B.Sc III Year – Paper-III — **90 hrs (3 h / w)**

UNIT – I (Inorganic Chemistry – III) — **30 hrs (1 h / w)**

1. Coordination Chemistry	10 h
2. Spectral and magnetic properties of metal complexes	4 h
3. Reactivity of metal complexes	4 h
4. Stability of metal complexes	4 h
5. Hard and soft acids and bases	4 h
6. Bioinorganic Chemistry	4 h

UNIT – II (Organic Chemistry – III) — **30 hrs (1 h / w)**

1. Nitrogen compounds	9 h
2. Heterocyclic compounds	5 h
3. Carbohydrates	6 h
4. Amino acids and Proteins	5 h
5. Mass spectroscopy	5 h

UNIT – III (Physical Chemistry – III) — **30 hrs (1 h / w)**

1. Chemical kinetics	9 h
2. Photochemistry	5 h
3. Thermodynamics	16 h

Paper-IV — **90 hrs (3 h / w)**

Chemistry and Industry

UNIT – I (Physico chemical methods of Analysis) — **30 hrs (1 h / w)**

1. Separation techniques	12 h
2. Spectrophotometry	4 h
3. Molecular spectroscopy	14 h

UNIT – II (Drugs, Formulation, Pesticides & Green Chemistry) — **30 hrs (1 h / w)**

1. Drugs	17 h
2. Formulations	3 h
3. Pesticides	5 h
4. Green Chemistry	5 h

UNIT – III (Macromolecules, materials science and catalysis) — **30 hrs (1 h / w)**

1. Macromolecules	10 h
2. Materials Science	8 h
3. Catalysis	12 h

LABORATORY COURSE – III

90 hrs (3 h / w)

Practical Paper – III (Organic Chemistry)

1. Synthesis of organic compounds
2. Thin layer and Column chromatography
3. Organic qualitative analysis
    a. Identification of Individual organic compounds
    b. Separation of two component mixtures
4. Demonstration experiments
    a. Microwave assisted Green synthesis
    b. Steam distillation experiment

LABORATORY COURSE – IV

90 hrs (3 h / w)

Practical Paper – IV (Physical Chemistry)

1. Chemical kinetics
2. Distribution Law
3. Electrochemistry
4. pH metry
5. Colorimetry
6. Adsorption
7. Project work

Note: From above experiment one experiment of 40 marks and project work of 10 marks at the University examination.

B.Sc III Year

Paper – III **90 hrs (3h / w)**

Unit – I (Inorganic Chemistry-III) **30 hrs (1 h/w)**

1. **Coordination Chemistry:** IUPAC nomenclature, bonding theories – review of Werner's theory and Sidgwick's concept of coordination, Valence bond theory, geometries of coordination numbers 4-tetrahedral and square planar and 6-octahedral and its limitations, crystal filed theory, splitting of d-orbitals in octahedral, tetrahedral and square-planar complexes – low spin and high spin complexes – factors affecting crystal-field splitting energy, merits and demerits of crystal-field theory. Isomerism in coordination compounds – structural isomerism and stereo isomerism, stereochemistry of complexes with 4 and 6 coordination numbers.

10 h

2. **Spectral and magnetic properties of metal complexes:** Electronic absorption spectrum of $[Ti(H_2O)_6]^{3+}$ ion. Types of magnetic behavior, spin-only formula, calculation of magnetic moments, experimental determination of magnetic susceptibility – Gouy method.

4 h

3. **Reactivity of metal complexes:** Labile and inert complexes, ligand substitution reactions – S_N1 and S_N2, substitution reactions of square planar complexes – Trans effect and applications of trans effect.

4 h

4. **Stability of metal complexes:** Thermodynamic stability and kinetic stability, factors affecting the stability of metal complexes, chelate effect, determination of composition of complex by Job's method and mole ratio method.

4 h

5. **Hard and soft acids bases (HSAB):** Classification, Pearson's concept of hardness and softness, application of HSAB principles – Stability of compounds / complexes, predicting the feasibility of reaction.

