study of the following rearrangements.

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

IV. Photochemistry -

(a) Photochemical Reactions :

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

(b) Photochemistry of Alkenes :

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

(c) Photochemistry of Carbonyl compounds :

Intramolecular reactions of carbonyl compounds- Saturated, cyclic and acyclic, β , γ -unsaturated and α , β - unsaturated compounds, cyclohexadienones.

(d) Photochemistry of Aromatic compounds.

Isomerisations, additions and substitutions.

(e) Miscellaneous Photochemical Reactions :

Photo-Fries reactions of anilides, Photo-Fries rearrangement, Barton reaction, Singlet molecular oxygen reactions.

M.Sc. Semester - III
Elective Paper - III A
(Coordination Chemistry)

1. Electronic configuration in multi electron system :

Quantum numbers and vectors, coupling of orbital angular momenta, coupling of spin angular momenta, coupling of spin angular momenta, Spin-orbit coupling, L-S Coupling scheme, i-coupling scheme, relation between electron configurations and terms, hole formation, Hund's rules, Inter electron repulsion parameters, spin-orbit coupling parameters.

2. Molecular orbital theory :

Symmetry consideration for formation of a and its molecular orbitals in Oh, Td, D. complexes, molecular orbital energy level diagrams of Oh, Td, D. Complexes.

3. Term Diagrams :

Effect of weak crystal fields on free ion terms in octahedral, square planar and tetrahedral symmetries, Orgel diagrams, mixing of terms, Transition from weak to strong field and correlations for only d case. Non crossing rule, Tanabe-Sugano diagrams, ligand field theory. spectrochemical and nephelauxetic series.

4. Electronic spectra of complexes :

Selection rules, band intensities, factors influencing band width, effect of temperature, interpretation of spectra of aqueous solution of M (II) spectra of spin free paired MA Jahn Teller distortion and its effect on electronic spectra.

5. Magnetic properties

Magnetic susceptibility - Curie strength, magnetic induction, intensity of magnetization, magnetic moment, diamagnetism, paramagnetism ferromagnetism and anti ferromagnetism.

Sources of paramagnetism (orbital and spin magnetic moment)- thermal energy and magnetic property, magnetic moment for multiplet width large as compared to kT , small as compared to kT and comparable to kT , magnetic properties of Oh, Td, D complexes based on crystal field model, spin cross over, quenching of orbital magnetic moment by crystal field, spin pairing in Oh and non-Oh complexes, spin cross over by inter electronic repulsion, b_9 substitution in ligands, effect of pressure, elucidation of structure of complexes by magnetic nature in tetrahedral cobalt(II) ions, isothiocyanatobis (p-toluidine) cobalt (II), Td & Oh complexes of Ni(II), square planar complexes.

M.Sc. Semester - III
Elective Paper - IV A
(Structural Inorganic Chemistry)

1. Nuclear Magnetic spectroscopy:-

The contact & pseudo Contact shifts, factors affecting nuclear relaxation, some applications including biochemical systems, an overview of NMR of metal nuclides with emphasis on ^{195}Pt and ^{119}Sn NMR.

2. Electron resonance spectroscopy-

Hyperfine coupling spin polarization atoms and transition metal ions, spin-orbital 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 pH_4 , F_2^- and $[\text{BH}_3]$.

3. Mossbaucr spectroscopy :-

Basic Principles, spectral parameters and spectrum display. Application of the technique to studies of (1) bonding and structures of Fe^{+2} and Fe^{+4} compounds including those of intermediate spin, (2) Sn^{+2} and Sn^{+4} compounds - natures of M-L Bond, coordination number, structure and (3) Detection of oxidation state and inequivalent MB atoms.

4. Vibrational Spectroscopy :

Symmetry and shapes of AB_z , AB_3 , AB_4 , AB_5 and AB_6 mode of bonding of ambidentate ligands, etylenediamine and diketonate complexes.

