Course Structure for M Sc (Chemistry)

Bundelkhand University, Jhansi

Paper No.	Nomenclature	Marks
Ist Sem.		50
CHY - 101	(a) Mathematics for chemist or (b) Biology for Chemist	
CHY - 102	Computer for Chemist	50
CHY - 103	Inorganic Chemistry	50
CHY - 104	Organic Chemistry	50
CHY - 105	Physical Chemistry	50
	Practical (Organic & Physical)	100
IInd Sem.		
CHY - 106	Chemical bonding & Group theory	50
CHY - 107	Inorganic Chemistry	50
CHY - 108	Organic Chemistry	50
CHY - 109	Physical Chemistry	50
CHY - 110	Spectroscopy	
	Practical (Inorganic & Analytical)	100
IIIrd Sem.		
CHY - 111	Application Of Spectroscopy	50
CHY - 112	Bio-Chemistry	50
CHY - 113	Analytical Techniques	50
CHY - 114	Elective paper – I (a/b/c/d)	50
CHY - 115	Elective paper – II (a/b/c/d)	50
	Practical (Organic, Inorganic & Physical)	100
IVth Sem.		
CHY - 116	Photochemistry & Solid state Chemistry	50
CHY - 117	Environmental Chemistry	50
CHY - 118	Elective paper – III (a/b/c/d)	50
CHY - 119	Elective paper – IV (a/b/c/d)	50
	Practical (Organic, Inorganic & Physical)	100

Total Marks:1400

I st Semester

CHY - 101: (a) Mathematics for chemist:

1. Vector and matrix algebra
2. Differential calculus
3. Integral calculus
4. Elementary differential equations
5. Permutation and probability
6. Statistics

Or (b) Biology for Chemist

1. Cell structure and function
2. Carbohydrates
3. Lipids
4. Proteins
5. Nucleic acid

CHY - 102: Computer for Chemist:

1. Introduction to computers and computing,
2. Computer programming in FORTRAN / Basic
3. Programming in Chemistry
4. Use of Computer Programmes

CHY - 103: Inorganic Chemistry

1. Stereochemistry and Bonding in Main Group Compounds,
2. Metal - Ligand Equilibria in Solution,
3. Metal-Ligands Bonding,
4. Metal π-Complexes,
5. Isopoly and Heteropoly Acids and Salts.

CHY - 104: Organic Chemistry

1. Nature of bonding in organic molecules:
2. Stereochemistry
3. Reaction mechanism- Structure and reactivity
4. Pericyclic Reactions

CHY - 105: Physical Chemistry

1. Quantum Chemistry

(a) Introduction to Exact quantum mechanical results
(b) Approximate methods
(c) Angular momentum
(d) Electronic structure of atoms
(e) Molecular orbital theory

2. Thermodynamics:

(a) Classical thermodynamics
(b) Statistical thermodynamics:
(c) Non Equilibrium thermodynamics

CHY - 101: (a) Mathematics for Chemist

1. **Vector and matrix algebra: A. Vectors**- Vectors, dot, cross and triple products etc. the gradient, divergence & curl, vector calculus, Gauss' theorem, divergence theorem. **B. Matrix algebra**: addition and multiplication, inverse, adjoint and transpose of matrices, special matrices (symmetric, skew symmetric, hermitian, skew hermitian, unit, diagonal, unitary etc) and their properties, matrix equations: homogeneous, non homogeneous linear equations and conditions for the solution, linear dependence and independence, introduction to vector spaces, matrix eigenvalues and eigenvectors, diagonalization, determinants (examples from Huckel theory), introduction to tensors, polarizability and magnetic susceptibility as examples.
2. **Differential calculus:** Functions, continuity and differentiability, rules for differentiation, applications of differential calculus including maxima and minima (examples related to maximally populated rotational energy levels, Bohr's radius and most probable velocity from Maxwell distribution etc), exact and inexact differentials with their applications to thermodynamic properties.
3. **Integral calculus**: basic rules for integration, integration by parts, partial fraction and substitution, reduction formulae, applications of integral calculus, functions of several variables, partial differentiation, co-ordinate transformations (e.g. Cartesian to spherical polar, curve sketching.
4. **Elementary differential equations:** variables-separable and exact first-order differential equations, homogeneous, exact and linear equations, applications to chemical kinetics, secular equilibria, quantum chemistry etc, solutions of differential equations by the power series method, Fourier series, solutions of harmonic oscillator and legendre equation etc, spherical harmonics, second order differential equations and their solutions.
5. **Permutation and probability:** permutations and combinations, probability and probability theorems, probability curves, average, root mean square and most probable errors, example from the kinetic theory of gases etc, curve fitting (including least squares fit etc) with a general polynomial fit.
6. **Statistics:** mean, median, mode, standard deviations, and Correlation coefficient, student t-test.

