1. Name of the Course - M.Sc.(Chemistry)

2. Need of the course:

Chemistry (from Egyptian $k\bar{e}me$ (chem), meaning "earth") is the science concerned with the composition, structure, and properties of matter, as well as the changes it undergoes during chemical reactions. It is a physical science for studies of various atoms, molecules, crystals and other aggregates of matter whether in isolation or combination, which incorporates the concepts of energy and entropy in relation to the spontaneity of chemical processes. Modern chemistry evolved out of alchemy following the chemical revolution (1773).

Disciplines within chemistry are traditionally grouped by the type of matter being studied or the kind of study. These include inorganic chemistry, the study of inorganic matter; organic chemistry, the study of organic matter; biochemistry, the study of substances found in biological organisms; physical chemistry, the energy related studies of chemical systems at macro, molecular and submolecular scales; analytical chemistry, the analysis of material samples to gain an understanding of their chemical composition and structure. Many more specialized disciplines have emerged in recent years, e.g. neurochemistry the chemical study of the nervous system

Chemistry is the central science and impacts on all facets of our lives. An understanding of chemistry is necessary to all other sciences from astronomy to zoology. All of the materials used by engineers and technologists are made by chemical reactions and we all experience chemical reactions continuously, whether it be breathing or baking a cake, driving a car or listening to a battery driven minidisk player. Chemistry is concerned with all aspects of molecules, their physical and chemical properties, their composition and structure, their synthesis and use in the 21st

Chemistry is fundamental. To understand why an autumn leaf turns red, or why a diamond is hard, or why soap gets us clean, requires an understanding of chemistry. To design a synthetic fiber, a life-saving drug, or a space capsule requires knowledge of chemistry. The behavior of atoms, molecules, and ions determines the sort of world we have to live in, our shapes and sizes, and even how we feel on a given day. Chemists are very much involved in tackling the problems faced by our modern society. On a given day, a chemist may be studying the mechanism of the recombination of DNA, measuring the amount of insecticide in drinking water, comparing the protein content of meats, developing a new antibiotic, or analyzing a moon rock. So chemistry is worth studying, just because it is such a good antidote for ignorance.

3. Objectives:

The broad objectives of the course have been listed below:

- 1. Demonstrate broad knowledge of descriptive Chemistry.
- 2. Demonstrate the basic analytical and technical skills to work effectively in the various fields of chemistry.
- 3. Demonstrate critical thinking and analysis skills to solve complex chemical problems, e.g., analysis of data, synthetic logic, spectroscopy, structure and modeling, team-based problem solving, etc.
- 4. Demonstrate the ability to calculate the physical properties of chemical reagents, predict outcomes of chemical reactions, and perform critical analysis of data.
- 5. Demonstrate an ability to conduct experiments in the above sub-disciplines with mastery of appropriate techniques and proficiency using core chemical instrumentation and modeling methods.
- 6. Demonstrate the ability to perform accurate quantitative measurements with an understanding of the theory and use of contemporary chemical instrumentation, interpret experimental results, perform calculations on these results and draw reasonable, accurate conclusions.
- 7. A mastery of a broad set of factual chemical knowledge concerning the properties of substances, molecules and atoms.
- 8. Develop skills in quantitative modeling of static and dynamic chemical systems.
- 9. Develop a detailed understanding of the relationship between changes in chemical composition or state and changes in energy content.
- 10. Develop laboratory competence in relating chemical structure to spectroscopic phenomena.
- 11. Students need to learn and understand the concepts of safe laboratory practices. Students should learn and understand safe disposal techniques, understand and comply with safety regulations, understand and use material safety data sheets (MSDS) and recognize and minimize potential chemical and physical hazards in the laboratory.
- 12. Demonstrate the ability to synthesize, separate and characterize compounds using published reactions, protocols, standard laboratory equipment, and modern instrumentation.

4. Learning and Teaching

Seminar sessions will be organized to discuss the learning objectives and to review progress at regular intervals and to provide support in topics of polymer science and technology. Students will bring their own case studies to the seminars for discussion. The seminars will also provide opportunities for students to reflect on individual jobs and to discuss the wide range of careers available and use this to expand their personal development plans.

5. Learning Outcomes

On successful completion of this module students should have the ability to:

1. think critically and analyze chemical problems.

- 2. present scientific and technical information resulting from laboratory experimentation in both written and oral formats.
- 3. work effectively and safely in a laboratory environment.
- 4. to use technologies/instrumentation to gather and analyze data.
- 5. use the power of computers in applications in chemistry.
- 6. work in teams as well as independently.
- 7. to apply modern methods of analysis to chemical systems in a laboratory setting.

Prof. A.K. Srivastav

Dr. R.K. Soni

Dean, Faculty of Science

Coordinator

Biochemistry, PSCT

M.SC. CHEMISTRY

(Two Year Course) M.Sc. I Year

I Sem

Paper	Course	Hours	Marks		Total	Duration of Exam
			External	Internal		
CH 101	Inorganic Chemistry-I	60	50	50	100	3 Hours
CH 102	Organic Chemistry-I	60	50	50	100	3 Hours
CH 103	Physical Chemistry-I	60	50	50	100	3 Hours
CH 104	Mathematics for Chemists* OR Biology for Chemists*	30 2 Hrs/week	25	25	50 Qualifying only (40%)	2 Hours
CH 105	Computer for Chemists	60	50	50	100	3 Hours
Total		270	200	200	400	14 Hours
Lab I Inorganic Chemistry Organic Chemistry Physical Chemistry		240	100	100	200	18 Hours 6 x 3
Grand Total		510	300		600	32 Hours

^{*} To be qualified during the course.