5. Molecular Spectroscopy :

Energy levels, molecular orbitals, vibronic transitions, vibrational progression and geometry of the excited states, internal conversion. charge-transfer spectra. Franck-Condon Principle, Spectra of Transition metal Complexes.

M.Sc. Semester - III
Elective Paper - III B
(Medicinal Chemistry)

1. Drug Design :

Introduction, Concept of lead compound, concept of pro drugs, structure activity relationship (SAR), factors affecting bioactivity, resonance, inductive effect, isosterism, biososterism, spatial consideration, theories of drug activity occupancy theory, rate theory, induce fit theory.

2. ANTIBIOTICS :

Cell wall biosynthesis inhibitors, B-lactam ring, Antibiotics inhibiting bio synthesis of Protein. Synthesis of Penicillin Penicillin V. Chloramphenicol.

3. Antimalarials :

Chemotherapy of malaria : SAR, synthesis of Primaquin Chloroquin and Dapsone.

4. Antineoplastic Drugs:

Cancer chemotherapy, role of alkylating agents and antimetabolite in the treatment of cancer. Synthesis of Cyclophosphamide, Uraci Mustards and 6 mcrcaptopurine.

Introduction to hormone and natural products in cancer therapy.

5. A general study of following classes of drugs : (Structure and mode of action only).

1. Antifungal Drugs
2. Antiviral Drugs
3. General anesthetics
4. Hypnotics and Sedatives

M.Sc. Semester - III
Elective Paper - IV B
(Chemistry of Natural Products)

1. Terpenoids and Carotenoids :

Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule.

Structure determination, stereochemistry and synthesis of the following representative molecules: Citral, Menthol and Carotene.

2. Alkaloids :

Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic role of alkaloids in plants.

Structure, stereochemistry, synthesis of the following: Nicotine, Quinine.

3. Steroids:

Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry, Isolation, structure determination and synthesis of Cholesterol, Testosterone, Progesterone, Aldosterone.

4. Plant Pigments:

Occurrence, nomenclature and general methods of structure determination, Isolation and synthesis of Quercetin, Cyanidin, Biosynthesis of flavonoids : Acetate pathway and Shikimic acid pathway.

5. Porphyrins :

Structure and synthesis of Haemoglobin and Chlorophyll.

6. Prostaglandins :

Occurrence, nomenclature, classification and physiological effects. Synthesis of PGE₂ and PGF₂.

M.Sc. Semester - III
Elective Paper - III C
(Solid State Chemistry)

1. Imperfection in Crystals:-

Point defects: Schottky and Frenkel defects. Colour centers line defects : Edge and screw Dislocations. Burgers vector, dislocation densities. dislocation multiplicity and slip dislocation and crystal growth.
Surface imperfection: grain boundaries.

2. Band theory of Solids :

Metals, insulators, semiconductor, electronic structure of solids Band theory, Band structure of metals, insulators and semiconductors intrinsic-Extrinsic semiconductor :p-n junction. Hall effects seebeck coefficient. p-n junction. Organic semiconductors.

3. Superconductivity :

Zero resistance and the transition temperature. Super conductivity and periodic table. Magnetic properties. Theory of superconductivity (BCS theory). Type I and Type II superconductors Hard superconductors. Surface energy, superconducting magnet preparation of 1-2-3 & 2-1-4 materials.

4. Nucleation and crystal growth :

Homogenous and heterogenous nucleation. Equilibrium condition for a curved interface. Critical nuclei. Theory of nucleation Crystallisation of lamellar eutectics. Dendritic growth and peritect solidification.
Preparation of single crystals from vapour melt and solution.

5. Solid State Reaction :

Classification, Nature of solid state reactions. Reaction involving single solid phase, solid-gas reaction, solid reaction, solid liquid reaction, intercalation chemistry. Reaction of organic solid factors affecting solid state reactivity.

6. Magnetic dielectric and optical properties of solids. Behaviour substances in a magnetic field. Effect of temp. Curie and Cur Weiss Laws, Selected examples on magnetic materials (TM alloys, TM oxides Spinelles) their structure and properties. Dielectric constant and dielectric materials-Luminescence. Photosensors, Laser ruby lasers & Nd Lasers.

