COMPULSORY PAPERS
APPLICATION OF SPECTROSCOPY, PHOTOCHEMISTRY AND SOLID STATE CHEMISTRY

A. APPLICATION OF SPECTROSCOPY

Application inorganic and organic chemistry

i. Vibrational Spectroscopy:
Symmetry and shapes of AB_2, AB_3, AB_4, AB_5 and AB_6, mode of bonding of ambidentate ligands, nitrosyl, ethylenediamine and diketonato complexes, application of resonance Raman spectroscopy particularly for the study of active sites and metallo-priteins.

ii. Electron Spin Resonance Spectroscopy:
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 system and to inorganic free radical such as $pH_4.F_{2.}BH_{3.}$

iii Infra-red Spectroscopy:
Instrumentation and sample handling. Characteristic Vibrational frequencies of alkenes, alkenes and alkynes, Aromatic compounds, alcohols, ethers phenols and amines. Detailed study of Vibrational frequencies of carbony compounds (Ketones, aldehydes, ester, amides, acids anhydrides and conjugated carbony system). Effect of hydrogen bonding Vibrational frequencies, overtones.

iv. Ultraviolet and Visible spectroscopy:
Various electronic transitions (185-800 nm) 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 compounds. Steric effect in biphenyls.

v. Nuclear Magnetic Resonance Spectroscopy:
General introduction and definition, Chemical shift, spin– spin interaction, shielding and deshilding mechanism, mechanism of measurement of chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, and amides & mercapto). Chemical exchange, effect of deuteration, Complex spin – spin interation between two, three, four and five nuclei (I order spectra) Stereochemistry, hindered rotation, Karplus curve-variation of coupling constant with disordered angle, NMR shift reagents, solvent effects, Nuclear overhauser effect (NOE). Resonance of other unclei - F.P.

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

vi. C-13 NMR Spectroscopy:

General considerations, chemical shift (aliphatic olefinic, alkyne, aromatic, heteroaromatic and carboynl carbon), coupling constants. Two dimension NMR spectroscopy.

COSY, NOESY, DEPT, HMBC and HMQC techniques.

vii. Mossbauer Spectroscopy

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 in equivalent MB atoms.

viii. Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD):

Definition, deduction of absolute configuration, Octant rule for ketones

ix. Mass Spectrometry

Introduction ion production E1, C1, FD, ESI and FAB, factors affecting fragmentation, ion analysis, ion abundance Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, meta-stable peak, Me Lafferty rearrangement, Nitrogen rule, High resolution mass spectrometry, Examples of mass spectral fragmentation of organic compounds with respect to their structural determination.

B. PHOTOCHEMISTRY

i. Photochemical Reactions

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

ii. Determination of Reaction Mechanism

Classification, rate constants and life times of reactive energy state 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 Alkene

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

iv. Photochemistry of Carbonyl Compounds

Intramolecular reactions of carbonyl compounds-saturated, cyclic and acyclic, α, β, γ unsaturated and α, β, unsaturated compounds, cyclohexadienones, Intermolecular cyloaddition reactions-dimerisations and oxetane formation.

v. Photochemistry of Aromatic Compounds

Isomerisations, additions and substitutions.

vi. Miscellaneous Photochemical Reactions.

Photo-Fries reactions of annelids, Photo-Fries rearrangement, Barton reaction, Singlet molecular oxygen and its reactions, Photo-chemical formation of smog, Photo-degration of polymers, Photochemistry of vision

C. SOLID STATE CHEMISTRY

i. Solid State Reactions

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

ii. Crystal Defects and Non- Stoichiometry

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

iii. Electronic Properties and Band Theory

Metals insulators and semiconductors, electronic structure of solid 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 paramagnetic, co-operative phenomenon

iv. Organic Solids

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

Book Suggested

1. Physical Methods for Chemistry, R.S. Drago, Saunders Compnay.
2. Structural Methods in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H. Rankin and S. Cradock, ELBS.
3. Infrared and Raman Spectral : 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, .V. Parish, Ellis Haywood.
8. Practical NMR Spectroscopy, M.L. Martin. J.J. Deepish and G.J. Martin, Heyden.
9. Spectrometric Identification of Organic Compounds, R.M. Silverstein, G.C. Bassler adn 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-Hill.
13. Solid state chemistry and its applications, A.R. West. Peenum.
14. Principles of the Solid State, H.V. Keer, Wiley Eastern.
15. Solid State Chemistry, N.B. Hannay.
16. Solid State Chemistry, D.K. Chakrabarty, New Wiley Eastern.