II Sem

Paper	Course	Hours	Marks		Total	Duration of Exam
			External	Internal		23.4
CH 201	Inorganic Chemistry-II	60	50	50	100	3 Hours
CH 202	Organic Chemistry-II	60	50	50	100	3 Hours
CH 203	Physical Chemistry-II	60	50	50	100	3 Hours
CH 204	Group Theory & Solid State	60	50	50	100	3 Hours
	Total	240	200	200	400	12 Hours
Lab II Inorganic Chemistry Organic Chemistry Physical Chemistry		240	100	100	200	18 Hours 6 x 3
Grand Total		480	300		600	30 Hours

M.Sc. II Year

III Sem

Paper	Course	Hours	Marks		Total	Duration of Exam
			External	Internal		23.4.1.1
CH 301	Photochemistry & Bioorganic Chemistry	60	50	50	100	3 Hours
CH 302	Spectroscopy	60	50	50	100	3 Hours
СН 303	Bioinorganic & Biophysical Chemistry	60	50	50	100	3 Hours
CH 304	Elective I	60	50	50	100	3 Hours
	Total	240	200	200	400	12 Hours
Lab III Analytical Chemistry Biochemistry		240	100	100	200	12 Hours 6 x 2
Grand Total		480	300		600	24 Hours

IV Sem

Paper	Course	Hours	Marks		Total	Duration of Exam
			External	Internal		23.44.11
CH 401	Environmental Chemistry	60	50	50	100	3 Hours
CH 402	Elective II	60	50	50	100	3 Hours
CH 403	Elective III	60	50	50	100	3 Hours
CH 404	Elective IV	60	50	50	100	3 Hours
Total		240	200	200	400	12 Hours
Lab IV Organic Synthesis		240	100	100	200	6 Hours
Grand Total		480	300		600	18 Hours

The students has to select the Elective papers from the set of Elective Papers in the following areas of Specialization

- 1. Organic Chemistry
- 2. Inorganic Chemistry
- 3. Physical Chemistry

M.Sc Chemistry

Ist Semester

CH-101 Inorganic Chemistry-I (PG-312)

60Hrs

1. Stereochemistry and Bonding in Main Group Compounds

12 Hrs

VSEPR, Walsh diagrams (tri atomic molecules), $d\pi$ -P π bonds, Bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules.

2. Metal-Ligand Equilibria in Solution

8 Hrs

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. Reaction Mechanism of Transition Metal Complexes

24 Hrs

Energy profile of a reaction, reactivity of metal complexes, inert and labile complexes, kinetic application of valence bond and crystal field theories.

Kinetics of Substitution Reactions- acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidences in favour of conjugate mechanism. Anation reactions, reactions without Metal-Ligand bond cleavage. Substitution reactions in square planer complexes, the trans effect, mechanism of the substitution reaction.

Redox reactions (electron transfer reactions) -Mechanism of one electron transfer reactions [such as Henry Taube's classical reaction of $(NH_3)_5Co^{3+}-Cr^{2+}$, Inner sphere type reactions]. Outer-sphere type reactions (cross reactions) and Marcus-Hush theory (No mathematical treatment).

4. Metal-Ligand Bonding

16 Hrs

Adjusted CFT, Limitations of crystal field theory. Octahedral, tetrahedral and square planar complexes.

1. Nature of Bonding in Organic Molecules

10 Hrs

Delocalized chemical bonding, Conjugation, hyperconjugation, bonding in fullerenes, tautomerism. Aromaticity in benzenoid and non-benzenoid compounds, alternant and non-alternant hydrocarbons, Huckel's rule, energy level of n-molecular orbitals, annulenes, antiaromaticity, w-aromaticity, homo-aromaticity, PMO approach. Bonds weaker than covalent- addition compounds, crown ether complexes and cryptands, inclusion compounds, cyclodextrins, catenanes and rotaxanes.

2. Stereochemistry 15 Hrs

Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity, conformation of sugars, 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

15 Hrs

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, carbanions, 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, substituent and reaction constants. Taft equation.

4. Aliphatic Nucleophilic Substitution

15 Hrs

The SN2, SN1, mixed SN1 & SN2 and SET mechanisms.

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

Classical and nonclassical carbocations, Phenonium ions, nonbornyl system, Common carbocation rearrangements. Application of NMR spectroscopy in the detection of

carbocations.

The SNi mechanism, Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium. Phase transfer catalysis and ultrasound, ambident nucleophile, regioselectivity.

5. Aliphatic Electrophilic Substitution

5 Hrs

Bimolecular mechanisms- SE2 and SE1. The SE1 mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity.

I Quantum Chemistry

30 Hrs

1. 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.

2. 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.

3. 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, anti symmetry and Pauli's exclusion principle.

4. Electronic Structure of Atoms

Electronic configuration, Russell-Saunders terms and coupling schemes, Slater-Condon parameters, term separation energies of the pn configuration, term separation energies for the dn configurations, magnetic effects: spin-orbit coupling and Zeeman splitting, introduction to the methods of self-consistent field, the virial theorem.

5. Molecular Orbital Theory

Huckel theory of conjugated systems, bond order and charge density calculations. Applications to ethylene, butadiene, cyclopropenyl radical, cyclobutadiene etc. Introduction to extended Huckel theory.

II Thermodynamics

30 Hrs

1. Classical Thermodynamics

Brief resume of concepts of laws of thermodynamics, free energy, chemical potential and entropies. Partial molar properties; 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.

2. 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 partition 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 statistics - distribution law and application to helium.

3. 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.

Vectors and Matrix Algebra

10 Hrs

A Vectors

Vectors, dot, cross and triple products etc. The gradient, divergence and curl. Vector calculus, Gauss' theorem, divergence theorem etc.

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 Hückel theory).

Introduction to tensors; polarizability and magnetic susceptibility as examples.