Or CHY - 101: (b) Biology for Chemist

1. **Cell structure and function:** structure of prokaryotic and eukaryotic cells, intracellular organelles and their functions, comparison of plant and animal cells, overview of metabolic processes-catabolism and anabolism, ATP- the biological energy currency, origin of life- unique properties of carbon, chemical evolution and rise of living systems, introduction to biomolecules, building blocks of bio-macromolecules.
2. **Carbohydrates:** conformation of monosaccharides, structure and functions of important derivatives of monosaccharides like glycosides, deoxy sugars, myoinosital, amino sugars, N-acetylmuramic acid, sialic acid, disaccharides and polysaccharides, structural polysaccharides-cellulose and chitin, storage polysaccharides-starch and glycogen, structure and biological functions of glucosaminoglycans or mucopolysaccharides, carbohydrates of glycoproteins and glycolipids, role of sugars in biological recognition, blood group substances, ascorbic acid, carbohydrate metabolism-Krebs' cycle, glycolysis, glycogenesis and glycogenolysis, gluconneogenesis, pentose phosphate pathway.
3. **Lipids:** Fatty acids, essential fatty acids, structure and function of triacylglycerols, glycerophopholipids, sphingolipids, cholesterol, bile acids, prostaglandins, lipoproteins-composition and function, role in atherosclerosis, properties of lipid aggregates-micelles, bilayers, liposomes and their possible biological functions, biological membranes, fluid mosaic model of membrane structure, lipid metabolism-β-oxidation of fatty acids.
4. **Proteins:** chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing, secondary structure of proteins, forces responsible for holding of secondary structures, α-helix, β-sheets, super secondary structure, triple helix structure of collagen, tertiary structure of protein-folding and domain structure, quaternary structure, amino acid metabolism-degradation and biosynthesis of amino acids, sequence determination: chemical/enzymatic/ mass spectral/racemization /detection, chemistry of oxytocin and tryptophan releasing hormone (TRH).

5. **Nucleic acids:** purine and pyrimidine bases of nucleic acids, base pairing via H-bonding, structure of ribonucleic acid (RNA) and deoxyribonucleic acid (DNA), double helix model of DNA and forces responsible for holding it. Chemical and enzymatic hydrolysis of nucleic acids, the chemical basis for heredity, an overview of replication of DNA, transcription, transpation and genetic code, chemical synthesis of mono and tri nucleosides.

CHY - 102: Computer for Chemist

1. **Introduction to computers and computing:** Basic structure and functioning of computers with a PC as an illustrative example, Memory, I/O devices, secondary storage, computer language, operating systems with DOS as an example, introduction to UNIX and WINDOWS, data processing, principles of programming, algorithms and flow-charts.

2. **Computer programming in FORTRAN / Basic**: Elements of the computer language, constants and variables, operations and symbols, expressions, arithemetic assignment statement, input and output. Format statement, termination statements, and branching statements such as IF or GO TO statement. Logical variables double precision variables, subscribed variables and Dimension, DO statement, FUNCTION and SUBROUTINE, COMMON and DATA statements.

3. **Programming in Chemistry:** Development of small computer codes involving simple formulae in chemistry, such as Vander Waals equation, pH titration, kinetics, radioactive decay, evaluation of lattice energy and ionic radii from experimental data, linear simultaneous equations to solve secular equations within the Huckel's theory, elementary structural features such as bond lengths, bond angles, dihedral etc of molecules extracted from a database such as Cambridge data base.

4. **Use of Computer Programmes**: The students will learn how to operate a PC and how to run standard programmes and packages, execution of linear regression, X-Y plot, numeriacal integration and differentiation as well as differential equation solution programmes, monte carlo and

molecular dynamics, programmes with data preferably from physical chemistry laboratory, further, the students will operate one or two or the packages such as MATLAB, EASYPLOT, LOTUS, FOXPRO, FOXPRO and Word processing software such as WORDSTAR/MS-WORD.

CHY - 103: Inorganic Chemistry

1. **Stereochemistry and Bonding in Main Group Compounds:** VSEPR, Walsh diagram (tri- and penta- atomic molecules), d_{π}-p_{π} bonds, Bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules.

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

3. **Metal-Ligands Bonding:** Crystal field splitting in an octahedral and tetrahedral field, factors affecting the crystal field stabilizing energy, consequence of crystal field splitting, Dynamic & Static John-Teller Effect, Limitation of crystal field theory, Site selection in spinals, molecular orbital theory, octahedral, tetrahedral and square planar complexes, π-bonding and molecular orbital theory.

4. **Metal π-Complexes:** Metal carbonyls, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls, preparation, bonding, structure and important reactions of transition metal nitrosyl, dinitrogen and dioxygen complexes, tertiary phosphine as ligands.

5. **Isopoly and Heteropoly Acids and Their Salts**.

CHY - 104: Organic Chemistry

1. **Nature of bonding in organic molecules:** Delocalized chemical bonding-conjugation, cross conjugation, resonance, hyperconjugation, bonding in fullerenes, tautomerism, Aromaticity in benzenoid and non-benzenoid compounds, alternant and non-alternant hydrocarbons, Huckel's rule, energy level of π-molecular orbitals, annulenes, anti-aromaticity, ψ-aromaticity, homo-aromaticity, PMO approach, bonds weaker than covalent – addition compounds, crown ether complexes and cryptands, inclusion compounds, cyclodextrins, catenanes and rotaxanes.

2. **Stereochemistry:** Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity. Conformation of sugar, steric strain due to unavoidable crowding, elements of symmetry, chirality, molecules with more than one chiral center, threo and erythro isomers, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis, asymmetric synthesis, optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape, stereochemistry of the compounds containing nitrogen, sulphur and phosphorus.

3. **Reaction mechanism- Structure and reactivity:** Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle, potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects, hard and soft acids and bases, generation, structure, stability and reactivity of carbocations, free radicals, carbenes and nitrenes, effect of structure on reactivity-resonance and field effects, steric effect, quantitative treatment, the Hammett equation and linear free energy relationship, substitutent and reaction constants, Taft equation.

4. **Pericyclic Reactions:** Molecular orbital symmetry, Frontier orbitals of ethylene, 1, 3-butadiene, 1,3,5-Hexatriene and allyl system, classification of pericyclic reactions, Woodward-Hoffmann correlation diagrams, FMO

and PMO approach, Electrocyclic reactions-conrotatory and disrotatory motions, 4n and 4n + 2 systems, 2 + 2 addition of ketenes, 1, 3dipolar cycloadditions and cheleotropic reactions. Sigmatropic rearrangements-suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 3,3-and 5,5-sigmatropic rearrangements, claisen, cope and aza-cope rearrangements, fluxional tautomerism, Ene reaction.