M.Sc. Semester - III
Elective Paper - IV C
(Chemical Kinetics)

1. Transition State Theory

Application of statistical mechanics to transition state theory with experimental results. Theories of unimolecular reactions-treatment of Lindmann, Hinshelwood, RiceRampsperger-Kassel (RRK) and Rice-Rampsperger Kassel-Murcus (RRKM).

2. Reaction in solution :

Reaction between ions: effect of solvent (single and double sphere models), interpretation of frequency factor and entropy of activation, influence of ionic strength, salt effect and reaction mechanism. reaction involving dipoles, influences of pressure on reaction rates in solution, significance of volume of activation, influence of substituent on reaction rates, electronic theories of organic reactivity, linear free energy relationship, the Hammett equation, significance of the Taft equation.

3. Kinetics of polymerization reaction:

Condensation, addition and ring opening polymerization, mechanism of polymerization (molecular free radical, cationic, and anionic mechanism), degree of polymerization and kinetics, chain length, kinetics of co polymerization.

4. Experimental Techniques for Fast Reaction : flow techniques, relaxation method, flash photolysis.

M.Sc. Semester - IV
Chemistry Paper - I
Environmental Chemistry (Compulsory)

1. Environment :

Biogeochemical cycles of C, N, P, S and O.

Hydrosphere :

Aquatic pollution - inorganic, organic, pesticides, agricultural, industrial and sewage. detergents, oil spills and oil pollutants. Water quality parameters - dissolved oxygen, biochemical oxygen demand, solids, metals, content of chloride, sulphate, nitrate and micro-organism. Water quality standards.

Analytical methods of measuring BaD, DO, COD, F, Oils, Metals (As, Cd, Cr, Hg, Pb, Se etc.) residual chloride and chlorine demand. Purification & treatment of water.

2. Soils :

Pollution - fertilizers, pesticides, and metals. waste treatment.

3. Atmosphere :

Chemical composition of atmosphere-particles, ions. and radicals and their formation. Chemical and photochemical reactions in atmosphere, smog formation, oxides of N, C, S, O and their effect, pollution by chemicals, petroleum, minerals; chlorofluorohydrocarbons Green house effect, acid rain, air pollution controls and their chemistry.

4. Industrial Pollution :

Cement, Sugar, distillery, drug, paper and pulp, thermal power plants, nuclear power plants, metallurgy polymers, drug etc. Radionuclide analysis. Disposal of wastes and their management.

5. Environmental Toxicology :

Chemical solutions to environmental problems, biodegradability, principles of decomposition, better industrial processes. Bhopal gas tragedy, hemobyl, Three mile island. Sewozo and Minamata disasters.

M.Sc. Semester - IV
Chemistry Paper - II
(Orange Transition Metal Chemistry)

I. Fluxional Organometallic compounds : Fluxionality and dynamic equilibria in compounds such as η^2 olefin η^3 -allyl and dienyl complexes.

II. Metal Carbonyl and nitrosyl compounds : Structural aspects of metal carbonyls, vibrational spectra for the structural diagnosis, Force constants and bonding Preparations, Properties and structure of some metal nitrosyls, Substitution reaction using donor and acceptors, hydrocarbonyls and metal carbides.

III. Homogeneous catalytic reactions: Coordinative unsaturation, Acid - Base behaviour of metal atoms in complexes. Insertion reaction, Reactions of coordinated ligands, catalytic reactions of alkenes, Hydrogenation of alkene, hydroformylation of alkenes. Alkene polymerization & oligomerization, Fischer- Tropsch process. Reactions involving molecular oxygen. Fluxional isomerism, Redistribution reactions, Wacker process (Smidt reaction), oxopalladation reaction, activation of C-H bond.

IV- Complexes with- bonding ligands :

(a) arene complexes of the transitional metals, origin of bis- arene concept bis-arene complexes of Cr & Fe, mixed arene & arene metal carbonyl compounds.