II Differential Calculus

10 Hrs

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's distribution etc), exact and inexact differentials with their applications to thermodynamic properties.

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.

III Elementary Differential Equations

7 Hrs

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.

IV Permutation and Probability

3 Hrs

Permutations and combinations, probability and probability theorems, probability curves, average, root mean square and most probable errors, examples from the kinetic theory of gases etc., curve fitting (including least squares fit etc.) with a general polynomial fit.

- 1. The Chemistry Mathematics Book, E. Steiner, Oxford University Press.
- 2. Mathematics for Chemistry, Doggett and Sutcliffe, Longman.
- 3. Mathematical Preparation for Physical Chemistry, F. Daniels, McGraw Hill.
- 4. Chemical Mathematics, D.M. Hirst, Longman.
- 5. Applied Mathematics for Physical Chemistry, J.R. Barrante, Prentice Hall.
- 6. Basic Mathematics for Chemists, Tebbutt, Wiley.

l Cell Structure and Functions

5 Hrs

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 earbon, chemical evolution and rise of living systems. Introduction to biomolecules, building blocks of bio-macromolecules.

ll Carbohydrates

8 Hrs

Conformation of monosaccharides, structure and functions of important derivatives of monosaccharides like glycosides, deoxy sugars, myoinositol, amino sugars. Nacetylmuramic acid, sialic acid, disaccharides and polysaccharides. Structural polysaccharides - cellulose, and chitin. Storage polysaccharides - starch and glycogen. Structure and biological functions of glucosaminoglycans or mucopolysaccharides.

Carbohydrate metabolism - Kreb's cycle, glycolysis, glycogenesis and glycogenolysis, gluconeogenesis, pentose phosphate pathway.

Carbohydrates of glycoproteins and glycolipids. Role of sugars in biological recognition.

III Lipids

6 Hrs

Fatty acids, essential fatty acids, structure and function of triacylglycerols, glycerophospholipids, 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.

IV Amino-acids, Peptides and Proteins

Blood group substances. Ascorbic acid.

6Hrs

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 exytocin and tryptophan releasing hormone (TRH).

Purine and pyrimidine bases of nucleic acids base pairing via H-bonding. Structure of ribonucleic acids (RNA) and deoxyribonucleic acids (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, translation and genetic code. Chemical synthesis of mono and trinucleoside.

- 1. Principles of Biochemistry, A. L. Lehninger, Worth Publishers.
- 2. Biochemistry, L.Stryer, W.H.Freeman.
- 3. Biochemistry, J. David Rawn, Neil Patterson.
- 4. Biochemistry, Voet and Voet, John Wiley.
- 5. Outlines of Biochemistry, E. E.Conn and P. K. Stumpf, John Wiley.

60Hrs

This is a theory-cum-Laboratory course with more emphasis on laboratory work.

1. Introduction to Computers and Computing

8 Hrs

Basic structure and functioning of computers with a PC as an illustrative example. Memory, I/O devices. Secondary storage. Computer languages. 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/C/BASIC

12 Hrs

The language feature are listed here with reference ton FORTRAN. The instructor may choose another language such as BASIC or C and the feature may be replaced appropriately. Elements of the computer language. Constants and variables. Operations and symbols. Expression. Arithmetic assignment statement input and output. Format statement. Termination statements. Branching statements such as IF or GO TO statement. LOGICAL variables, Double Precision variables. Subscripted variables and DIMENSIONS. DO statements. FUNCTION and SUBROUTINE. COMMON and DATA statements.

Decision control structure, case4 control structure, functions, introduction ton arrays, programmes based on above.

3. Programming in Chemistry

15 Hrs

Development of small computer course involving simple formula in chemistry such as Vander Waal's equation, pH titration, kinetics, radioactive decay. Evaluation of lattice energy and ionic radii from experimental data. Linear simultaneous equations to solve secular equation with in the Huckel theory. Elementary structural features such as bond lengths, bond angels, dihedral angels etc. of molecule extracted from a database such as Cambridge database.

4. Use of Computer Programmes

25 Hrs

Execution of linear regression, X-V plot, Numerical integration and differentiation as well as differential equation solution programmes. Monte –Carlo and Molecular dynamics. Introduction to MS Office (MS Word, MS Excel, MS PowerPoint). Lab sessions based on MS Office package, Introduction to Internet Explorer.

- 1. Computers and Common Sense, R, Hunt and J, Shelly, Prentice Hall.
- 2. Computational Chemistry, AC, Norris.
- 3. Microcomputer Quantum Mechanics, J.P., Killngbeck. Adam Hilger.
- 4. Computer Programming in FORTRAN IV, V. Rajaraman, Prentice Hall.
- 5. An Introduction to Digital Computer Design, V. Rajaraman and T. Radhakrishnan, Prentice Hall.

PRACTICAL SYLLABUS <u>I- SEMESTER</u>

PHYSICAL PRACTICAL

- 1. To find out the strength of the given HCl solution by titrating it against N/10 NaOH using pH meter.
- 2. To find out the strength of the given CH₃COOH solution by titrating it against N/10 NaOH using pH meter.
- 3. To find out the strength of HCl and CH₃COOH in a mixture of both by titrating it against N/10 NaOH using pH meter.
- 4. To determine the solubility of a given salt at room temperature and also draw its solubility curve.
- 5. To find out the heat of solution of oxalic acid by solubility method.
- 6. To standardize the given KMnO₄ solution by titrating it against standard Ferrous Ammonium Sulphate solution.
- 7. To determine the critical solution temperature of phenol water system.
- 8. To determine the viscosity of given sample of oil at different temperature using Red Wood Viscometer.

