INORGANIC CHEMISTRY

UNIT I  Vibrational Spectroscopy
Symmetry and shapes of $\text{AB}_2$, $\text{AB}_3$, $\text{AB}_4$, $\text{AB}_5$ and $\text{AB}_6$, mode of bonding of ambidentate ligands, ethylenediamine and diketonato complexes, application of resonance Raman spectroscopy particularly for the study of active sites of metalloproteins.

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 systems and to inorganic free radicals such as $\text{PH}_4$, $\text{F}_2$ and $[\text{BH}_3]$.

UNIT II  Nuclear Magnetic Resonance of Paramagnetic Substances in Solution
The contact and 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 $^{199}$Sn NMR.

Mossbauer Spectroscopy
Basic principles, spectral parameters and spectrum display. Application of the technique to the studies of (1) bonding and structures of $\text{Fe}^{2+}$ and $\text{Fe}^{3+}$ compounds including those of intermediate spin, (2) $\text{Sn}^{2+}$ and $\text{Sn}^{4+}$ compounds nature of M-L bond, coordination number, structure and (3) detection of oxidation state and inequivalent MB atoms.

ORGANIC CHEMISTRY

UNIT III 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 and heterocyclic compounds. Steric effect in biphenyls.

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.

UNIT IV  Infrared Spectroscopy
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.

**Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD)**
Definition, deduction of absolute configuration, octant rule for ketones.

**UNIT V Nuclear Magnetic Resonance Spectroscopy**
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.

**Carbon-13 NMR Spectroscopy**
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.

**Books Suggested:**

5. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Horwood.
CH-502 PHOTOCHEMISTRY AND SOLID STATE CHEMISTRY

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

Determination of Reaction Mechanism
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- photodissociation, gas-phase photolysis.

UNIT II Photochemistry of Alkenes
Intramolecular reactions of the olefinic bond – geometrical isomerism, cyclisation reactions, rearrangement of 1,4- and 1,5- dienes,

Photochemistry of Carbonyl Compounds
Intramolecular reactions of carbonyl compounds – saturated, cyclic and acyclic, \( \beta,\gamma \)-unsaturated and \( \alpha,\beta \)-unsaturated compounds. Cyclohexadienones.

Intermolecular cycloaddition reactions – dimerisations and oxetane formation.

UNIT III Photochemistry of Aromatic Compounds
Isomerisations, additions and substitutions.

Miscellaneous Photochemical Reactions
Photo-Fries reactions of anilides. Photo-Fries rearrangement.
Barton reaction. Singlet molecular oxygen reactions. Photochemical formation of smog.

UNIT IV Solid State Reactions
General principles, experimental procedures,
Crystal Defects – Perfect and imperfect crystals, intrinsic and extrinsic defects – point defects, line and plane defects. Thermodynamics of Schottky and Frenkel defect formation, colour centers.

UNIT V Solid State Chemistry
Electronic Properties and Band Theory
Metals, insulators and semiconductors, band theory of solids(qualitative treatments), band structure of metals, insulators and semiconductors. Intrinsic and extrinsic semiconductors, p-n junctions.
Superconductors- factors affecting the super conductivity, magnetic properties, persistent current and BCS theory of superconductors.
Optical properties – photoconduction.
Magnetic Properties – Classification of materials, Magnetic domains, hysteresiuis.

Organic Solids
Electrically conducting solids, organic charge transfer complex - new superconductors.

Books Suggested:
CH-503 ENVIRONMENTAL CHEMISTRY

UNIT I Environment

UNIT II Hydrosphere
Chemical composition of water bodies: lakes, streams, rivers and wet lands, etc. Hydrological cycle.
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.