PAPER- II
BIOINORGANIC, BIOORGANIC, BIOPHYSICAL AND ENVIRONMENTAL CHEMISTRY

A. BIOINORGANIC CHEMISTRY

i. Metal ions in biological systems
Essential and trace metals.

ii. Na+ /K+ pump:
Role of metal ions in biological processes

iii. Bioenergotic6 and ATP cycle:
DNA polymerisation, glucose storage, metal complexes in transmission of energy, chlorophyll photo system I and photo-system in cleavage to water Model systems

iv. Transport and Storage Di-oxygen
Heme proteins and oxygen uptake, structure and function of hemoglobin, myoglobin, haemocyanins and haemerythrin, model synthetic complexes of iron, cobalt and copper

v. Electron Transfer in Biology:
Structure and function of metolloproteins in electron transport processes-cyto-chromes and iron-sulphur proteins, synthetic models

vi. Nitrogenase:
Biological nitrogen fixation, Molybdenum Nitrogenase, Spectroscopic and other evidence, other Nitrogenase Model Systems

B. BIOORGANIC CHEMISTRY

i. Introduction
Basic considerations, Proximity effects and molecular adaptation

ii. 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-Mentien and Lineweaver-Burk plots, reversible and irreversible inhibition.

iii. Mechanism of Enzyme action:
Transition state theory, acid-base catalysis, covalent catalysis, strain or distortion. Examples of some typical enzyme mechanisms for chymotrypsin, ribonuclease, lysozyme and carboxypeptidase A.

iv. Kinds of reactions catalysed by Enzymes:
Nucleophilic displacement on a phosphorus atom, multiple displacement reactions and the coupling of ATP cleavage to endergonic processes. Transfer of sulphate, addition and elimination reactions, enolic intermediates in isomerization reactions, β cleavage and condensation, some isomerization and rearrangement reactions. Enzyme catalysed carboxylation and decarboxylation.

v. Co-Enzyme Chemistry:
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 catalysed by the above cofactors.

vi. Enzyme Models:
Host-guest chemistry. chiral recognition and catalysis, Molecular recognition Molecular asymmetry and prochirality, Btomimetic chemistry. Crown ether cryptates cyclodextrin, cyclodextdn-based enzyme models, calixarenes. ionophores, micelles synthetic enzymes or synzymes

vii. Biotechnological Applications of Enzymes:
Large-scale production and purification of enzymes, techniques and methods of immobilization of 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

B. BIOPHYSICAL CHEMISTRY:

i. Biological Cell and its Constituents:
Biological cell, Structure and Functions of Proteins, Enzymes, DNA and RNA in living cell systems, Helix coil transition.

ii. Bioenergetics:
Standard free energy change in biochemical reactions exergonic, endergonic hydrolysis of ATP, synthesis of ATP from ADP.

iii. Statistical Mechanics in Biopolymers:
Chain configuration of macro molecules, Statistical distribution end to end dimensions, calculation of average dimensions for various chain structure Potypeptide and protein structure, introduction to protein folding problem.

iv. Biopolymer Interactions :
Force involved in biopolymer interactions Electrostatic changes and molecular expansion. hydrophobic forces, dispersion force interactions, Multiple equilibria and various types of binding processes in biological systems, H^+ion titration.

v. Thermodynamics of biopolymer Solutions :
Thermodynamics of biopolymer solutions, osmotic pressure, membrane equilibrium, muscular contraction and energy generation in mechano-chemical systems.

vi. Cell membrane and transport of ions :
structure and functions of Cell Membrane, ion transport through cell membrane, ion transport through cell membranes, irreversible thermodynamic treatment of membrane transport. Nerve conduction.

vii. Biopolymer and their molecular weights:
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 totational motions.

viii. Diffraction Methods :
Light scattering, low angle x-ray scattering, x-ray diffraction and photo correlation spectroscopy.