4 h

6. **Bioinorganic chemistry:** Essential elements, biological significance of Na, K, Mg, Ca, Fe, Co, Ni, Cu, Zn and chloride (Cl^-). Metalloporphyrins – hemoglobin, structure and function, Chlorophyll, structure and role in photosynthesis.

4 h

UNIT – II (Organic Chemistry – III) 30 hrs (1h/w)

1. Nitrogen compounds 9 h

Nitro hydrocarbons: Nomenclature and classification – nitro hydrocarbons – structure. Tautomerism of nitroalkanes leading to aci and keto form. Preparation of Nitroalkanes. Reactivity – halogenation, reaction with HONO (Nitrous acid), Nef reaction and Mannich reaction leading to Michael addition and reduction.

Amines (Aliphatic and Aromatic): Nomenclature, Classification into 1^0, 2^0, 3^0 Amines and Quarternary ammonium compounds. Preparative methods -1. Ammonolysis of alkyl halides 2. Gabriel synthesis 3. Hoffman's bromamide reaction (mechanism).
4. Reduction of Amides and Schmidt reaction. Physical properties and basic character – Comparative basic strength of Ammonia, methyl amine, dimethyl amine, trimethyl amine and aniline – comparative basic strength of aniline, N-methylaniline and N,N-dimethyl aniline (in aqueous and non-aqueous medium), steric effects and substituent effects. Use of amine salts as phase transfer catalysts. Chemical properties: a) Alkylation b) Acylation c) Carbylamine reaction d) Hinsberg separation e) Reaction with Nitrous acid of 1^0, 2^0, 3^0 (Aliphatic and aromatic amines). Electrophilic substitutions of Aromatic amines – Bromination and Nitration, oxidation of aryl and 3^0 Amines, diazotization
Cyanides and isocyanides: Nomenclature (aliphatic and aromatic) structure. Preparation of cyanides from a) Alkyl halides b) from amides c) from aldoximes. Preparation of isocyanides from Alkyl halides and Amines. Properties of cyanides and isocyanides, a) hydrolysis b) addition of Grignard reagent iii) reduction iv) oxidation.

2. Heterocyclic Compounds 5 h

Introduction and definition: Simple 5 membered ring compounds with one hetero atom Ex. Furan. Thiophene and pyrrole. Importance of ring system – presence in important natural products like hemoglobin and chlorophyll. Numbering the ring systems as per Greek letter and Numbers. Aromatic character – 6- electron system (four-electrons from two double bonds and a pair of non-bonded electrons from the hetero atom). Tendency to undergo substitution reactions.
Resonance structures: Indicating electron surplus carbons and electron deficient hetero atom. Explanation of feebly acidic character of pyrrol, electrophillic substitution at 2 or 5 position, Halogenation, Nitration and Sulphonation under mild conditions. Reactivity of furan as 1,3-diene. Diels Alder reactions (one example). Sulphonation of thiophene purification of Benzene obtained from coal tar). Preparation of furan, Pyrrole and thiophene from 1,4,- dicarbonyl compounds only, Paul-Knorr synthesis, structure of pyridine, Basicity – Aromaticity – Comparison with pyrrole – one method of preparation and properties – Reactivity towards Nucleophilic substitution reaction – chichibabin reaction.

3. Carbohydrates 6 h

Monosaccharides: All discussion to be confined to (+) glucose as an example of aldo hexoses and (-) fructose as example of ketohexoses. Chemical properties and structureal elucidation: Evidences for straight chain pentahydroxy aldehyde structure (Acetylation, reduction to n-hexane, cyanohydrin formation, reduction of Tollen's and Fehling's