UNIT III Lithosphere : All types of soils

UNIT IV 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.
Analytical methods for measuring air pollutants. Continuous monitoring instruments.
UNIT V Industrial Pollution and Environmental Toxicology

Books Suggested:

4. Environmental Pollution analysis, S.M. Khopkar, Wiley Eastern.

CH-504 BIO-CHEMISTRY

UNIT I

UNIT II Enzymes
Introduction and historical perspective, chemical and biological catalysis, remarkable properties of enzymes like catalytic power, specificity and regulation. Nomenclature and classification. Fischer’s lock and key and Koshland’s induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labelling and enzyme modification by site directed muta genesis. Transition state theory, orientation and stearic effect, acid-base catalysis, covalent catalysis, strain or distortion. Coupling of ATP cleavage to endergonic processes, β-cleavage and condensation.
UNIT III Co-Enzyme Chemistry
Cofactors as derived from vitamins, coenzyme, prosthetic groups, apoenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD⁺, NADP⁺, FMN, FAD, lipoic acid, vitamin B₁₂. Mechanism of reaction catalysed by the above cofactors. 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.

UNIT IV Bioenergetic and Biopolymer Interactions:

UNIT V Diffraction Methods and Statistical Mechanics in Biopolymers.
Evaluation of size, shape, molecular weight and extent of hydration of biopolymers by various experimental techniques. Light scattering, low angle X-ray scattering, X-ray diffraction and photo correlation spectroscopy. ORD Chain configuration of macromolecules, statistical distribution end to end dimensions, calculation of average dimensions for various chain structure. Polypeptide and protein structures, introduction to protein folding problem.

Books Suggested:

10. Immobilized Enzymes: An Introduction and Applications in Biotechnology, Michael D. Tevan, John Wiley.
15. Biochemistry, L. Strver, W.H. Freeman
17. Biochemistry, Voet and Voet, John Wiley.

Laboratory Course - I
Course No. 511: Inorganic Chemistry

Experiment No. 1:
Preparation of some Inorganic coordination compounds.

Experiment No. 2:
Analyse the given mixture for four rare elements.

Experiment No. 3:
Estimation of three constituent in the given mixture (Two gravimetrically and one volumetrically).

Experiment No. 4: Iron phenanthroline complex: Job’s Method of continuous variations.

Experiment No. 5: Find out the stability constant of metal complex by Bjerrum’s Method.

Laboratory Course - II
CH 512: Instrumental Lab.

I. pH metry:
1. To determine the dissociation constants of dibasic and tribasic acids.
2. Titration of mixture of acids (HCl + CH₃COOH) against strong base.

II. Spectrophotometry:
1. Determination of PKₐ of an indicator (e.g. methyl red) in (a) aqueous and (b) micellar media.
2. Determination of stoichiometry and stability constant of inorganic (e.g. ferri–salicylic acid) and organic (e.g. amine–iodine).
3. To determine the concentration of chromium and manganese in a binary mixture.

III. Polarography:
1. To study oxygen wave by polarography.
2. To characterize and determine Pb\(^{2+}\), Cd\(^{2+}\) and Zn\(^{2+}\), ions by polarography/cyclic voltammetry

**IV Fluorometry**
1. Determination of strength of Vitamin B (Riboflavin) and Aluminium.

**V. Nephelometry**
1. Determination of sulphate content in water sample.
2. Determination of phosphate content in water sample.

**VI. Flame photometry**
1. Estimation of Ma, K and Ca.
2. Estimation in a mixture (Na and K; K and Ca).

**VII Water and Waste Water examination:**
1. DO and BOD determination.
2. COD estimation.
3. Fluoride and nitrate determination.

**VIII Cement Analysis**

**IX Chromatography: Coloumn**

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**M Sc II YEAR (Affiliated college)-2015**

**SEMESTER IV**

**LIST of ELECTIVE PAPERS IN THE M.Sc. CHEMISTRY.**

**GROUP A**

CH 601: Organotransition Metal Chemistry.

CH 602: Advanced Analytical Techniques

CH 603: Liquid State

CH 604: Polymers

**ELECTIVE PAPER 1**

**CH-601 Organotransition Metal Chemistry**

**UNIT I**

**Organotransition metal compounds**: Definition, Classification and nomenclature of organotransition metal compounds. Difference in nature of bonding between metal carbonyls and organotransition metal compounds.

**UNIT II**

**Alkyls and Aryls of Transition Metals**: Types, methods of synthesis, thermal stability and decomposition pathways.

**UNIT III**
**Transition Metal π-Complexes:** Transition metal π-complexes with unsaturated organic molecules, alkenes, cyclopentadienyls and arenes, methods of synthesis, properties, nature of bonding and structural features.