(b) Compounds of Transition metals and Carbon-Multiple bonds: Alkylindenes, Alkylidynes, low valent Carbenes and Carbynes-Synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reaction on the ligand.

(c) Cyclopentadienyl metal compounds of Fe. Structure & bonding of cyclopentadienyl metal compounds.

M.Sc. Semester - IV
Elective Paper - III A
(Photo inorganic Chemistry)

1. Basics of Photochemistry: 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.

2. Properties of Excited States : Structure dipole-moment, acid base strength, reactivity. Photo chemical kinetics-calculation of rates of radiative process. Bi molecular deactivation-quenching.

3. Excited States of Metal complexes : Excited States of Metal complexes:- Comparison with organic compounds electronically excited states of Metal complexes, charge transfer spectra, charge transfer excitations. method for obtaining charge transfer spectra.

4. Ligand Field Photochemistry : Photo substitution, photo oxidation, lability and selectivity, Zero vibrational levels of ground states and excited states, energy content of excited state, Lero-zero spectroscopic energy, development of equation for redox potentials os the excited states.

5. Redox Reactions by Excited Metal Complexes : Energy transfer under conditions of weak interaction and strong interactions- exciplex formation, conditions of the excited states to be useful as redox reactants, exited electron transfer, metal complexes as attractive candidates (2,2-bi pyridine and 1,10 phcnonthroline complexes), illustration of reducing and oxidizing character of Ruthenium²⁺ (bipyridil complex, comparison with Fe(bipy)₃; role of spin-orbit coupling-life time of these complexes. Application of redox processes of electronically exited states for catalytic purpose, transformations of low energy reactants into high energy products, transformations of low energy reactants into high energy products, chemical energy into light.

VI. Metal Complex sensitizers : Metal Complexes sensitizers, electron relay, metal colloid systems, semi conductors Supported metal oxide systems, water photolysis, nitrogen fixation and CO₂ reduction.

M.Sc. Semester - IV
Elective Paper - IV A
(Analytical Chemistry-II)

1. Food Analysis :

Moisture, ash, crude protein, fat, crude fiber, carbohydrates, 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. Extration and purification of sample. HPLC, Gas Chromatography for organophosphates. Thin -layer chromatography for identification of chlorinated pesticides in food products.

2. Analysis of Water 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, General survey of instrumental techniques for the analysis of heavy metals In aqueous systems. Pesticides as water pllutants and analysis. Water pollution Standards.

3. Analysis of Soil, Fuel, Body Fluids and Drugs :

(a) Analysis of solids; 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 & alkaline phosphates. Immunoassay : principles of radio immunoassay (RIA) & applications. The blood gas analysis trace element in the body.

(d) Drug analysis : Narcotics & dangerous drugs. Classification of drugs screening by gas and thin layer chromatography and spectrophotometric measurement.

M.Sc. Semester - IV
Elective Paper - III
(Organic Synthesis-II)

1. Disconnection Approach :

An introduction to synthons Disconnection Approach functional group inter conversion and one group C-X and two group C-X Disconnections.

2. protecting Groups :

Principle of protection of alcohol, amine, carbonyl and carboxyl groups.

3. One group C-C Disconnections :

Alcohol and carbonyl compounds, alkene synthesis.

4. Two group C-C Disconnections :

Diels alder reactions, Micheal addition Robinson annelation, 1,3 difunctionalised and 1,5 difunctionalised compounds.

5. Ring synthesis :

Saturated heterocycles (Piperidine, oxetane, THF, only)
aromatic heterocycles (3,4,5 and 6 membered rings) for example Aziridine, Pyyrole, Oxetene, Thiazole and Pyridine.

6. Synthesis of some complex molecules :

Application of above in the synthesis of following.
Camphor, Reserpine and Vitamin D.

M.Sc. Semester - IV
Elective Paper - IV B
(Heterocyclic Chemistry)

1. Nomenclature of Heterocycles :

Replacement and systematic nomenclature (Hantzsch-Widman system) for monocyclic fused and bridged heterocycles.