D. ENVIRONMENTAL CHEMISTRY

i. Environment:

Introduction. Composition of atmosphere, vertical temperature, heat budget of the earth atmospheric system, vertical stability atmosphere, Biochemical cycles of C,N,P, S and O Bio distribution of elements.

ii. Hydrosphere:

Chemical composition of water bodies-lakes, streams, rivers and wetlands etc.. Hydrological cycle, Aquatic Pollution : Inorganic, organic, pesticide, agricultural, industrial and sewage, detergents, oil spills and oil pollutants.

Water quality parameter - dissolved oxygen biochemical oxygen demand, solids metals, sulphate, phosphate, nitrate, microorganism, Water Quality standard. analytical methods for measuring BOD, DO, COD, F, oils metals (As, Cd, Hg, Pb) Residual chloride and chloride demands, Purification and treatment of water.

iii. Industrial Pollution:

Cement, Sugar, distillery, paper and pulp, Thermal power plants, Nuclear power plants, Radio Nuclide analysis disposal of waste and their management.

PAPER - III
SECTION- A
ORGENOTRANSITION METAL CHEMISTRY

i. Alkyls and Ary ls of Transitioin Metals:
Types, routes of synthesis, stability and decomposition pathways, organo copper in organic synthesis

ii. Compounds of Transition Metal-Carbon Multiple Bonds
Alkylidenes, alkylidynes, low valent carbenes and carbyn es- synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions on the ligands, ro le in organic synthesis.

iii. Transition Metal π Complexes:
Transition Metal π Complexes with unsaturated organic molecules, alkenes, alkynes, allyl, diene, dienyl, arene and trienyl complexes, preparations, properties, nature of bonding and structural features. Important reactions relating to nucleophilic and electrophilic attack on ligands and to organic synthesis.

iv. Transition Metal Compounds with Bonds to Hydrogen:
Transition Metal Compounds with Bonds to Hydrogen

v. Homog eneous Catalysis:
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 reactions, activation of C-H bond.

vi. Fluxiona l Organometallic compounds:
Fluxionality and dynamic equilibria in compound such as n^2 olefin, n^2 allyl and dienyl complexes.

SECTION - B
PHOTOINORCANIC CHEMISTRY

i. Basics of Photochemistry:

Absorption, excitation, photochemical laws, quantum yield, electronically excited states-life times-measurements of the times. Radiative and Non-radiative Processes Energy dissipation by radiative and non radiative processes, bimolecular quenching, absorption spectra, Franck condon principle, photochemical kinetics, photochemical stages-primary and secondary process.

ii. Prooertles of Excited States:

Structure, dipole moment, acid-base shengths, reactivity. Photochemical kinetics-calculation of rates of radiative processes. Bimolecular deactivation quenching.

iii. Excited States of Metal Complexes:

Excited states of metal complexes: Cornparison 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:

Photosubstitution, photooxidation and photoreduction, lability and selectivity. Zero vibretional 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:

Energy transfer under conditions of weak interction and strong interaction exciplex formation : Conditions of the excited states to be useful as redox reactants. excited electron transfer metal complexes as attractive candidates (e,2'-bipyridine and 1, 10-phenonthroline complexes), illustration of reducing and oxidising character of Ruthenium^{2+} (bipyridal complex). comparison with fe $(bipy)_3$, role of spin-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:

Metal complex sensitizer, electron relay, metal or oxide systems water photolysis, nitrogen fixation and carbon dioxide reduction.