**UNIT IV**
**Homogeneous Catalysis:** Homogeneous catalytic hydrogenation of Alkenes, Zeigler Natta polymerization of olefins, Isomerisation of Alkenes, Hydroformylation, Dimerisation and polymerization of Alkenes and Alkynes.

**UNIT V**
**Organocopper in Organic Synthesis:** Conjugated additions, halogen substitution, alkylation of epoxides, alkylation of allylacettes, ketones from acid chlorides.

**Books Suggested:**


**ELECTIVE PAPER 2**

**Ch-602 Advanced Analytical Techniques**

**Unit I Basics of Instrumentation and Gas Chromatography**
Basic Electronics for Analytical Instruments; Automation in Analysis: Introduction to On-line/ Process control analyzer, Discrete, Continuous analysis and Flow injection analysis
Gas Chromatography (GC): Theory, General layout of equipment, detectors for GC, Applications; Gas Chromatography with Mass Spectrometry (GC-MS).

**Unit II Column and Thin Layer Chromatography**
High performance Liquid Chromatography (HPLC): Types of Liquid Chromatography, General layout of equipment & detectors for HPLC, Applications of HPLC in pharmaceutical Analysis.
Thin Layer Chromatography (TLC), Application of TLC special reference to forensic analysis; High Performance Thin Layer Chromatography (HPTLC).

**Unit III X-ray and Emission Techniques:**
Production of X-rays, Instrumentation, direct X-ray method, X-ray Absorption Spectroscopy, X-ray Fluorescence Spectroscopy.
Inductively Coupled Plasma Emission Spectroscopy (ICPES): theory,
instrumentation and applications.

**Unit IV Surface Techniques:**
Basic Principle, Theory; Chemical & Surface applications of:
Electron Spectroscopy for Chemical Analysis (ESCA), Auger Emission Spectroscopy (AES), Photoacoustic Spectroscopy (PAS)

**Unit V Tools for Nanotechnology:**

**Books:**
3. Instrumental Methods of Analysis, Strobel

**ELECTIVE PAPER 3**

**CH-603 Liquid State**

**UNIT I General Properties of Liquids**
Properties of liquids, Structure of liquids, Comparison of liquid Argon and liquid sodium. Some thermodynamic relations, equations of state, critical constants. Different types of intermolecular forces in liquids, Order on liquids.

**UNIT II Theories of Liquids**
A classical partition function for liquids, correspondence principle, configuration properties: configuration integral. Theory of liquids: cell theory, model approach; single cell models, communal energy and entropy.

**UNIT III Distribution Function and Related Equations**
Molecular distribution functions, pair distribution function. Internal energy of liquids. Relationship between pair distribution function and pair potential function. The YBG equation, the HNC equation, the PY equation, cluster expansion.

**UNIT IV Methods for Structure Determination and Computational Techniques**
Spectroscopic techniques for liquid dynamic structure studies, Neutron and X-ray scattering spectroscopy.
Computation Techniques-Monte Carlo and molecular dynamics methods.

UNIT V Super cooled and Ionic Liquids
Super cooled and ionic liquids, theories of transport properties; non Arrhenius behaviour of transport properties,
Quantum liquids: Comparison of classical and quantum liquids. Critical velocity for superfluids.

Books Suggested:

2. The Dynamic Liquid State, A.F.M. Barton, Longman.
4. The Liquid State, J.A. Pryde.
6. Properties of liquids and solutions, Murrel & Boucher, John Wiley & Sons

ELECTIVE PAPER 4
CH-604 Polymers

UNIT I Basic
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.

UNIT II Polymer Characterization

UNIT 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 series, 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.

**UNIT IV Polymer Processing**
Plastics, elastomers and fibres. Compounding. Processing techniques: Calendering, die casting, rotational casting, film casting, injection moulding, blow moulding, extrusion moulding, thermoforming, foaming, reinforcing and fibre spining.

**UNIT V Properties of 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.

**Books Suggested:**


**Laboratory Courses-III**

**CH 513 : Organic Chemistry**

**I. Qualitative Analysis**
Separation, purification and identification of three components of a mixture of organic compounds (three solids or two liquids and one solid, two solids and one liquid).