reagents and oxidation to gluconic and saccharic acid). Number of optically active isomers possible for the structure, configuration of glucose based on D-glyceraldehyde as primary standard (no proof for configuration is required). Evidence for cyclic structure of glucose (some negative aldehydes tests and mutarotation). Cyclic structure of glucose. Decomposition of cyclic structure (Pyranose structure, anomeric Carbon and anomers). Proof for the ring size (methylation, hydrolysis and oxidation reactions). Different ways of writing pyranose structure (Haworth formula and chair conformationa formula). Structure of fructose: Evidence of 2 – ketohexose structure (formation of penta acetate, formation of cyanohydrin its hydrolysis and reduction by HI to give 2-Carboxy-n-hexane). Same osazone formation from glucose and fructose, Hydrogen bonding in osazones, cyclic structure for fructose (Furanose structure and Haworth formula).
Interconversion of Monosaccharides: Aldopentose to aldo hexose – eg: Arabinose to D-Glucose, D-Mannose (Kiliani - Fischer method). Epimers, Epimerisation – Lobry de bruyn van Ekenstein rearrangement. Aldohexose to Aldopentose eg: D-glucose to D-arabinose by Ruff'f degradation. Aldohexose (+) (glucose) to ketohexose (-) (Fructose) and Ketohexose (fructose) to aldohexose (Glucose)

4. Amino acids and proteins **5 h**

Introduction: Definition of Amino acids, classification of Amino acids into alpha, beta, and gama amino acids. Natural and essential amino acids – definition and examples, classification of alpha amino acids into acidic, basic and neutral amino acids with examples. Methods of synthesis: General methods of synthesis of alpha amino acids (specific examples – Glycine, Alanine, valine and leucene) by following methods: a) from halogenated carboxylic acid b) Malonic ester synthesis c) strecker's synthesis.
Physical properties: Optical activity of naturally occurring amino acids: L-configuration, irrespective of sign rotation, Zwitterion structure – salt like character - solubility, melting points, amphoteric character , definition of isoelectric point.
Chemical properties: General reactions due to amino and carboxyl groups – lactams from gamma and delta amino acids by heating peptide bond (amide linkage). Structure and nomenclature of peptides and proteins.

5. Mass Spectroscopy: **5 h**

Basic principles – Molecular ion / parent ion, fragment ions / daughter ions. Theory – formation of parent ions. Representation of mass spectrum. Identification of parent ion, (M+1), (M+2), base peaks (relative abundance 100%) Determination of molecular formula – Mass spectra of ethylbenzene, acetophenone, n-butyl amine and 1- proponal.

Unit-III (physical chemistry-III) **30hrs (1 h / w)**

1. Chemical kinetics 9 h

Rate of reaction, factors influencing the rate of a reaction-concentration, temperature, pressure, solvent, light, catalyst. Experimental methods to determine the rate of reaction. Definition of order and molecularity. Derivation of rate constants for first, second, third and zero order reactions and examples. Derivation for time half change. Methods to determine the order of reactions. Kinetics of complex reactions (first order only): opposing reactions, parallel reactions. consecutive reactions and chain reactions. Effect of temperature on rate of reaction. Arrhenius equation. concept of activation energy. Theories of reaction rates- collision theory-derivation of rate constant for bimolecular reaction. The transition state theory (elementary treatment).

2. Photochemistry 5 h

Difference between thermal and photochemical processes. Laws of photochemistry-Grothus-Draper's law and Stark-Einstein's law of photochemical equivalence. Quantum yield. Ferrioxalate actinometry. Photochemical hydrogen- chlorine, hydrogen-bromine reaction. Jablonski diagram depicting various processes occurring in the excited state, qualitative description of fluorescence, phosphorescence, non-radiative processes (internal conversion, intersystem crossing). Photosensitized reactions- energy transfer processes (simple example)

3. Thermodynamics 16 h

The first law of thermodynamics-statement, definition of internal energy and enthalpy. Heat capacities and their relationship. Joule's law-Joule-Thomson coefficient. Calculation of w, q, dU and dH for the expansion of perfect gas under isothermal and adiabatic conditions for reversible processes. State function.

Temperature dependence of enthalpy of formation-Kirchoff's equation.