PAPER - IV
SECTION - A
BIOINORGANIC CHEMISTRY

i. Metal Storage Transport and Biomineralization:
Ferritin, transferring, and siderophores.

ii. Calcium in Biology:
Calcium in living cells, transport and regulation, molecular aspects of intramolecular processes, extra cellular binding proteins.

iii. Metalloenzymes:
Zinc enzymes – carboxypeptidase and carbonic anhydrase, Iron enzymes – catalase, proxidase and cytochrome P-450. Copper enzymes- superoxide dismutase. Molybdenum oxatransferase enzymes – xanthine oxidase. Coenzyme vitamin B12.

iv Metal—Nucleic Acid Interactions:
Metal ions and metal complex interactions. Metal complexes – nucleic acids.

v. Metals in Medicine:
Metal deficiency and disease, toxic effects of metals, metals used for diagnosis and chemotherapy with particular reference to anticancer drugs.

vi. Concepts and language of Supramolecular Chemistry:

(A) Molecular recognition: Molecular receptors for different types of molecules including arisonic substrates, design and synthesis of co receptor molecules 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

SECTION - B
ANALYTICAL CHEMISTRY

i. Introduction:

Role of analytical chemistry Classification of analytical methods - classical and instrumental. types of instrumental analysis Selecting an analytical method. Neatness and cleanliness. Laboratory operation and practices. Analytical balance. Techniques of weighing errons. Volumetric glass water - cleaning and calibration of glassware Sample Preparation- dissolution and decompositions. Gravirietric techniques Selecting and handling of reagents, Laboratory notebooks. Safe try in the analytical laboratory

ii. Errors and Evaluation:

Definition of terms in mean and median, Precision standard deviation, relative standard deviation. Accuracy - absolute error, relative error, relative error Types of error in experimental data ieterminate (systematic), indeterminate (or random) and gross Sources of errors and the effects upon the analytical results. Methods for reporting analytical data. Statistical evolution of data - indeterminate errors. The uses of Statistical.

iii. Food Analysis:

Moisture, ash, crude potein, fat, crude fiber, carbohydrates calcium potassium, sodium and phosphate. Food adulteration - common adulterants in food. contamination of food stuffs. 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:

Origin of waste water, types, water pollutants and their effects. Sources of water pollution -domestic, industrial, agricultural soil and radio active wastes as sources ol pollution. Objectives bf 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.

v. Analysis of Soil Fuel:

(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 coat Liquid fuels flash point. aniline point octane number and carbon residue. Gaseous fuels _ producer gas and water gas - calorific value.

PAPER- III
SECTION- A
CHEMISTRY IN NATURAL PRODUCTS

i. Terpenoids and Carotenoids

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

Structure determination, stereochemistry, biosynthesis and synthesis of the following representative molecules: Citral, Geraniol α-Terpeneol, Menthol, Farnesol, Zingiberence, Santonin, Phytol, Abietic acid and β-Carotene.

ii. Alkaloids

Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, role of alkaloids in plants. Structure, stereochemistry, synthesis and biosynthesis of the following: Ephedrine, (+) - Coniine, Nicotine, Atropine, Quinine and Morphine.

iii. Steroids

Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry, Isolation, Structure determination and synthesis of Cholesterol, Bile acids, Androsterone, Testosterone, Estrone, Progesterone, Aldosterone, Biosynthesis of Steroids.

iv. Plant Pigments

Occurrence, nomenclature and general methods of structure determination. Isolation and synthesis of Apigenin, Luteolin Quercetin, Myrcetin, Quercetin 3-glucoside, Vitexin, Diadzein, Aureusin, Cyanidin-7arabinoside, Cyanidin, Hirsutidin, Biosynthesis of flavonoids: Acetate pathway and Shikimic acid pathway.