**II. Multi-step Synthesis of Organic Compounds**

Benzophenone → Benzpinacol → Benzpinacolone

→ Benzophenone → Benzophenone oxime → Benzanilide

Benzoin → Benzil → Benzilic acid

Skraup synthesis: Preparation of quinoline from aniline.

Synthesis using microwaves
To carry out oxidation of alcohols and oxime by PCC.

Synthesis using phase transfer catalyst

Alkylation of diethyl malonate or ethyl acetoacetate with an alkyl halide.

III. 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 piperine from black pepper.
5. Isolation of lycopene from tomatoes.
6. Isolation of carotene from carrots.
7. Isolation of eugenol from cloves.

IV. Paper Chromatography / TLC

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.

V. Spectroscopy

Identification of organic compounds by the analysis of their spectral data (UV, IR, PMR, Ms).

Spectrophotometric (UV/VIS) Estimations

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

Books Suggested

1. Systematic Qualitative Organic analysis by H. Middleton.
2. Qualitative and Quantitative hand book of Organic analysis by H. Clark

Laboratory Courses-IV

CH 514- Physical Chemistry

I. Chemical Kinetics
(i) To investigate the kinetics of the reaction between I\(^-\) and persulphate ion
   (a) Order of the reaction
   (b) Energy of activation of the reaction.
   (c) Effect of ionic strength on rate.

(ii) To find out the order of the reaction of saponification of ester using unequal concentrations of reactants.

II. Chemical kinetics
   (i) To investigate the kinetics of the reaction between ceric ammonium sulfate and glycollic acid.
      (a) Order with respect to ceric ion.
      (b) Order with respect to glycollic acid.
      (c) Energy of activation of the reaction.
      (d) Effect of ionic strength on rate.

   (ii) To study the reaction between ceric ammonium nitrate and primary alcohol.

III. Thermodynamics
   (i) Determination of partial molar volume of solute (e.g., KCl) and solvent in a binary mixture.
   (ii) Determination of the temperature dependence of the solubility of a compound in two solvents having similar intermolecular interactions (benzoic acid in water and in DMSO-water mixture) and calculate the partial molar heat of solution.

IV. Phase Equilibrium
   (i) To find out the equilibrium constant for the triiodide formation.
   (ii) To find the formula of complex cuprammonium ion by distribution method.

V. Conductometry
   (i) To find out the equivalent conductance of strong electrolytes at different dilutions and to verify Debye-Huckel Onsagar equation.
   (ii) To determine the equivalent conductance of a weak electrolyte at infinite dilution.
   (iii) To determine the dissociation constant of acetic acid/Oxalic acid and verify the Ostwald’s dilution law.
   (iv) To determine the degree of hydrolysis and hydrolysis constant of ammonium chloride at room temperature.
   (v) To determine the activity coefficient of zinc ions in the solution of 0.002 M ZnSO\(_4\) using Debye-Huckel’s Limiting Law.
(vi) Determination of the velocity constant, order of the reaction and energy of activation for saponification of ethyl acetate by NaOH conductometrically.

(vii) To determine the solubility and solubility product of sparingly soluble salt (PbSO₄, BaSO₄)

VI. Potentiometry/pHmetry

(i) To determine the dissociation constants of weak acids (oxalic, tartaric, phosphoric) using pH meter.

(ii) To determine the temperature dependence of emf of a cell.

(iii) To determine the degree of hydrolysis of aniline hydrochloride for three different solutions at room temperature and hence calculate the hydrolysis constant of the salt and dissociation constant of the base.

(iv) To study the acid-base titration in a non-aqueous media using a pH meter.

(v) To find out thermodynamic constants ΔG, ΔS and ΔH for the reaction by emf measurements.

\[ \text{Zn} + \text{H}_2\text{SO}_4 \rightarrow \text{ZnSO}_4 + \text{H}_2 \]

Books suggested:

1. Practical Physical Chemistry, A.M. James and F.E. Prichard, Longman.
2. Findley’s Practical Physical Chemistry, B.P. Levitt, Longman.