2. Heterocyclic Synthesis :

Principles of heterocyclic synthesis involving cyclization reactions and cycloaddition reactions.

3. Small Ring Heterocycles :

Three-membered and four-membered heterocycles-synthesis and reactions of aziridines, azetidines, oxetanes.

4. Benzo-Fused Five-Membered Heterocycles :

Synthesis and reactions including medicinal applications of benzopyrroles, benzofurans and benzothiophenes.

5. Six-Membered Heterocycles with one heteroatom :

One Heteroatom

Synthesis and reaction of pyrylium salts and pyrones and their comparison with pyridinium & thiopyrylium salts and pyridones.

Synthesis and reactions of quinolizium and benzopyrylium salts, coumarins and chromones.

6. Six-Membered Heterocycles with Two or More Heteroatoms :

Synthesis and reactions of diazines and thiazines.

7. Mesoionic Heterocycles :

General classification, chemistry or some important mesoionic heterocycles of type A & type B their applications.

8. Seven & Large Membered Heterocycles :

Synthesis and reaction of azepines, oxepines, Thiepinines and diazepines.

M.Sc. Semester - IV
Elective Paper - IV C
(Enzyme Chemistry)

1. Introduction :

Basic consideration, Proximity effects and molecular adaptation.

2. Enzymes : 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.

3. Mechanism of Enzyme Action : Transition-state theory, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortion, Example of some typical enzyme mechanism for chymotrypsin, ribonuclease, lysozyme and carboxypeptidase A.

4. Kinds of Reactions Catalysed by Enzymes : Nucleophilic displacement on phosphorus atom, multi displacement reactions and the coupling of ATP cleavage to endergonic processes. Addition and elimination reactions, enolic intermediates in isomerization reaction, some isomerization and rearrangement reactions. Enzyme catalyzed carboxylation and decarboxylation.

5. Co-enzyme chemistry : Cofactor as derived from vitamins, coenzymes, prosthetic groups, apoenzymes. Structure and biological function of coenzyme A, NAD⁺, NADP⁺, FAD, Vitamin B₁₂ Mechanisms of reactions catalyzed by the above cofactors.

6. Enzyme Model : 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.

M.Sc. Semester - IV
Elective Paper - III C
(Advanced Quantum Chemistry)

1. Principles of Quantum Mechanics :

Review of the principles of quantum mechanics. Treatment of H-atom , harmonic oscillator, rigid rotor. Born -Oppenheimer Approximation. Slater-Condon rules . Theory of angular momentum .

2. Ab initio and Semi-Empirical SCE-ME Calculations for Closed Shell System :

Roothaan-Hartree-Fock method. Methods based on neglect of differential overlap.

3. Molecular Orbital Theory :

MOT of H_2^+ , MO treatment of HOMO and Heteronuclear diatomics, Shapes of tritomic molecules. Huckle theory of conjugated system, bond order and charge density calculations. Applications of ethylene, butadiene, cyclopropenyl radical, cyclobutadiene etc. Introduction to extended Huckel theory.

4. Time dependent perturbation theory- radiative transition Einstein coefficient.

Introduction to the methods of self-consistent field.

M.Sc. Semester - IV
Elective Paper - IV D
(Statistical Thermodynamics)

1. Review of Basic Statistical Mechanics :

Phase Space, Ensembles, Equal a priori probability, Microcanonical ensemble, canonical ensemble & Grand Canonical ensembles, Probability and most probable distribution. Entropy & information. Stirling's approximation. Energy levels. Entropy & third law of thermodynamics.

2. Distribution law :

(i) Boltzmann distribution law : Molecular partition functions for non-interacting particles, relation of partition function to thermodynamic functions (H,U,G,S,A) & equilibrium constant $X_{2(g)} \rightleftharpoons 2X_{(g)}$.

(ii) Fermi-Dirac statistic : Electrons in metals.

(iii) Bose-Einstein statistics : Application to Helium.