SECTION- B
MEDICINAL CHEMISTRY

i. Pharmacokinetics:

introduction to drug absorption, disposition, elimination using Pharmacokinetics. important Pharmacokinetic parameters in defining drug disposition and in therapeutics. Mention of uses of Pharmacokinetics in drug development Process.

ii. Antineoplastic Agents :

introduction cancer chemotherapy, special problems, role of alkylating agents and anti metabolites in treatment of cancer. Mention of carcinolytic antibiotics and mitotic inhibitors. Synthesis of mechloreethamine, cyclophosphamide, melphalan, uracil, mustards and 6-mercaptopurine. Recent development in cancer chemotherapy Hormone and natural Products.

iii. Cardiovascular Drug:

introduction, cardiovascular diseases, drug inhibitors of peripheral svmpathetic function central intervention of cardiovascular output, Direct acting arteriolar dilators. Synthesis of anyl nitrate, sorbitrate, diltiazem quiniidine, verapamil, melhyldopa, atenolol oryprenolol.

iv. Loca Antiinfective Drugs:

Introduction and general mode of action, Synthesisof sulphonamides, furazolidone, nalidixic acid, ciprofloxacin, norfloxacin, dapsone, aminosalicylic acid, isoniazid. ethionamide, ehtambutal, fluconazole, econozole, griseofulvin, cholroquin and primaquin.

v. Psychoactive Drugs -The Chemotherapy of Mind:

introduction. neurotransmitters, CNS depressants general anaesthetics, mode of action of hypnotics, sedatives, anti-anxiety drugs, benzodiazipines, buspirone neurochemistry of mental diseases. Antipsychotic drugs - the neuroleptics, antidepressants, butyrophenones, serendipity and drug development, stereochemical aspects of psychotropic drugs.

synthesis of diazepam, oxazepam, chlorazepam, alprazolem, phenytoin. ethosuximide. trimethadione, barbitrates, thiopental sodium, glutethimide.

GROUP 'B'
SECTION- A
PAPER- IV
PHYSICAL ORGANIC CHEMISTRY

i. Concepts In Molecular Orbital(MO) and Valence Bond (VB) Theory :

Introduction to Juckel molecular orbital (MO) method as a means to explain modem theoretical methods. Advanced techniques in PMO and FMO theory. Molecular mechanics, semi empirical methods and ab inito and density functional methods. Quantitative MO theory - Huckel molecular orbital (HMO) method as applied to ethene allyl and butadiene. Qualitative MO theory - ionisation potential. Electron affinities MO energy levels. Orbital symmetry Orbital interaction diagrams. MO of simple organic systems such as ethene, allyl, butadiene, methane and methyl group Conjugation and hyper conjugation. Aromaticity. Valence bond (VB) configuration mixing diagrams. Relationship between VB configuration mixing and resonance theory Reaction profiles. Potential energy diagrams Curve-crossing model- nature of activation barrier in chemical reactions.

ii. Principals of Reactivity:

Mechanistic significance of entropy, enthalpy and Gibb's free energy. Arrhenius equation. Transition state theory Uses of activation parameters. Hammond's postulate. Bell-Evans-Polanyi principle. Potential energy surface model. Marcus theory of electron transfer reactivity and selectivity principles.

iii. Solvation and Solvent Effects

Qualitative understanding of solvent solute effects on reactivity, Classification of solvents, Solvation, Thermodynamics of Solvation, effects of solvation on Reaction Rates and Equilibria, Various Empirical indexes based on Physical properties, Dielectric Constant, Grunwald- Winstein Parameters. Koppel Palm Treatment, Solvent sensitive Reaction Rates, Spectroscopic parameters and Scales for Specific Solvation, use of solvation Scales in Mechanistic studies, solvent effect from curve Crossing models.

iv. Acids, Bases, Electrophiles, Nucleophiles and Catalysis

Acid-base dissociation, Electronic and structural effects, acidity and basicity. Acidity functions and their application. Hard and soft acids and bases. Nucleophilicity scales. Nucleofugacity. The α-effect. Ambivalent nucleophiles. Acid-base catalysis-specific and general catalysis. Brőnsted catalysis, Nucleophilic and electrophilic catalysis. Catalysis by non-covalent binding-micellar catalysis.