CHY - 105: Physical Chemistry

1. Quantum Chemistry

A. Introduction to Exact quantum mechanical results: The Schrodinger equation and the postulates of quantum mechanics, discussion of solutions of the Schrodinger equation to some model systems viz., particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom.

B. Approximate methods: The variation theorem, linear variation principle, perturbation theory (first order and non-degenerate). Applications of variation method and perturbation theory to the helium atom.

C. Angular momentum: Ordinary angular momentum, generalized angular momentum, eigen functions for angular momentum, eigen values of angular momentum, operator using ladder operators, addition of angular momenta, spin, antisymmetry and pauli exclusion principle.

D. Electonic structure of atoms: Electronic configuration, Russell-Saunders terms and coupling schemes, Slater-Condom parameters, term seperation energies of the p^n configuration, term seperation energies for the d^n configurations, magnetic effects: spin-orbit coupling and Zeeman splitting, introduction to the methods of self-consistent field, the virial theorem.

E. Molecular orbital theory: Huckel theory of conjugated systems, bond order and charge density calculations, applications to ethylene, butadiene, cyclopropeneyl radical, cyclobutadiene etc, introduction to external Huckel theory.

2. Thermodynamics:

A. Classical thermodynamics: Brief resume of concepts of laws of thermodynamics, free energy, chemical potential and entropies, partial molar free energy, partial molar volume and partial molar heat content and their significances, determinations of these quantities, concept of fugacity and determination of fugacity. Non-ideal systems: Excess functions for non-ideal solutions, activity, activity coefficient, Debye-Huckel theory for activity coefficient of electrolytic solutions, determinations of activity and activity coefficients, ionic strength, application of phase rule to three component systems, second order phase transitions.

B. Statistical thermodynamics: Concept of distribution, thermodynamic probability and most probable distribution, Ensemble averaging, postulates of ensemble averaging, canonical, grand canonical and microcanonical ensembles, corresponding distribution laws (Using Lagrange's method of undetermined multipliers), partition functions-translational, rotational, vibrational and electronic partion functions, calculation of thermodynamic properties in terms of partition functions, applications of partition functions, heat capacity behaviour of solids-chemical equilibria and equilibrium constant in terms of partition functions, Fermi-dirac statistics, distribution law and applications to metal, bose-einstein statics-distribution law and application to helium.

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

Syllabus of M Sc Chemistry Practical (Ist Semester)

M M 100 (30 + 25 + 25 + Viva 10 + Record 10)

(Inorganic, Organic and Physical)

Qualitative and quantitative analysis in Inorganic Chemistry

(a) Less common metlions: Ti, Mo, W, Ti, Zr, Th, V, U (two metal ions in cationic/anionic forms)

(**b) Insolubles** - oxides, sulphates and halides

Chromatography

Separation of cations and anions by

(a) Paper Chromatography

(b) Column Chromatography -Ion exchange.

Organic Chemistry:

Qualitative Analysis

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

Organic Synthesis Acetylation:

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

Oxidation: Adipic acid by chromic acid, oxidation of cyclohexanol

Grignard reaction: Synthesis of triphenylmethanol from benzoic acid

Physical Chemistry:

Error Analysis and Statistical Data Analysis

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

Apparatus: burette, pipette and standard flask.

Adsorption

To study surface tension - concentration relationship for solutions (Gibbs equation).

Phase Equilibria

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

(ii) Determination of glass transition temperature of a given salt (e.g., $CaCl_2$) conductometrically.

(Hi) To construct the phase diagram for three component system (e.g. chloroform-acetic acid-water).

Chemical Kinetics

(i) Determination of the effect of (a) Change of temperature (b) Change of concentration of reactants aad' catalyst and (c) Ionic strength of the media on the velocity constant of hydrolysis of an ester/ionic reactions.

(ii) Determination of the velocity constant of hydrolysis of an ester/ionic reaction in micellar media.

(iii) Determination of the rate constant for the oxidation of iodide ions by hydrogen peroxide studying the kinetics as an iodine clock reaction.

(iv) Flowing clock reactions (Ref: Experiments in Physical Chemistry by Showmaker)

(v) Determination of the primary salt effect on the kinetics of ionic reactions and testing of the Bronsted relationship (iodide ion is oxidised by persulphate ion)

(vi) Oscillatory reaction.

Solutions

(i) Determination of molecular weight of non-volatile and non-electrolyte/electrolyte by cryoscopic method and to determine the activity coefficient of an electrolyte .

. (ii) Determination of the degree of dissociation of weak electrolyte and to study the deviation from ideal behaviour that occurs with a strong electrolyte.

M Sc – IInd semester

CHY - 106: Chemical bonding & Group theory

CHY - 107: Inorganic Chemistry

1. Reaction mechanism of transition metal complexes
2. Electronic spectra and magnetic properties of transition metal complexes
3. Metal-Clusters

CHY - 108: Organic Chemistry

1. Aliphatic Nucleophilic substitution
2. Aliphatic Electrophilic substitution
3. Aromatic Electrophilic substitution
4. Aromatic Nucleophilic substitution
5. Free radical reactions
6. Addition to Carbon-Carbon multiple bonds
7. Addition to Carbon – Hetero multiple bonds
8. Elimination Reactions

CHY - 109: Physical Chemistry

1. Chemical Dynamics
2. Surface Chemistry
   (a) Adsorption
   (b) Micelle
   (c) Macromolecules
3. Electrochemistry

CHY - 110: Spectroscopy

1. Microwave spectroscopy
2. Vibrational spectroscopy
   A. Infrared spectroscopy
   B. Raman spectroscopy
3. Electronic spectroscopy
   A. Atomic spectroscopy
   B. Molecular spectroscopy
4. Magnetic resonance spectroscopy
   a. Nuclear Magnetic resonance spectroscopy
   b. Electron spin resonance spectroscopy
   c. Nuclear Quadrupole resonance spectroscopy:
5. X-ray Diffraction

CHY - 106: Chemical bonding & Group theory

1. Concepts in Molecular Orbital and Valence Bond Theory:

Quantitive MO theory: Huckel molecular orbital (HMO) method as applied to ethane, allyl and butadiene, Qualitative MO theory, Ionization potential, Electron affinities, MO energy levels, Orbital symmetry, Orbital interaction diagrams, MO of simple Organic systems such as ethane, allyl, butadiene, methane and methyl group, conjugation, hyper conjugation and 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.