INORGANIC PRACTICAL

- 1. To analyze the mixture of two components.
- 2. To analyze the mixture of three components.
- 3. To prepare Hexa-Ammine (II) Chloride.
- 4. To prepare potassium Dioxalato Cuprate (II) Dihydrate.
- 5. To prepare Potassium Trioxalato Chromate (III).
- 6. To prepare Tetrammine Cupric Sulphate.
- 7. To prepare Sodium Ferric Oxalate.

8. To prepare crystals of Potassium Tris Oxalate Aluminate (III).

ORGANIC PRACTICAL

- 1. To identify the given organic compound and prepare its derivatives.
- 2. To analyze the given organic mixture (water separation).
- 3. Single step preparations
 - Hydrolysis
 - Bromination
 - Nitration
 - Oxime formation
 - Reduction
 - Hoffmann Bromide reaction
 - Benzoin condensation reaction etc.
- 4. To determine the iodine value of the given fat sample.
- 5. To determine the saponification value of the given fat sample.

IInd Semester

CH-201 Inorganic Chemistry-II (PG-326)

60Hrs

1. Electronic Spectra and Magnetic Properties of Transition Metal Complexes

22 Hrs

Spectroscopic ground states, correlation, Orgel and Tanabe-Sugano diagrams for transition metal complexes (d1-d9 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

2. Metal π -Complexes

18 Hrs

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 Ligand

3. Metal Clusters 12 Hrs

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

4. Nuclear Chemistry

8 Hrs

Radioactive decay & equilibrium. Nuclear Reactions, Q-value cross-sections, types of reactions, Chemical effects of nuclear transformations Fission & Fusion, Fission products & fission yields. Radioactive techniques, tracer techniques.

- 1. Advanced Inorganic Chemistry, FA Cotton and Wilkinson, John Wiley.
- 2. Inorganic Chemistry, J.E. Huhey, Harpes & Row.
- 3. Chemistry of the Elements, N.N. Greenwood and A. Earnshaw, Pergamon.
- 4. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
- 5. Magnetochemistry, R.L. Carlin, Springer Verlag.
- 6. Comprehensive Coordination Chemistry eds., G. Wilkinson, RD. Gillars and J.A.

CH-202 Organic Chemistry-II (PG-327)

60Hrs

1. Aromatic Electrophilic Substitution

6 Hrs

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 substrates and electrophiles. Diazonium coupling, Vilsmeir reaction, Gattermann-Koch reaction.

2. Aromatic Nucleophilic Substitution

5 Hrs

The SNAr, SN 1, benzyne and SRN 1 mechanisms. Reactivity - effect of substrate structure, leaving group and attacking nucleophile. The von Richter, Sommelet-Hauser, and Smiles rearrangements.

3. Free Radical Reactions

8 Hrs

Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. Reactivity in the attacking radicals. The effect of solvents on reactivity. Allylic halogenations (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. Hunsdiecker reaction.

4. Addition to Carbon-Carbon Multiple Bonds

6 Hrs

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.

5. Addition to Carbon-Hetero Multiple Bonds

12 Hrs

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 condensation reactions involving enolates – Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions. Hydrolysis of esters and amides, ammonolysis of esters.

The E2, E1 and E1 CB 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.

7. Pericyclic Reactions

18 Hrs

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, 4n+2 and allyl systems. Cycloaddditions - antarafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3 dipolar 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, Sommelet Hauser Rearrangement, Ene reaction.

- 1. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.
- 2. Advanced Organic Chemistry, F. A. Carey and R. J. Sundberg, Plenum.
- 3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
- 4. Structure and Mechanism in Organic Chemistry, C. K. Ingold. Cornell University Press.
- 5. Organic Chemistry, R. T. Morrison and R. N. Boyd, Prentice-Hall.
- 6. Modern Organic Reactions, H. O. House, Benjamin.
- 7. Principles of Organic Synthesis, R. O. C. Norman and J. M. Coxon, Blackie Academic & Professional.
- 8. Pericyclic Reactions, S. M. Mukherji, Macmillan, Irdia.
- 9. Reaction Mechanism in Organic Chemistry, S. M. Mukherji and S. P. Singh, Macmillan.
- 10. Stereochemistry of Organic Compounds, D. Nasipuri, New Age International.
- 11. Stereochemistry of Organic Compounds, P.S. Kalsi, New Age International.

1. Chemical Dynamics

20 Hrs

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-chlorine reactions) and oscillatory reactions (Belousov -Zhabotinsky reaction), homogeneous catalysis, kinetics of enzyme, reactions, 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 unimolecular reactions (Lindemann Hinshelwood and Rice-Ramsperger - Kassel-Marcus [RRKM] theories of unimolecular reactions).

2. Surface Chemistry

20 Hrs

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), Elementary treatment of BET equation, 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, solubilization, micro emulsion, reverse micelles.

C. Macromolecules

Polymer - definition, types of polymers, kinetics of radical polymerization, mechanism of polymerization.

Molecular mass, number and mass average molecular mass, molecular mass determination (Elementary treatment of Osmometry, Viscometry, Sedimentation and Light scattering methods), chain configuration of macromolecules, calculation of average dimensions of various chain structures.

Electrochemistry of solutions. Debye-Huckel - Onsager treatment and its extension, ion solvent interactions. 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.

20 Hrs

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. Electrocatalysis - influence of various parameters. Hydrogen electrode. Bioelectrochemistry, Polarography theory, Ilkovic equation, half wave potential and its significance.

Introduction to corrosion, homogenous theory, forms of corrosion, corrosion monitoring and prevention methods.