Second law of thermodynamics. Different Statements of the law. Carnot cycle and its efficiency. Carnot theorem. Thermodynamic scale of temperature. Concept of entropy, entropy as a state function, entropy changes in cyclic, reversible, and irreversible processes and reversible phase change. Calculation of entropy changes with changes in V & T and P&T. Entropy of mixing inert perfect gases. Entropy changes in spontaneous and equilibrium processes.

The Gibbs (G) and Hlmholtz (A) energies. A & G as criteria for thermodynamic equilibrium and spontaneity-advantage over entropy change. Gibbs equations and the Maxwell relations. Variation of G with P, V and T.

Paper-IV Chemistry and Industry **90 hrs (3 h / w)**

Unit – I (Physico Chemical methods of analysis) **30 hrs (1 h / w)**

1. Separation techniques **12 h**

1. Solvent extraction: Principle and process, Batch extraction, continuous extraction and counter current extraction. Application – Determination of Iron (III)
2. Chromatography: Classification of chromatography methods, principles of differential migration adsorption phenomenon, Nature of adsorbents, solvent systems, Rf values, factors effecting Rf values.
    a. Paper Chromatography: Principles, Rf values, experimental procedures, choice of paper and solvent systems. developments of chromatogram – ascending, descending and radial. Two dimensional chromatography, applications.
    b. Thin layer Chromatography (TLC): Advantages. Principles, factors effecting Rf values. Experimental procedures. Adsorbents and solvents. Preparation of plates. Development of the chromatogram. Detection of the spots. Applications.
    c. Column Chromatography: Principles. experimental procedures, Stationary and mobile Phases, Separation technique. Applications
    d. High Performance Liquid Chromatography (HPLC): Principles and Applications.
    e. Gas Liquid Chromatography (GLC): Principles and Applications

2. Spectrophotometry **4 h**

General features of absorption – spectroscopy, Beer-Lambert's law and its limitations, transmittance, Absorbance, and molar absorptivity. Single and double beam spectrophotometers. Application of Beer-Lambert law for quantitative analysis of

1. Chromium in $K_2Cr_2O_7$
2. Manganese in manganous sulphate
3. Iron (III) with thiocyanate.

3. Molecular sectorscopy **14 h**

(i) Electronic spectroscopy:

Interaction of electromagnetic radiation with molecules and types of molecular spectra. Potential energy curves for bonding and antibonding molecular orbitals. Energy levels of molecules (σ,π, n) . Selection rules for electronic spectra. Types of electronic transitions in molecules effect of conjugation. Concept of chromophore.

(ii) Infra red spectroscopy

Energy levels of simple harmonic oscillator, molecular vibration spectrum, selection rules. Determination of force constant. Qualitative relation of force constant to bond energies. Anharmonic motion of real molecules and energy levels. Modes of vibrations in polyatomic molecules. Characteristic absorption bands of various functional groups. Finger print nature of infrared spectrum.

(iii) Raman spectroscopy

Concept of polarizavility, selection rules, pure rotational and pure vibrational Raman spectra of diatomic molecules, selection rules.

(iv) Proton magnetic resonance spectroscopy

Principles of nuclear magnetic resonance, equivalent and non-equivalent protons, position of signals. Chemical shift, NMR splitting of signals – spin-spin coupling, coupling constants. Applications of NMR with suitable examples – ethyl bromide, ethanol. acetaldehyde. 1.1.2-tribromo ethane, ethyl acetate, toluene and acetophenone.

(v) Spectral interpretation

Interpretation of IR, UV-Visible, 1H-NMR and mass spectral data of the following compounds 1. Phenyl acetylene 2. Acetophenone 3.Cinnamic Acid 4. para-nitro aniline.