2. Supramolecular Chemistry:

Properties of covalent bonds: Bond length, Inter bond – angles, Force constant, bond and molecular dipole moments. Molecular and bond polarizability, bond dissociation enthalpy, Intermolecular forces, hydrophobic effects, electrostatic, induction, dispersion and resonance energy, Magnetic interactions, magnitude of interaction energy, forces between macroscopic bodies, medium effects, hydrogen bond.

Principles of molecular association and organization as exemplified in biological macromolecules like enzymes, nucleic acids, membranes and model systems like micelles and vesicles. Molecular receptors and design principles, cryptands, cyclophanes, calixeranes, cyclodextrines, supramolecular reactivity and catalysis, molecular channels and transport processes, molecular devices and nanotechnology.

3. Symmetry and group theory in chemistry: symmetry elements and symmetry operation, definition of group, subgroup, relation between orders of a finite group and its subgroup, conjugacy relation and classes, point symmetry group, schonfiles symbols, representations of groups by matrices (representation for the C_n, C_{nv}, C_{nh}, D_{nh} etc groups to be worked out explicity). character tables and their use, spectroscopy.

CHY - 107: Inorganic Chemistry

1. **Reaction mechanism of transition metal complexes**: Energy profile of a reaction, reactivity of metal complexes, inert and labile complexes, kinetic application of valence bond and crystal field theories, kinetics of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidences in favor of conjugate mechanism, anation reactions, reactions without metal ligand bond cleavage, substitution reactions in square planar complexes, the trans effect, mechanism of the substitution reaction, redox reactions, electron transfer reactions, mechanism of one electron transfer reactions, outer-sphere type reactions, cross reactions and Marcus-hush theory, inner sphere type reactions.

2. **Electronic spectra and magnetic properties of transition metal complexes:** Spectroscopic ground states, correlation, Orgel and Tanabe –Sugano diagrams for transition metal complexes (d^1-d^9 states), calculations of Dq, B and β parameters, charge transfer spectra, spectroscopic method of assignment of absolute configuration in optically active metal chelates and their stereochemical information, anomalous magnetic moments, magnetic exchange coupling and spin crossover.

3. **Metal-Clusters:** Higher boranes, carboranes, metalloboranes and metallocarboranes, metal carbonyl and halide clusters, compounds with metal-metal multiple bonds.

CHY - 108: Organic Chemistry

1. **Aliphatic Nucleophilic substitution:** The S_N2, S_N1, mixed S_N2 and S_N1, and SET mechanism, the neighboring group mechanism, neighboring group participation by π and σ bonds, anchimeric assistance, classical and non classical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements, application of NMR spectroscopy in the detection of carbocations, the Sn^i mechanism, nucleophilic substitution at an allylic, aliphatic trigonal and vinylic carbon, reactivity effects of substrate

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

2. **Aliphatic Electrophilic substitution:** Biomolecular mechanism-S_E2 and S_E1, The S_E1 mechanism, electrophilic substitution accompanied by double bond shifts, effect of substrates, leaving group and solvent polarity on the reactivity.

3. **Aromatic Electrophilic substitution:** The arenium ion mechanism, orientation and reactivity, energy profile diagrams, the ortho/para ratio, ipso attack, orientation in other ring systems, quantitative treatment of reactivity in substrate and electrophiles, diazonium coupling, vilsmeir reaction, Gatterman Koch reaction.

4. **Aromatic Nucleophilic substitution:** The S_NAr, S_N1, benzyne and $S_{RN}1$ mechanisms, reactivity-effect of substrate structure, leaving group and sttacking nucleophile, the Von Richter, Sommlet-Houser and Smiles rearrangements.

5. **Free radical reactions:** Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighboring assistance, reactivity for aliphatic and aromatic substrates at a bridgehead, reactivity in the attacking radicals, the effect of solvents on reactivity. allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts, Sandmeyer reaction, free radical rearrangement, Hunsdicker reaction.

6. **Addition to Carbon-Carbon multiple bonds:** Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemoselectivity, orientation and reactivity, addition to cyclopropane ring, hydrogenation of double and triple bonds, hydrogenation of aromatic rings, hydroboration, Michael reaction, sharpless asymmetric epoxidation.

7. **Addition to Carbon – Hetero multiple bonds:** Mechanism of mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds,

acids, esters and nitriles, addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds, Wittig reaction, mechanism of condensationr involving enolates-aldol, knovenagel, Claisen, Mannich, benzoin, Perkin and Stobbe Reactions. hydrolysis of esters and amides, ammonolysis of esters.

8. **Elimination Reactions:** The E^2, E^1 and E^1cb mechanisms and their spectrum, orientation of the double bond, reactivity - effects of substrate structures, attacking base, the leaving group and the medium, mechanism and orientation in pyrolytic elimination.