v. Steric and Conformation Properties:

Various type of steric strain and their influence on reactivity. Steric acceleration. Molecular measurements of steric effects upon rates. Steric LFER, Conformational barrier to bond rotation-spectroscopic detection of individual conformers. Acyclic and monocyclic systems. Rotation around partial double bonds. Winstein-Holness and Curtin-Hammett principle.

vi. Nucleophilic and Electrophilic Reactivity

Structural and electronic effects on S_N1 and S_N2 reactivity. Solvent effect. Kinetic isotope effects. Intramolecular assistance. Electron transfer nature of S_N2 reaction. Nucleophilicity and S_N2 reactivity based on curvecrossing mode. Relationship between polar and electron transfer reactions $S_{RN}1$ mechanism. Electrophilic reactivity, general mechanism. Kinetic of $S_E{}^{ZAr}$ reaction. Structural effects on rates and selectivity. Curve-crossing approach to electrophilic reactivity.

vii. Radical and Pericyclic Reactivity

Radical stability, polar influences, solvent and steric effects. A curve crossing approach to radical addition, factors affecting barrier heights in addition, redioselectivity in radical reactions.

Reactivity, specificity and periselectivity in pericyclic reactions.

SECTION B
HETEROCYCLIC CHEMISTRY

i. Nomenclature of Heterocycles

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

ii. Aromatic Heterocycles

General chemical behaviour 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 escalations).

Heteroaromatic reactivity and tautomerism in aromatic heterocycles.

iii. Non-aromatic Heterocycles

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 elctrophilic interactions.

iv. Heterocyclic Synthesis

Principles of heterocyclic synthesis involing cyclization reactions and cyclo addition reactions.

v. Small Ring Heterocycles

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

vi. Benzo-Fused Five-Membered Heterocycles

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

vii. Six-Membered Heterocycles with one Heteroatom

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

Synthesis and reactions of quinolizinium and benzopyrylium salts, coumarins and chromones

viii. Six Membered Heterocycles with Two or More Heteroatoms

Synthesis and reactions of diazones, triazines, tetrazines and thiazines.

ix. Seven-and Large-Membered Heterocycles

Synthesis and reactions of azepines, oxepines, thiepines, diazepines thiazepines, azocines, diazocines, dioxocines and dithiocines.

GROUP C
SECTION– A
PAPER- III
ADVANCED QUANTUM CHEMISTRY

i. **Theoretical and computational Treatment of Atoms and Molecules, Hartree-Fock Theory :**
Review of the principles of quantum mechanics, Bom- Oppenheimer approximation. Slater-Condon rules, Hartree-Fock equation: Koopmans and Brilouin theories, Roothan equation, Gaussion basis sets.

ii. **Configuration Interaction and Mc-SCF**
Introduction to CL full and truncated Cl theories, size consistency introductory treatment of coupled cluster and MC-SCF methods.

iii. **Semi-Empirical Theories**
Areview of the Huckel, 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**
Derivation of Hohenberg-Kohn theorem, Kohn-Sham formulation, N and V-represent abilities, review of the performance of the existing local (e.g slate Xa and other methods) and non-local functionals,, treatment of chemical concepts, concepts with the density functional theory.

v. **Computer experiments**
Computer experiments using quantum chemistry-software packages such as GASSIAN/GAMESS/MOPAC and modeling software. e. g. MM2/AMBER/CHARM etc.

SECTION - B
LIQUID STATE

i. General properties of Liquids

(a) Liquids as dense gases, Liquids as disordered solids, some thermodynamics reactions, internal pressure and its significance in liquids equations of state, critical constants, Different types of intermolecular forces in liquids, different potential functions for liquids additively of pair potential approximation.