3. Determination (Evaluation) of partition function :

Localized & non-localized particles, separation of partition function, Review of rotational, vibrational, translational & electronic partition functions. The Sackur-Tetrode equation. Derivation of thermodynamic properties of ideal gases from partition function.

4. Statistics Mechanics of Crystals :

Heat capacity of Solids. The Einstein's theory. The Debye theory.

5. Statistical of Non-equilibrium States :

Boltzmann transport equation. Electrical conductivity.

6. Statistical mechanics to liquids :

Radial distribution functions. Distribution function for classical monoatomic fluids.

M.Sc. Semester - IV
Elective Paper - IV E
(Chemistry of Materials)

1. Multiphase Materials :

Ferrous alloys: Fe-C phase transformations in ferrous alloys: stainless steels, non-ferrous alloys, properties of ferrous and non-ferrous alloys and their applications.

2. Ceramics, Composites and Nanomaterials :

Ceramic structures, mechanical properties, clay product, Refractories characterization, properties and applications. Microscopic composites; dispersion-strengthened and particle-reinforced. fibre-reinforced Composites, macroscopic composites, Nanocrystalline phase, preparation procedures, special properties applications.

3. Thin Films and Langmuir-blodgett Films :

Preparation techniques: evaporation / sputtering, chemical Processes, MOCVD, Langmuir-blodgett (LB) Films. Growth techniques, properties and applications of thin LB film.

4. Polymeric Materials :

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

5. Ionic Conductors :

Types of ionic conductors, mechanism of ionic conduction, interstitial jumps (Frenkel) : Vacancy mechanism, diffusion.

6. High T_C Materials :

Defects perovskites, high T_C superconductivity in cuprates, normal state properties: anisotropy: temperature dependence of electrical resistance.

M.Sc. Part-II
Semester - III
(Chemistry Practical)

Estimation of three component mixture of cations like M.N. 50 Cu, Ni, Zn, or Cu, Ni, Mg or Ag, Cu, Ni, or Cu, Ag, Zn or Ag, Ni, Zn or Ag, Ni, Mg or Fe, Ni, Zn or analysis of solder and type metal (Pb, Sb, Sn), analysis of Silver coin for (Ag, Cu, Ni) etc. Involving volumetric and gravimetric methods.

Spectrophotometric Determinations

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

Flame Photometric Determinations

- a) Sodium and potassium when present together
- b) Lithium / calcium / barium / strontium
- c) Cadmium and magnesium in tap water.

Nephelometric Determinations

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

M.Sc. Part-II
Semester - III
(Chemistry Practical)

Qualitative Analysis

Separation, purification and identification of the components of a mixture of three organic compounds (three solids or two liquids and one solid, two solids and one liquid), using tlc for checking the purity of the separated compounds. Chemical analysis, IR, PMR and mass spectral data.

Paper Chromatography

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

Spectroscopy

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

Spectrophotometric (UV/VIS) Estimations

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

Quantitative Analysis

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

Determination of DO, COD and BOD of water sample.

M.Sc. Part-II
Semester - IV
(Chemistry Practical)

Preparation

Preparation of selected inorganic compounds and their study by IR, electronic spectra, Mossbauer, ESR and magnetic susceptibility measurements. Handling of air and moisture sensitive compounds involving vacuum lines.