CHY - 109: Physical Chemistry

1. Chemical dynamics:

Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation and the activated complex theory, ionic reactions, kinetic salt effects, steady state kinetics, kinetic and thermodynamic control of reactions, treatment of unimolecular reactions. Dynamic chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogen-bromine and hydrogen–chloride reactions) and oscillatory reactions (Belousov-Zhabotinsky reaction), homogeneous catalysis, kinetics of enzyme reaction, general features of fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis and the nuclear magnetic resonance method. dynamics of molecular motions, probing the transition state, dynamics of barrierless chemical reactions in solution, dynamics of unimolecular reactions (Lindmann- Hinshelwood and Rice-Ramsperger-Kassel-Marcus [RRKM], theories of unimolecular reactions)

2. 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 surface area (BET

equation), surface films on liquids (electro-kinetic phenomenon), catalytic activity at surfaces.

B. Micelles: Surface active agents, classification of surface active agents, micellization, Hydrophobic interaction, Critical 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.

C. Macromolecules: Polymer-Definition, Types of Polymers, Electrically conducting, Fire Resistant, Liquid Crystal Polymers, Kinetics of Polymerization, Mechanism of Polymerization, Molecular Mass, Number and Mass Average Molecular Mass, Molecular Mass Determination (Osmometry, viscometry, Diffusion and light scattering methods), Sedimentation, Chain Configuration of Macromolecules, Calculation of Average Dimensions of Various Chain Structures.

3. Electrochemistry: Electrochemistry of solutions, Debye-Huckel-Onsager electro treatment and its extension, ion solvent intractions, Debye-Huckel-Jerum mode, Thermodynamics of electrified interface equations, Derivation of electro-capillarity, Lippmann equations (surface excess), Methods of determination, structure of electrified interfaces, Guoy –Chapman, Stern, Graham- Devanathan-mottwatts, Tobin, Bockris, Devanathan models, over potentials, exchange current density, derivation of Butler-Volmer equation, Tafel plot, quantum aspects of charge transfer at electrodes-solution interfaces, quantization of charge transfer, tunneling, semiconductor interfaces-theory of double layer at semiconductor, electrolyte solution interfaces, structure of double layer interfaces, effect of light at semiconductor solution interface.

Electrocatalysis – Influence of various parameters, hydrogen electrode. bioelectrochemistry, threshold membrane phenomena, Nernst-Plank equation, Hodges-polarography theory, Ilkovic equation, half wave potential and its significance, introduction to corrosion, homogenous theory, forms of corrosion, monitoring and prevention methods for corrosion

CHY - 110: Spectroscopy

1. **Microwave spectroscopy:** classification of molecules, molecular requirement for rotational spectra, the molecule as a rigid rotor, non-rigid rotor, effect of isotopic substitution on the transition frequencies, intensities, stark effect, nuclear and electron spin interaction and effect of external field, application.

2. **Vibrational spectroscopy:**
   - **A. Infrared spectroscopy:** linear harmonic oscillator, features of vibrational-rotational spectra, vibrational energies of diatomic molecules, zero point energy, frequency, force constant and bond strengths, molecules as anharmonic oscillator, morse potential energy diagram, the interaction of rotations and vibrations, molecules as vibrating rotator: fine structure of infra red bands, P, Q and R branches, breakdown of oppenheimer approximation, vibration of polyatomic molecules, selection rules, normal modes of vibration, group frequencies, overtones, Thermal distribution of vibrational & rotational levels, factors affecting the band positions and intensities, analysis and application of infrared spectroscopy.
   - **B. Raman spectroscopy:** Classical and Quantum theories of Raman effect, pure rotational, vibrational and vibrational-rotational raman spectra, coherent anti stokes and stokes lines, selection rules, mutual exclusion principle, resonance Raman spectroscopy, infra red *vs* raman spectroscopy.

3. **Electronic spectroscopy:**
   - **A. Atomic spectroscopy:** structure of atoms, atomic quantum number, energies of atomic orbital, electronic angular momentum, vector representation of momenta and vector coupling, spectra of hydrogen atom and alkali metal atoms.
   - **B. Molecular spectroscopy:** Energy levels, molecular orbitals, vibronic transitions, vibrational progressions and geometry of the excited states, Frank condon principle, electronic spectra of polyatomic molecules,

predissociation, emmision spectra, radiative and non-radiative decay, internal conversion, spectra of transition metal complexes, charge transfer spectra.

4. Magnetic resonance spectroscopy:

A. **Nuclear Magnetic resonance spectroscopy:** Nuclear spin, interaction between spin and a magnetic field, nuclear resonance, shielding of magnetic nuclei, chemical shift and its measurnments, factors influencing chemical shift, deshielding, spin-spin interactions, factors influencing coupling constant 'J', classification to AX, A_2, AMX, ABC etc, spin decoupling, basic idea about instrument, NMR studies of nuclei other than proton-^{13}C, ^{19}F and ^{31}P, FTNMR, advantages of FTNMR, use of NMR in medical diagnostics.

B. **Electron spin resonance spectroscopy:** basic principles, zero field splitting and Kramer's degeneracy, factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densities and McConnell relationship, measurement techniques, applications**.**

C. **Nuclear Quadrupole resonance spectroscopy:** Quadrupole nuclei, quadrupole moments, electric field gradient, coupling constant, splitting, applications.

5. X-ray diffraction: Bragg condition, miller indices, laue method, Bragg method, Debye-Scherrer method of X-ray structural analysis of crystals, index reflections, identification of unit cells from systematic absences in diffraction pattern, structure of simple lattices and X-ray intensities, structure factor and its relation to intensity and electron density, phase problem, description of the procedure for an X-ray structure analysis, absolute configuration of molecules, Ramchandran diagram.