- 1. Physical Chemistry, P.W Atkins, ELBS.
- 2. Introduction to Quantum Chemistry, AK. Chandra, Tata McGraw Hill.
- 3. Quantum Chemistry, Ira N. Levine. PrentCe Hall.
- 4. Coulson's Valence, R. McWeeny, ELBS.
- 5. Chemical Kinetics, K. J. Laidler, Mcgraw-Hill.
- Kinetics and Mechanism of Chemical Transformations, J. Rajaraman and J. Kuriacose, McMillan.
- 7. Micelles, Theoretical and Applied Aspects, V. Moroi, Plenun
- 8. Modern Electrochemistry Vol. I and Vol. II, J.O.M. Bockris and AK.N. Reddy, Plenum.
- 9. Introduction to Polymer Science, V.R. Gowarikar, N.V. Vishwanathan and J. Sridhar, Wiley Eastern.

CH-204 Group Theory, Spectroscopy & Diffraction Methods & Solid State (PG-329) 60Hrs

1. Symmetry and Group Theory in Chemistry

11 Hrs

Symmetry elements and symmetry operation, definitions of group, subgroup, relation between orders of a finite group and its subgroup. Conjugacy relation and classes. Point symmetry group. Schonflies symbols, representations of groups by matrices (representation for the Cn, Cnv, Cnh. Dnh etc. groups to be worked out explicitly). Character of a representation. The great orthogonality theorem (without proof) and its importance. Character tables and their use; spectroscopy.

2. Unifying Principles

5 Hrs

Electromagnetic radiation, interaction of electromagnetic radiation with matterabsorption, emission, transmission, reflection, refraction, dispersion, polarisation and scattering. Uncertainty relation and natural line width, and natural line broadening, transition probability, results of the time dependent perturbation theory, transition moment, selection rules, intensity of spectral lines, Born-Oppenheimer approximation, rotational, vibrational and electronic energy levels.

3. Vibrational Spectroscopy

12 Hrs

A. Infrared Spectroscopy

Review of linear harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constant and bond strengths; anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy, p,a,R branches. Breakdown of Oppenheimer approximation; vibrations of poly atomic molecules. Selection rules, normal modes of vibration, group frequencies, overtones, hot bands, factors affecting the band positions and intensities, far IR region, metal-ligand vibrations, normal co-ordinate analysis.

B. Raman Spectroscopy

Classical and quantum theories of Raman effect. Pure rotational, vibrational and Vibrational-rotational Raman spectra, selection rules, mutual exclusion principle. Resonance Raman spectroscopy, coherent anti Stokes Raman spectroscopy (CARS).

4. Electronic Spectroscopy

10 Hrs

A. Atomic Spectroscopy

Energies of atomic orbitals, 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, Franck-Condon principle, electronic spectra of polyatomic molecules. Emission spectra; radiative and non-radiative decay, internal conversion, spectra of transition metal complexes, charge-transfer spectra.

C. Photoelectron Spectroscopy

Basic principles; photo-electric effect, ionization process, Koopman's theorem. Photoelectron spectra of simple molecules, ESCA, chemical information from ESCA. Auger electron spectroscopy - basic idea.

5. Magnetic Resonance Spectroscopy

10 Hrs

A. Nuclear Magnetic Resonance Spectroscopy

Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurements, factors influencing chemical shift, deshielding, spin-spin interactions, factors influencing coupling constant 'J'. Classification (ABX, AMX, ABC, A2B2 etc.), spin decoupling; basic ideas about instrument, NMR studies of nuclei other than proton - 13C.

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.

6. X-ray Diffraction

10 Hrs

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.

Books Suggested

1. Applied Electron Spectroscopy for Chemical Analysis Ed. H. Windawi and F.L. Ho, Wiley Interscience.

- 2. NMR, NOR, EPR and M6ssbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Harwood.
- 3. Physical Methods in Chemistry, R.S. Drago, Saunders College.
- 4. Chemical Applications of Group Theory, F. A. Cotton.
- 5. Introduction to Molecular Spectroscopy, G.M. Barrow, McGraw Hill.
- 6. Basic Principles of Spectroscopy, R. Chang, McGraw Hill.
- 7. Theory and Applications of UV Spectroscopy, H.H. Jaffe and M. Orchin, ISH-Oxford.
- 8. Introduction to Photoelectron Spectroscopy, P. K. Ghosh, John Wiley.
- 9. Introduction to Magnetic Resonance, A Carrington and A.D. Maclachalari, Harper & Row.
- 10. Modern Spectroscopy, J.M. Hollas, John Wiley

PRACTICAL SYLLABUS II- SEMESTER

PHYSICAL PRACTICAL

- 1. To find out the surface tension of the given liquid by drop weight method at room temperature.
- 2. To determine the parachor value of given liquid.
- 3. To find out the surface tension of CH₃COOH, C₂H₅OH, n-Hexane at room temperature and hence calculate the atomic parachors of C, H, and O.
- 4. To compare the cleaning powers of two samples of detergents supplied to you.
- 5. To determine the critical micelle concentration of soap.
- 6. To find out the strength of HCl solution by titrating it against N/10 NaOH using conductometer.
- 7. To find out the strength of given NH₄OH by titrating it against HCl solution using conductometer.
- 8. To find the velocity constant of the hydrolysis of methyl acetate catalyzed by
 - i. HCl
 - ii. H_2SO_4
- 9. Determine the relative strengths of two acids i.e. HCl & H₂SO₄ by studying the hydrolysis of methyl acetate.

INORGANIC PRACTICAL

- 1. Acidimetry- Alkalimetry titration.
- 2. Oxidation Reduction titration.
- 3. Silver Nitrate titration.
- 4. Complexometric EDTA titration.
- 5. pH-metry titration.
- 6. To estimate Copper and Nickel in the given solution.

7. To estimate Iron and Nickel in a given solution.

ORGANIC PRACTICAL

- 1. Analysis of binary organic mixtures
 - Separartion with NaHCO₃
 - Separation with NaOH
 - Separation with HCl
- 2. Two step preparations
 - To prepare Anthranilic Acid from Phthaic Anhydride.
 - To prepare o- Chlorobenzoic Acid from Phthalamide.
 - To prepare Benzil from Benzaldehyde.
 - To prepare Benzanilide from Benzophenone.