(b) A classical pattern functions for liquids, correspondence principle, configuration Integral configuration properties.

ii. Theory of Liquids:

Theory of liquids, partition, function methods of model approach, single cell models, communal energy and entropy, LTD model, significant structure model.

iii. Distribution Function and Related Equation

Radial distribution function methods, equation of state in term of RDF molecular distribution function. Relationship between pair distribution function and pair potential function, The IBG equation, the HNC equation the PY equation, clusters expansion

iv. Methods for Structure Determination and Computation Techniques

Spectroscopic techniques for liquid dynamic structure studies, Neutron and X-ray scattering spectroscopy

Computation Techniques - Monte Carlo and Molecular dynamics methods.

v. Super cooled and ionic Liquids

Super cooled and ionic liquids, theories of transport properties non- Arrhenius behavior of transport properties, Cohen-Tumbull free volume model Configurational entropy model, Macedo-Litovitz hybrid model glass transition in super cooled liquids.

PAPER IV
SECTION A
CHEMISTRY OF MATERIALS

i. Multiphase Materials

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

ii. Glasses, Ceramics, Composites and Nonmaterial

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

Microscopic composites; dispersion-strengthened and particle reinforced. fibrerein forced composites macroscopic composites Nano crystalline phase, preparation procedures, special properties' applications.

iii. Thin Films and Langmuil-Blodgett Films

Preparation techniques; evaporation/sputtering Chemical processes MOCVD soi-gell etc, Langmuir-Blodgett (LB) film, growth techniques, photolithography, properties and application of thin and LB films

iv. Liquid Crystals

Mes morphic behavior, thermo tropic liquid crystals positional order, bond orientational order, nematic and smectic mesophases. smecticnematic transition and clearing temperature - home tropic, planar and schlieren textures, twisted nematics. chiral nematics, molecular arrangement in smectic A and smectic C phases, optical properties of liquid crystals, Di electric susceptibility and dielectric constants. Lyotropic phases and their description of ordering in liquid crystals

v. Poly materials

Molecular shape, structure and configuration, crystalllnity, stress strain behavior thermal behaviour, polymer types and their application, conducting and Ferro-electric polymers

vi. Ionic Conductors

Types of ionic conductors, mechanism of ionic conduction, Interstitial Jumps (Frenkel) vacancy mechanism, diffusion super ionic conductors: phase transitions and mechanism of conduction in super ionic conductors, examples and applications of ionic conductors.

vii. High Tc Materials

Defect perosovkites, high Tc superconductivity in cuprtales, 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 multi gap structure in high Tc materials. applications of high Tc materials.

viii. Materials tor Solid State Devices

Rectifirers, transistors, capacitors - lV-V compounds, Low-di-rnensional quantum structures; optical properties.

ix. Organic Solids, Fullerenes, Molecular Devices

Conducing organics, organic super conductors, magnetism in organic materials. fullerenes-doped fullerenes as super conductors.

Molecular rectifiers and transistors, artificial photosynthetic devices, optical storage 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.

SECTION - B
POLYMERS

i. Basics:

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 plmer reactions. Polymerization in homogeneous and heterogeneous systems.

ii. Polymer Characterization:

Poly dispersion -average molecular weight concept. Number, weight and viscosity average molecular weights Poly dispersity and molecular weight distribution. The practical significance of molecular weight. Measurement of molecular weights. End-group, viscocity, 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.esistance. Hardness and abrasion resistance,

iii. Structure and Properties:

Morphology and order in crystalline polymers - configurations 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 Tm melting points of homogeneous sides, effect of chain flexibility and other steric factors, entropy and heat of fusion. The glass transition temperature, Tg - Relationship between Tm and Tg, effects of molecular weight diluents. Chemical structure, chain topology, branching and cross linking. Property requirements and polymer utilization.

iv. Polymer Processing

Plastics. elastomers and fibres, Compounding Processing techniques calendaring, die-casting, rotational casting, lilm casting' injection moulding, blovi, moulding, extrustion moulding, thermoforming. foaming, reinforcing and fibre spinning.

v. Properties to Commercial Polymers:

Polyethylene, polyvinyl chloride, polyamides, polyesters, phenolic resins. epoxy resins 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.s