Syllabus of M Sc Chemistry Practical (II nd Semester)

M M 100 (30 + 25 + 25 + Viva 10 + Record 10)

INORGANIC CHEMISTRY:

Preparations

Preparation of selected inorganic compounds and their studies by I.R., Electronic spectra, Mossbauer, E.S.A. and magnetic susceptibility measurements. Handling of air and moisture sensitive compounds

(1) $VO(acac)_2$

(2) $TiO(C_9H_8NO)_2.2H_20$

(3) cis-$K[Cr(C_20_4)_2(H_20)_2]$

(4) $Na[Cr(NH_3)_2(SCN)_4]$

(5) $Mn(acac)_3$

(6) $K_3[Fe(C_20_4)_3]$

(7) Prussian Blue, Turnbull's Blue.

(8) $Co(NH_3)_6][Co(N0_2)_6]$.

(9) cis-$[Co(trien)(N0_2)_2]CI.H_20$

(10) $Hg[Co(SCN)_4]$

(11) $[Co(Py)_2CI_2]$

(12) $[Ni(NH_3)_6]CI_2$

(13) $Ni(DMG)_2$

(14) $[Cu(NH_3)_4]S0_4.H_20$

ORGANIC CHEMISTRY:

Aldol condensation: Dibenzal acetone from benzaldehyde

Sandmeyer reaction: p-Chlorotoluene from p-toluidine

Acetoacetic ester Condensation:

Synthesis of ethyl-n-butylacetoacetate by A.E.E. condensation.

Cannizaro Reaction: 4- chlorobenzaldehyde as substrate

Friedel Craft Reaction: β-Benzoyl propionic acid from succinic anhydride and benzene **Aromatic electrophilic sustitutions**: Synthesis of p-nitroaniline and p-bromoaniline

Quantitative Analysis

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

Estimation of amines/phenols using bromate bromide solution/or acetylation method. Determination of Iodine and Saponification value of an oil sample.

Determination of DO, COD and BOD of water sample

PHYSICAL CHEMISTRY

Electrochemistry

A. Conductometry

(i) Determination of the velocity constant, order of the reaction and energy of activation 'for saponification of ethyl acetate by sodium hydroxide conductometrically.

(ii) Determination ot solubility and solUbility product of sparingly soluble salts (e.g., $PbS0_4$, $BaS0_4$) conductometrically.

(III) Determination of the strength of strong and weak acids in a given mixture conductometrically.

(iv) To study the effect of solvent on the conductance of $AgNO_3$ /acetic acid and to determine the degree of dissociation and equilibrium constant in different solvents and in their mixtures (DMSO, DMF, dioxane, acetone, water) and to test the validity of Debye-Huckel - Onsager theory.

(v) Determination of the activity coefficient of zinc ions in the solution of 0.002 M zinc sulphate using Debye HOckel's limiting law.

B.· **Potentiometry/pH metry**

(i) Determination of strength of halides in a mixture potentiometrically.

(ii) Determination of the valency of mercurous ions potentiometrically.

(iii) Determination of the strength of strong and weak acids in a given mixture using a potentiometer/pH meter.

(iv) Determination of temperature dependence of EMF of a cell.

(v) Determination of the formation constant of silver-ammonia complex and stoichiometry of the complex potentiometrically.

(vi) Acid-base titration in a non-aqueous media using a pH meter. (Vii) Determination of activity and activity coefficient of electrolytes.

(Viii) Determination of the dissociation constant of acetic acid in DMSO, DMF, acetone and dioxane by titrating it with KOH.

(ix) Determination of the dissociation constant of monobasic/dibasic acid by Albert-Serjeant method.

(x) Determination of thermodynamic constants, ΔG, ΔS and ΔH for the reaction by e.m.f. method.

$$Zn + H_2S0_4 \longrightarrow ZnS0_4 + H_2$$

Polarimetry

(i) Determination of rate constant for hydrolysis/inversion of sugar using a polarimeter.

(ii) Enzyme kinetics - inversion of sucrose

Books Suggested

1. Vogel's Textbook of Quantitative Analysis, revised. J. Bassett. R. C. Denney, G. H. Jeffery and J. Mendham, ELBS .
2. Synthesis and Characterization of Inorganic Compounds. W. L. Jolly, Prentice Hall
3. Experiments and Techniques in Organic Chemistry, D. Pasto, C. Johnson and M. Miller, Prentice Hall
4. Macroscale and Microscale Organic Experiments, K. L. Williamson, D. C. Heath.
5. Systematic Qualitative Organic Analysis. H. Middleton, Adward Arnold.
6. Handbook of Organic Analysis, Qualitative and Quantitative. H. Clark, Adward Arnold.
7. Vogel's Textbook of Practical Organic Chemistry. A. R. Tatchell. John Wiley
8. Practical Physical Chemistry, A. M. James and F, E. Prichard. Longman
9. Findley's Practical Physical Chemistry, B. P. Levitt. Longman.
10 Experimental Physical Chemistry, R.C. Das and B. Behera, Tata McGraw Hill.

M.Sc.–3rd semester

CHY - 111: Application of spectroscopy

A. Inorganic Chemistry

1. **Vibrational spectroscopy:** Symmetry and shapes of AB_2, AB_3, AB_4, AB_5 and 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.

2. **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 PH_4, F_2^- and $[BH_3]^-$.

3. **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 ^{119}Sn NMR.

4. **Mossbauer Spectroscopy:** Basic principles, spectral parameters and spectrum display, application of the technique to the studies of (1) bonding and structures of Fe2+ and Fe3+ compounds including those of intermediate spin, (2) Sn+2 and Sn+4 compounds-nature of M-L bond, coordination number, structure and (3) detection of oxidation state and inequivalent MB atoms.

B. Organic Chemistry

5. **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 effects in biphenyls.

6. **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, FTIR, IR of gaseous, solids and polymeric materials

7. **Optical rotatory dispersion and Circular dichroism**: Definition, deduction of absolute configuration, octant rule for ketones.