IIIrd Semester

CH-301 Photochemistry & BioOrganic Chemistry (PG-317A) 60Hrs

I) Photochemistry

1. Photochemical Reactions

4 Hrs

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

2. Determination of Reaction Mechanism

4 Hrs

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.

3. Photochemistry of Alkenes

6 Hrs

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

4. Photochemistry of Carbonyl Compounds

8 Hrs

Intramolecular reactions of carbonyl compounds - saturated, cyclic and acyclic, β , γ - unsaturated and α , β -unsaturated compounds. Cyclohexadienones.

Intermolecular cyloaddition reactions - dimerisations and oxetane formation, Paterno-Buchi Reaction.

5. Photochemistry of Aromatic Compounds

4 Hrs

Isomerisations, additions and substitutions.

6. Miscellaneous Photochemical Reactions

4 Hrs

2 Hrs

Photo-Fries reactions of anilides. Photo-Fries rearrangement.

Barton reaction. Singlet molecular oxygen reactions. Photochemical formation of smog. Photodegradation of polymers. Photochemistry of vision.

II) Bioorganic Chemistry

1. Introduction

Basic considerations. Proximity effects and molecular adaptation.

2. Enzymes 6 Hrs

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, MichaelisMenten and Lineweaver-Burk plots, reversible and irreversible inhibition.

3. Mechanism of Enzyme Action

3 Hrs

Transition-state theory, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortion. Examples of some typical enzyme mechanisms for chymotrypsin, ribonuclease, lysozyme and carboxypeptidase A.

4. Kinds of Reactions Catalysed by Enzymes

6 Hrs

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, I)-cleavage and condensation, some isomerization and rearrangement reactions. Enzyme catalyzed carboxylation and decarboxylation.

5. Co-Enzyme Chemistry

4 Hrs

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. Mechani\$ms of reactions catalyzed by the above cofactors.

6. Enzyme Models

4 Hrs

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.

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, enzymes as targets for drug design. Clinical uses of enzymes, enzyme therapy, enzymes and recombinant DNA technology.

- 1. Bioorganic Chemistry: A Chemical Approach to Enzyme Action, Hermann Dugas and. Penny, SpringerVerlag.
- 2. Understanding Enzymes, Trevor Palmer, Prentice Hall.
- 3. Enzyme Chemistry: Impact and Applications, Ed. Collin J Suckling, Chapman and Hall.
- 4. Enzyme Mechanisms Ed, M. I. Page and A. Williams, Royal Society of Chemistry.
- 5. Fundamentals of Enzymology, N.C. Price and L. Stevens, Oxford University Press.
- 6. Immobilized Enzymes: An Introduction and Applications in Biotechnology, Michael D. Trevan, John Wiley.
- 7. Enzymatic Reaction Mechanisms, C. Walsh, W H. Freeman.
- 8. Enzyme Structure and Mechanism, A Fersht, W.H. Freeman.
- 9. Biochemistry: The Chemical Reactions of Living Cells, D. E. Metzler, Academic Press.
- 10. Fundamentals of Photochemistry, K. K. Rohtagi-Mukherji. Wiley- Eastern
- 11. Essentials of Molecular Photochemistry, A. Gilbert and J. Baggott, Blackwell Scientific Publication.
- 12. Molecular Photochemistry. N. J. Turro, W. A. Benjamin.
- 13. Introductory Photochemistry, A. Cox and T. Camp, McGraw-Hili
- 14. Photochemistry. R. P. Kundall and A. Gilbert, Thomson Nelson.

I) Inorganic Spectroscopy

1. Vibrational Spectroscopy

5Hrs

Symmetry and shapes of AB2, AB3, AB4, AB5 and AB6, mode of bonding of ambidentate ligand, ethylenediamine and diketonato complexes, application of resonance Raman spectroscopy particularly for the study of active sites of metalloproteins

2. Electron Spin Resonance Spectroscopy

8 Hrs

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 PH₄, F₂- and [BH3].

3. Nuclear Magnetic Resonance of Paramagnetic Substances in Solution 6 Hrs

The contact and pseudo contact shifts, factors affecting nuclear relaxation, some applications including biochemical systems.

4. Mossbauer Spectroscopy

6 Hrs

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

II) Organic Spectroscopy

1. Ultraviolet and Visible Spectroscopy

3 Hrs

6 Hrs

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.

2. 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.

3. Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD) 3 Hrs

Definition, deduction of absolute configuration, octant rule for ketones.

4. Nuclear Magnetic Resonance Spectroscopy

10 Hrs

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 curvevariation of coupling constant with dihedral angle. Simplification of complex spectranuclear magnetic double resonance, contact shift reagents, solvent effects. Fourier transforms technique, nuclear Overhauser effect (NOE). Resonance of other nuclei-F, P.

5. Carbon-13 NMR Spectroscopy

5 Hrs

General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants. Introduction to 2 D NMR.

6. Mass Spectrometry

8 Hrs

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. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

- 1. Physical Methods for Chemistry, R.S. Drago, Saunders Company.
- 2. Structural Methods in Inorganic Chemistry. E.AV. Ebsworth, D.W.H. Rankin and S. Cradock, ELBS
- 3. Infrared and Raman Spectra: Inorganic and Coordination Compounds, K. Nakamoto,

Wiley.