Unit – II (Drugs, formulations, pesticides and green chemistry) 30 hrs (1 h / w)

1. Drugs **17 h**

1. Introduction: Drug, disease (definition), Historical evolution, Sources – Plant, Animal synthetic, Biotechnology and human gene therapy
2. Terminology: Pharmacy, Pharmacology, Pharmacophore, Pharmacodynamics, Pharmacokinetics (ADME, Receptors – brief teartment) Metabolites and Anti metabolites.
3. Nomenclature: Chemical name, Generic name and trade names with examples
4. Classification: Classification based on structures and therapeutic activity with one example each.
5. Synthesis: Synthesis and therapeutic activity of the following drugs., L-Dopa, Chloroquin, Omeprazole, Albuterol and ciprofloxacin.
6. Drug Development: Pencillin, Separation and isolation, structures of different pencillins
7. HIV-AIDS: Immunity – CD-4 cells, CD-8 cells Retrovirus, replication in human body. Investigation available, prevention of AIDS. Drugs available – examples with structures: PIS: Indinavir (Crixivan), Nelfinavir (Viracept), NNRTIS: Efavirenz (Susrtiva), Nevirapine (Viramune) NRTIs: Abacavir (Ziagen), Lamivudine (Epivir, 3TC) Zidovudine (Retravir, AZT, ZDV)
8. Monographs of drugs: Eg Paracetamol, Sulpha methoxazole (Tablets)

2. FORMULATIONS 3 h

1. Need of conversion of drugs into medicine. Additives and their role (brief account only)
2. Different types of formulations

3. PESTICIDES 5 h

1. Introduction to pesticides – types – Insecticides, Fungicides, Herbicides, Weedicides, Rodenticides plant growth regulators, Pheremones and Hormones. Brief discussion with examples, Structure and uses.
2. Synthesis and presnt status of the following.
   DDT, BHC, Malathion, Parathion, Endrin, Baygon, 2,4-D and Endo-sulphon

4. GREEN CHEMISTRY 5h

Introduction: Definition of green Chemistry, need of green chemistry, basic principles of green chemistry

Green synthesis: Evalution of the type of the reaction i) Rearrangements (100% atom economic), ii) Addition reaction (100% atom economic), Pericyclic reactions (no by-product).

Selection of solvent:

i) Aqueous phase reactions ii) Reactions in ionic liquids iii) Solid supported synthesis iv) Solvent free reactions (solid phase reactions)

ii) Green catalysts: i) Phase transfer catalysts (PTC) ii) Biocatalysts

Microwave and Ultrasound assisted green synthesis:

1. Aldol condensation
2. Cannizzaro reaction
3. Diels-Alder reactions
4. Strecker synthesis
5. Willaimson synthesis
6. Dieckmann condensation

Unit-III: (Macromolecules, materials Science and catalysis) 30 hrs (1 h / w)

1. Macromolecules 10h

Classification of polymers, chemistry of polymerization, chain polymerization, step polymerization, coordination polymerization – tacticity. Molecular weight of polymers-number average and weight average molecular weight, degree of polymerization, determination of molecular weight of polymers by viscometry, Osmometry and light scattering methods. Kinetics of free radical polymerization, derivation of rate law. Preparation and industrial application of polyethylene, PVC, Teflon, polyacrylonitrile, terelene and Nylon66. Introduction to biodegradability.

2. Materials science 8h

Superconductivity, characteristics of superconductors, Meissner effect, types of superconductors and applications.

Nanomaterials- synthetic techniques, bottom-up-sol-gel method, top-down- electro deposition method. Properties and applications of nano-materials. Composites-definition, general characteristics, particle reinforce and fiber reinforce composites and their applications.

3. **Catalysis** **12h**

Homogeneous and heterogeneous catalysis, comparision with examples. Kinetics of specific acid catalyzed reactions, inversion of cane sugar. Kinetics of specific base catalyzed reactions, base catalyzed conversion of acetone to diacetone alcohol. Acid and base catalyzed reactions- hydrolysis of esters, mutarotation of glucose. Catalytic activity at surfaces. Mechanisms of heterogeneous catalysis. Langmuir-Hinshelwood mechanism. Enzyme catalysis: Classification, characteristics of enzyme catalysis. Kinetics of enzyme catalyzed reactions-Michaelis Menton law, significance of Michaelis constant (K_m) and maximum velocity (V_{max}). Factors affecting enzyme catalysis- effect of temperature, pH, concentration and inhibitor. Catalytic efficiency. Mechanism of oxidation of ethanol by alcohol dehydrogenase.