8. **Nuclear Magnetic resonance spectroscopy**: General introduction and definition, chemical shift, spin-spin interaction, shielding mechanism, 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, solvents effects, Fourier transform technique, nuclear overhouser effect, resonance of other nuclei-F, P.

9. **^{13}C 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

10. **Mass Spectroscopy:** 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.

CHY - 112: BIOCHEMISTRY

A. Bio-Inorganic Chemistry

1. **Metal ions in biological systems:** Essential and trace metals.
2. **Na+/k+ Pump:** Role of metals ions in biological processes,
3. **Bioenergetic and ATP Cycle:** DNA polymerization, glucose storage, metal complexes in transmission of energy, chlorophylls, photosystem I and photosystem II in cleavage of water, model systems.
4. **Transport and storage of Dioxygen:** Heme protein and oxygen uptake, structure and function of hemoglobin, myoglobin, hemocyanins and hemerythrin, model synthetic complexes of iron, cobalt and copper
5. **Electron Transfer in biology:** Structure and function of metalloproteins in electron transport processes-cytochromes and ion-sulphur proteins, synthetic models.
6. **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.
7. **Mechanism of enzyme action:** transport state theory, orientation and steric effect, acid-dase catalysis, covalent catalysis, strain or distortion, examples of some typical enzyme mechanisms for chymotrypsin, ribonuclease, Lysozyme and carboxypeptidase A.

8. **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.

9. **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 B12, mechanism of reactions catalysed by the above cofactors.

10. **Enzyme models:** 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.

11. **Biological cell and its constituents:** Biological cell, structure and functions of proteins, enzymes, DNA and RNA in living systems, Helix coil transition.

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

13. **Thermodynamics of biopolymer solutions:** Thermodynamics of biopolymer solutions, osmotic pressure, membrane equilibrium, muscular contraction and energy generation in mechanochemical system.

14. **Diffraction methods:** Light scattering, low angle X-ray scattering, X-ray diffraction and photo correlation spectroscopy, ORD.

CHY - 113 Analytical Techniques

1. Significant figures; Determinate and Indeterminate errors, absolute and relative errors, error curves, minimization of errors; precision and accuracy, determination of accuracy; mean, median and mode; standard deviation.
2. Principles, instrumentation and applications of the following techniques:
   (i). Complexometric, Chelatometric and Non-aqueous titration.
   (ii).Potentiometric and Conductometric Titrations.
   (iii)Polarography and Amperometry
   (iv)Coulometry and Voltametry (With special reference to cyclic voltametry and Annodic Stripping voltametry).
3. Principles and applications of solvent extraction and ion exchange resins.
4. Fundamental principles of chromatography. Principles, instrumentation and applications of column chromatography, paper chromatography, thin layer chromatography, gas chromatography, radial chromatography and HPLC.
5. Techniques and principles of Thermal Analysis: TGA, DTA and DSC.

ELECTIVE PAPER - I

CHY 114 Organic Synthesis - I

I Organometallic Reagents

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

Group I and II metal organic compounds

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

Transition metals

Cu, Pd, Ni, Fe, Co, Rh, Cr and Ti compounds.

Other elements

S, Si, B and I compounds.

II Oxidation

Introduction. Different oxidative processes .

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

Alcohols, diols, aldehydes, ketones, ketals and carboxyalic acids. Amines, hydrazines, and sulphides.

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

III Reduction

Introduction. Different reductive processes.

Hydrocarbons- alkanes, alkenes, alkynes and aromatic rings.

Carbonyl compounds-aldehydes, ketones, acids and their derivatives. Exposides. Nitro, nitroso, azo and oxime groups.

Hydrogenolysis.

IV 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, Hofman, Curtius, Schmidt, Baeyer-Viliger, Shapiro reaction.

ELECTIVE PAPER· II

CHY 115 Chemistry of Natural products

I Terpenoids and Carotenoids

Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Structure determination, stereochemistry, biosynthesis and synthesis of the following representative molecules: Citral, Geraniol, α-Terpeneol, Menthol, Farnesol, Zingiberene, Santonin, Phytol, Abiatic acid and β-Carotene.

II Alkaloids

Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradatin, classification based on nitrogen heterocyclic ring, role of alkeloids in plants. Structure, stereochemistry, synthesis and biosynthesis of the following:

Ephedrine, (+)- Conviine, 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, Progestrone, Aldosterone. Biosynthesis of steroids.

IV Plant Pigments

Occurrence, nomenclature and general methods of structure determination, isolation and synthesis of Apigenin, Luteoline, Quercetin, Myrectin, Quercetin-3-glucoside, Vitexin, Diadzein, Butein, Aureusin , Cyandin-7-arabinoside, cyanidin, Hirsutidin.

Biosynthesis of flavonoids : Acetate pathway and Shikimic acid pathway.

V Porphyrins

Structure and synthesis of Hemoglobin and Chlorophyll.

VI Prostaglandins

Occurrence, nomenclature, classification, biogenesis and physiological effects.

Synthesis of PGE_2 and $PGF_{2'}$

Pyrethroids and Rotenones

Syathesis and reactions of Pyrethroids and Retenones. (For structtJre elucidation, emphasis is to be place on the use of spectral parameters wherever possible).

M.Sc.- 4th semester

CHY - 116: Photochemistry and Solid State Chemistry

A. Photochemistry:

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

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-photo dissociation, gas-phase photolysis**.** Photochemistry of alkenes: **Intramolecular reactions of the olefinic bond-geometrical isomerization, cyclic reactions, rearrangement of 1,4- and 1,5-dienes.**

1. **Photochemistry of carbonyl compounds:** intramolecular reactions of the carbonyl compounds- saturated, cyclic and acyclic, βγ Unsaturated and αβ-unsaturated compounds, cyclohexadienones, intermolecular cycloaddition reactions-dimerisation and oxectane formation.