- 4. Progress in inorganic Chemistry vol., 8. ed, F.A. Cotton, vol., 15, ed. S.J. Lippard, Wiley.
- 5. Transition Metal Chemistry ed, R.L. Carlin vol. 3, Dekker
- 6. Inorganic Electronic Spectroscopy, A.P.B. Lever, Elsevier.
- 7. NMR, NOR, EPR and Mbssbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis
- 8. Horwood. Practical NMR Spectroscopy, M.L. Martin, J.J. DelpeuGh and G.J. NBrtin, Heyden.
- 9. Spectrometric Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler and T. C. Morrill, John Wiley
- 10. Introduction to NMR Spectroscopy, R. J. Abraham, J. Fisher and P. Loftus, Wiley.
- 11. Application of Spectroscopy of Organic Compounds, J. R. Dyer, Prentice Hall. Spectroscopic Methods in Organic Chemistry, D. H. Williams, I. Fleming, Tata McGraw-Hill.

CH-303 Biochemistry (PG-319)

60 Hrs

I) Bioinorganic Chemistry

30hrs

1. Metal Ions in Biological Systems

2 Hrs

Essential and trace metals.

2. Na+/K+ Pump

3 Hrs

Role of metals ions in biological processes.

3. Bioenergetics and ATP Cycle

6 Hrs

DNA polymerisation, glucose storage, metal complexes in transmission of energy; chlorophylls, photosystem I and photosystem II in cleavage of water.

4. Transport and Storage of Dioxygen

8 Hrs

Heme proteins 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

6 Hrs

Structure and function of metalloproteins in electron transport processes - cytochromes and ion-sulphur proteins, synthetic models

6. Nitrogenase 5 Hrs

Biological nitrogen fixation, molybdenum nitrogenase, spectroscopic and other evidence, other nitrogenases model systems.

- 1. Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.
- 2. Bioinorganic Chemistry, I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, University Science Books.
- 3. Inorganic Biochemistry vols I and II. ed. G.L. EichhHn, Elsevier.
- 4. Progress in Inorganic ChemiStry, Vois 18 and 38 ed. J.J. Lippard, Wiley.

II) Biophysical Chemistry

30 Hrs

1. Biological Cell and its' Constituents

2 Hrs

Biological cell, structure and functions of proteins, enzymes, DNA and RNA in living systems. Helix coil transition.

2. Bioenergetics 3 Hrs

Standard free energy change in biochemical reactions, exergonic, endergonic. Hydrolysis of ATP, synthesis of ATP from ADP.

3. Statistical Mechanics in Biopolymers

6 Hrs

Chain configuration of macromolecules, statistical distribution end to end dimensions, calculation of average dimensions for various chain structures. Polypeptide and protein structures, introduction to protein folding problem.

4. Biopolymer Interactions

6 Hrs

Forces involved in biopolymer interactions. Electrostatic charges and molecular expansion, hydrophobic forces, dispersion force interactions. Multiple equilibria and various types of binding processes in biological systems. Hydrogen ion titration curves.

5. Thermodynamics of Biopolymer Solutions

4 Hrs

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

6. Cell Membrane and Transport of Ions

3 Hrs

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

7. Biopolymers and their Molecular Weights

6 Hrs

Evaluation of size, shape, molecular weight and extent of hydration of biopolymers by various experimental techniques. Sedimentation equilibrium, hydrodynamic methods, diffusion, sedimentation velocity, viscosity, electrophoresis and rotational motions.

- 1. Principles of Biochemistry, A. L. Lehninger, Worth Publishers.
- 2. Biochemistry, L.Stryer, WH.Freeman.
- 3. Biochemistry, J. David Rawn, Neil Patterson.
- 4. Biochemistry, Voet and Voet, John Wiley.
- 5. Outlines of Biochemistry, E. E. Conn and P. K. Stumpf, John Wiley.
- 6. Biorganlc Chemistry: A Chemicak Approach to Enzyme Action, H. Duga, and C. Penny.
- 7. Macromolecules: Structure and Function, F. Wold, Prentice Hall.

60 Hrs

1. Introduction: 4 Hrs

Classification of analytical methods- classical and instrumental, types of Instrumental analysis, selecting an analytical method.

2. Errors and Evaluation:

6 Hrs

Definition of terms of mean and median, precision- standard deviation, relative standard deviation, accuracy, absolute error, relative error. Types of error in experimental data- determination (systematic), intermediate (random) and gross. Sources of errors and the effect upon the analytical results. Methods for reporting analytical data. Statistical evaluation of data indeterminate errors. The use of statistics.

3. Radiochemical methods:

10 Hrs

Elementary working, Principles of Giger Muller, Ionization, proportional and γ -ray counters. Neutron radiation sources, radio tracer techniques, Neutron Activation Analysis (NAA): Principle, techniques and applications in preparation of some commonly used radioactive isotopes. Use of radioactive isotopes in analytical and physiochemical problems, Isotopic Dilution Analysis (IDA), substoichiometric IDA, advantages and limitations of IDA and comparison of IDA with NAA. Principle of Radiometric Titrations, Types, Experimental techniques and its applications.

4. Thermal methods of Analysis:

10 Hrs

Introduction of different thermal methods, Thermogravimetry- TGA & DTG, static thermogravimetry, quasithermogravimetry and dynamic thermogravimetry, Instrumental and balances, X-Y recorder, thermogram, factors affecting thermograms. Application of thermogravimetry.

Differential Scanning Claorimetry (DSC): Introduction, instrumentation, DSC-curves, factors affecting DSC curves and applications.

Thermometric Titrations: Introduction, instrumentation, apparatus, theory and applications.

5. Chromatographic Techniques:

8 Hrs

Adsorption and Partition chromatography, Paper chromatography, Thin Layer chromatography, Ion exchange and Gas chromatography, HPLC, Size Exclusion Chromatography, their principles, techniques and important applications.

6. Electroanalytical Techniques:

15 Hrs

A. Voltametry:

General Introduction, Principle, Instrumentation, Types of Voltammetry: Polarography (Principle & Instrumentation), Cyclic Voltammetry, Pulse Methods.