Selection can be made from the following

1. Sodium amide, Inorg . Synth, 1946,2,128.
2. Synthesis and thermal analysis of group II metal oxalate hydrate. J. Chem. Ed., 1988,65,1024.
3. Atomic absorption analysis of Mg and Ca
4. Trialkoxyboranes- Preparation, IR and NMR spectra.
5. PhBCl₂ Dichlorophenylborane - Synthesis in vacuum line.
6. Preparation of Tin(IV) iodide, Tin(IV) chloride and Tin(II) iodide. Inorg. Synth., 1953, 4, 119.
7. Relative stability of Tin(IV) and Pb(IV). Preparation of ammonium hexachlorostannate (NH₄)₂SnCl₆, ammonium hexachloroplumbate (NH₄)₂PbCl₆.
8. Hexa-bis (4-nitrophenoxy) cyclotriphosphazene.
9. Synthesis of trichlorodiphenylantimony (V) hydrate. Inorg. Synth., 1985,23,194.
10. Sodium tetrathionate Na₂S₄O₆
11. Metal complexes of dimethyl sulfoxide (IR): CuCl₂·2DMSO, PdCl₂·2DMSO, RuCl₂·4DMSO. J. Chem. Educ., 1982,63,90.
12. Synthesis of metal acetylacetonate: Magnetic moment, IR, NMR. Inorg. Synth, 1957,5, 130; 1963, 1, 183.
13. Bromination of Cr(acac)₃ J.Chem. Edu., 1986, 63, 90.
14. Magnetic moment of Cu(acac)₂·H₂O.
15. Cis and Trans [Co(en)₂Cl₂]⁺.
16. Separation of optical isomer of cis- [Co(en)₂Cl₂] Cl. J. Chem. Soc., 1960, 4369.
17. Ion exchange separation of oxidation state of vanadium. J. Chem. Educ., 1980,57, 316, 1978, 55, 55.
18. Determination of Cr(III) Complexes.
[Cr(H₂O)₆]NO₃·3H₂O, [Cr(H₂O)₄Cl₂]Cl·2H₂O, [Cr(en)₃]Cl₃ Cr(acac)₃
Inorg. Synth., 1972, 13, 184.

19. Preparation of N, N bis (salicylaldehyde)ethylenediamine, salen $H_2Co(salen)$ J. Chem. Educ., 1977, 54, 443, 1973, 50, 670.
Determination of O_2 absorption by $Co(salen)$
Acct. Chem. Res. 1975, 8, 384.
Reaction of oxygen adduct with $CHCl_3$ (deoxygenation).
20. Preparation of $Fe(II)$ chloride (use it as Friedel-Craft chlorination source.
J. Org. Chem., 1978, 43, 2423; J. Chem. Edu., 1984, 61, 645.; 1986, 63, 361.
21. Reaction of $Cr(III)$ with a multidentate ligand: a kinetics experiment (visible spectra $Cr-EDTA$ complex.) J.A.C.S., 1953, 75, 5670.
22. Preparation of $[Co(phenanthroline-5,6-quinone)]$.
23. Preparation and use of Ferrocene.
J. Chem. Edu., 1966, 43, 73: 1976, 53, 730.
24. Preparation of copper glycine complex-cis and trans bis (glycinato Copper(II)). J.Chem. Soc., Dalton, 1979, 1901, J. Chem. Edu., 1982, 59, 1052.
25. Preparation of phosphine Ph_3P and its transition metal complexes.
26. Any other experimental such as conversion of p-xylene to terephthalic acid catalyzed by $CoBr_2$ (homogeneous catalysis)

Chromatography

Separation of cations and anions by

- (a) Paper Chromatography
- (b) Column Chromatography - Ion exchange.

Chromatographic Separations

- (a) Cadmium and Zinc
- (b) Zinc and magnesium
- (c) Thin-layer chromatography-separation of nickel, manganese, cobalt and zinc. Determination of R_f values.
- (d) Separation and identification of the sugars present in the given mixture of glucose, fructose and sucrose by paper chromatography and determination of R_f values.

M.Sc. Part-II
Semester - IV
(Chemistry Practical)

Multi-Step Synthesis of Organic compounds

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

Photochemical reaction



Beckmann rearrangement : Benzanilide from benzene



Benzilic acid rearrangement: Benzilic acid from benzoin



Synthesis of heterocyclic compounds

Skraup synthesis: Preparation of quinoline from aniline Fisher -Indole synthesis:

Preparation of 2-phenylindole 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 ethyl acetoacetate with alkyl halide

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 reactions of proteins).
3. Isolation of lactose from milk (purity of sugar should be checked by TLC and PC 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 (+) limonine from citrus rinds.