2. **Photochemistry of aromatic compounds:** isomerization, addition and substitutions.

3. **Miscellaneous photochemical reactions:** Photo-fries reactions of anilides, photo-fries rearrangement, Barton reaction, singlet molecular oxygen reactions, photochemical formation of smog, photo degradation of polymers, photochemistry of vision.

B. Solid State Chemistry:

4. **Solid State reactions:** General principles, experimental procedures, co-precipitation as a precursor to solid-state reactions, kinetics of solid-state reactions.

5. **Crystal Defects and Non-Stoichiometry**: Perfect and imperfect crystals, intrinsic and extrinsic defects-point defects, line and plane defects,

vacancies-Schotty defects and Frenkel defects, thermodynamics of Schotky and Frenkel defect formation, color centers, non-Stoichiometry and defects.

6. **Electronic properties and band theory:** Metals, insulators and semiconductors, electronic structure of solid-band theory, band structure of metals, insulators and semiconductor, intrinsic and extrinsic semiconductors, doping semiconductor, p-n-junction, super conductors, optical properties-optical properties - optical reflectance, photoconduction-photoelectric effects, magnetic properties-classification of materials: quantum theory of paramagnetic-cooperative phenomena-magnetic domains, hysteresis.
7. Organic solids: Electrically conducting solids, organic charge transfers complex, organic metals, new superconductors.

CHY - 117: Environmental Chemistry

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

1. Hydrosphere: Chemical composition of water bodies – lakes, streams, rivers and wetlands etc Hydrological cycle. 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, phosphate, nitrate and micro-organisms, water quality standards, Analytical methods for measuring BOD, DO, COD, F, OILS, METALS (As, Cd, Cr, Hg, Pb, Se), Residual chloride and chlorine demand, purification and treatment of water.

2. Soils: Composition, micro and macronutrients, pollution-fertilizers, pesticides, plastics and metals, waste treatment.

3. **Atmosphere:** Chemical Composition of Atmosphere-particles, ions and radical 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.

4. **Industrial pollution:** Cement, sugar, distillery, drug, paper and pulp, thermal power plants, nuclear power plants, metallurgy, polymers, drugs etc, radionuclide analysis, disposal of wastes and their management.
5. **Environmental Toxicology**: Chemical solutions to environmental problems, biodegradability, principles of decomposition, better industrial processes.

CHY 118 Organic Synthesis II

I Disconnection Approach

An introduction to synthons and synthetic equivalents, disconnection approach, functional group inter-conversions, the importance of the order of events in organic synthesis, one group C-X and two group C-X disconnections, chemoselectivity, reversal of polarity, cyclisation reactions, amine synthesis

II Protecting Groups

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

III One Group C-C Disconnections

Alcohols and carbonyl compounds, regioselectiviity. Alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis.

IV Two Group C –C Disconnections

Diels-Alder reaction, 1,3-difunctionalised compounds, unsaturated carbonyl compounds, control in carbonyl condensations, 1,5-difunctionalised compounds, Michael addition and Robinson annulations.

V Ring Synthesis

Saturated heterocycles, synthesis of 3-, 4-, 5- and 6-membered rings, aromatic heterocycles in organic synthesis.

VI Synthesis of Some Complex Molecules

Application of the above in the synthesis of following compounds:

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

BOOKS SUGGESTED

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

7 Advanced Organic Chemistry Part B, F. A. Carey and A. J. Sundberg, Plenum Press

CHY 119 Heterocyclic Chemistry

I Nomenclature of Heterocycles

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

II Aromatic Heterocycles

General chemical behavior of aromatic heterocycles, classification (structural type), criteria of aromaticity (bond lengths, ring current and chemical shifts in 1 H NMR-spectra, empirical resonance energy, delocalization energy and Dewar resonance energy, diamagnetic susceptibility exaltations).

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- electrophilic interactions

IV Heterocyclic Synthesis

Principles of heterocyclic synthesis involving cyclization reactions and cycloaddition reactions.

V Small Ring Heterocycles

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

VI Benzo Fused Five Membered Heterocycles

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

VII Mesoionic Heterocycles

General classification, chemistry of some important meso-ionic heterocycles of type-A and B and their applications.

VIII 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

IX Six-Membered Heterocycles with Two or More Heteroatoms

Synthesis and reactions of diazines, triazines, tetrazines and thiazines

X Seven and Large Membered Heterocycles

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

XI Heterocyclic System Containing P, As, Sb and B

Heterocyclic rings containing phosphorus:

Introduction; nomenclature, synthesis and characteristics of 5- and 6-membered ring systems-phosphorinanes, phosphorines, phospholanes and phospholes.

Heterocyclic rings containing As and Sb:

Introduction, synthesis and characteristics of S 5 and 6- membered ring systems.

Heterocyclic rings containing B:

introduction. synthesis, reactivity and spectral characteristics of 3-,5- and 6- membered ring systems.

BOOKS SUGGESTED:

1. Heterocyclic Chemistry, Vol 1-3, A. A. Gupta. M. Kumar and V. Gupta,

Springer Verlag

2. The Chemistry of Heterocycles, T. Eicher and S. Hauptmann, Thieme
3. Heterocyclic Chemistry, J. A. Joule, K. Mills and G.F. Smith, Chapman and Hall
4. Heterocyclic Chemistry,T.L Gilchrist,Longman Scietific Techinal
5. Contemporary Heterocyclic Chemistry, G. A. Newkome and W. W. Paudler, Wiley-Inter Science
6. An Introduction to the. Heterocyclic Compounds, A. M. Acheson, JohnWiley
7. Comprehensive Heterocyclic Chemistry, A. A. Katritzky and C. W. Rees. ads. Pergamon Press

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