LABORATORY COURSE – III

Practical Paper – III (Organic Chemistry) **90 hrs (3 h / w)**

1. Synthesis of Organic Compounds

i. Aromatic electrophilic substitution Nitration: Preparation of nitro benzene and p-nitro acetanilide, Halogenation: Preparation of p-bromo acetanilide – preparation of 2,4,6-tribromo phenol.
ii. Diazotization and coupling: Preparation of pheyl azo β-napthol
iii. Oxidation: Preparation of benzoic acid from benzoyl chloride
iv. Reduction: Preparation of m-nitro aniline from m-dinitro benzene
v. Esterfication: Preparation of methyl p-nitro benzoate from p-nitro benzoic acid.
vi. Methylation: Preparation of β-napthyl methyl ether
Condensation: Preparation of benzilidine aniline and Benzoyl aniline.

2. Thin layer Chromatography & Column Chromatography

i. Acetylation of salicyclic acid, aniline, Benzoylation of Aniline and Phenol
Determination of Rf values and identification of organic compounds: preparation and separation of 2,4-dinitrophenyl hydrazones of acetione and 2-butanone using toluene and light petroleum(40:60)
ii. Separation of ortho & para nitro aniline mixtures

III. Organic Qualitative Analysis:

i. Identification of an organic compound through the functional group analysis, determination of melting point and preparation of suitable derivatives.
ii. Separation of two component mixtures
1) Aniline + Naphthalene 2) Benzoic acid + Benzophenone 3) p-Cresol + Chlorobenzene.

4. Demonstration experiments:

1. Steam distillation experiment 2) microwave assisted synthesis, two examples.

LABORATORY COURSE - IV

Practical Paper IV (Physical Chemistry) **90hrs (3 h / w)**

1. Chemical kinetics

i. Determination of specific reaction rate of the hydrolysis of methyl acetate catalyzed by hydrogen ion at room temperature.
ii. Determination of rate of decomposition of hydrogen peroxide.
iii. Determination of overall order of saponification of ethyl acetate

2. Distribution law

i. Determination of distribution coefficient of iodine between water and carbon Tetrachloride.
ii. Determination of molecular status and partition coefficient of benzoic acid in Toluene and water.

3. Electrochemistry

i. Determination of concentration of HCl conductometrically using standard NaOH solution.
ii. Determination of concentration of acetic acid conductometrically using standard NaOH solution.
iii. Determination of dissociation constant (K_a) of acetic acid by conductivity measurements.
iv. Determination of solubility and solubility product of $BaSO_4$.
v. Determination of redox potentials of Fe^{2+}/Fe^{3+} by potentiometric titration of ferrous ammonium sulphate vs. potassium dichromate.

4. pH metry

i. Preparation phosphate buffer solutions
ii. pH metric titration of weak acid, acetic acid with strong base NaOH and calculation of dissociation constant.

5. Colorimetry

i. Verification of Beer-Lambert law for $KMnO_4$, $K_2Cr_2O_7$ and determination of concentration of the given solution.
ii. Verification of Beer-Lambert law for $CuSO_4$ and determination of concentration of the given solution.
iii. Composition of complex of Cu^{2+} - EDTA disodium salt

6. Adsorption

i. Surface tension and viscosity of liquids.
ii. Adsorption of acetic acid on animal charcoal, verification of Freundlich isotherm.

7. Project Work:

Collection of spectral data of a minimum of six compounds belonging to different functional groups (other than those included in the syllabus) and submission of the report.

NOTE: From the above experiments one experiment of 40 marks at the University examination and 10 marks for the project work.