Stripping Technique: Anodic and Cathodic Stripping Voltametry and their applications in the trace determination of metal ions and biologically important compounds.

B. Ion SelectiveElectrodes:

Electrical properties of membrane, Glass electrode with special reference to H+, Na+, K+ ions, operation of solid membrane electrode, operation of liquid membrane electrode, coated type ion electrode. Applications of ion selective electrode in determination of some toxic metals and some anions (F-, Cl-, Br-, I-, and NO3-).

7. Atomic Absorption Spectroscopy & Flame Photometry:

7 Hrs

Introduction, basic principle, instrumentation & application.

- 1. Quantitative Analysis: Day and Underwood
- 2. A text book of Quantitative Analysis A.I. Vogal
- 3. Advanced Analytical Chemistry: Meites and Thomas
- 4. Analytical Chemistry: Dr. R.K. Soni
- 5. Instrumental methods of Chemical Analysis: G.W. Ewing
- 6. Physical Methods in Inorganic Chemistry: R.S. Drago
- 7. Analytical Chemistry: G.D. Christian
- 8. Basic Concepts of Analytical Chemistry: S.M. Khopkar
- 9. Polarography: Kolltath and Lingane
- 10. Instrumental Methods of Chemical Analysis: Braun
- 11. Instrumental Methods of Analysis: Willard, Merritt & Dean
- 12. Analytical Chemistry: Strouts, Crifillan & Wilson
- 13. Introduction to radiation Chemistry: J.W.T. Spinks & R.J. Woods
- 14. Fundamentals of Analyttical Chemistry: S.A. Skoog & D.W. West
- 15. Analytical Chemistry: R.V. Dilts
- 16. EDTA Titration: Flaschka

PRACTICAL SYLLABUS III- SEMESTER"> III- SEMESTER

ANALYTICAL PRACTICAL

- 1. To verify Lambert's –Beer's Law with the help of U.V visible spectrophotometer.
- i. To determine λ_{max} of a given sample.
- ii. To determine the concentration of unknown sample with the help of U.V visible spectrophotometer.
- 2. To determine the concentration of Na⁺, Ca⁺, K⁺ with the help of flame photometer.
- 3. To scan the U.V visible spectra of unknown sample with the U.V-visible double beam spectrophotometer.
- 4. To determine the calorific value of unknown sample.
- 5. To determine the degradation peak, T_g , T_m of unknown sample with the help of DSC.
- To determine kinematics viscosity of plasticizer with the help of Redwood viscometer.
- 7. To determine the dynamic viscosity of polymeric plasticizer at different temperature with the help of Brukfield viscometer.
- 8. To separate the chlorophyll pigments with the help of TLC.
- 9. Apply paper chromatography to separate
 - i. The chlorophyll pigments
 - ii. Lead anions and cations
- 10. To separate the amino acids with the help of TLC.
- 11. To determine formation constant of FeSCN²⁺ compounds by conductometry.

12. To determine rate constants & formation constants of intermediate complex in the reaction of Cerium (IV) ammonium nitrate and hypophosphoric acid in acid medium.

BIOCHEMISTRY PRACTICAL

- 1. To make a phosphate buffer of pH.
- Qualitative test for carbohydrates
 Molisch's, Iodine, Scliwanhoff, Benedict, Anthrone, Barfoed, Fehling,
 Bial
- Qualitative tests for lipids
 Acrotien test, test for presence of FA, test for unsaturation of FA.
- 4. Determination of acid values of fats and oils
- 5. Determination of saponification value of fats and oils
- 6. Determination of iodine no. of a fat sample
- 7. Qualitative test for amino acid and protein
- 8. To detect ketone bodies in urine sample
- 9. Seperation of plant pigment by TLC
- 10. Estimation of amylase activity in saliva
- 11. To know blood sample in given sample of blood
- 12. To have RBC and WBC count
- 13. To estimate glucose in urine sample
- 14. To estimate sugar in blood
- 15. To prepare casein protein from milk and its estimation.

IVth Semester

CH-401 Environmental Chemistry (PG 330)

60 Hrs

1. Environment 8 Hrs

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. Biodistribution of elements.

2. Hydrosphere 12 Hrs

Chemical composition of water bodies-lakes, streams, rivers and wet lands etc. Hydrological cycle.

Aquatic pollution - inorganic, organic, pesticide, 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 etc.), residual chloride and chlorine demand.

Purification and treatment of water.

3. Soils 6 Hrs

Composition, micro and macro nutrients, Pollution - fertilizers, pesticides, plastics and metals. Waste treatment.

8 Hrs 4. Atmosphere

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

Analytical methods for measuring air pollutants. Continuous monitoring instruments

5. Industrial Pollution 12 Hrs

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.

6. Environmental Toxicology

14 Hrs

Chemical solutions to environmental problems, biodegradability, principles of decomposition, better industrial processes. Bhopal gas tragedy, Chernobyl, Three Mile

Island, Sewal D and Minamata disasters.

- 1. Environmental Chemistry, S. E. Manahan, Lewis Publishers.
- 2. Environmental Chemistry, Sharma & Kaur, Krishna Publishers.
- 3. Environmental Chemistry, A. K. De, Wiley Eastern.
- 4. Environmental Pollution Analysis, S.M. Khopkar, Wiley Eastern
- 5. Standard Method of Chemical Analysis, F.J. Welcher Vol. III, Van Nostrand Reinhold Co.
- 6. Environmental Toxicology, Ed. J. Rose, Gordon and Breach Science Publication.
- 7. Elemental Analysis Airborne Particle,. Ed. S. Landsberger, and M. Cealchmao, GO'doo and Beach Scleoce
- 8. Environmental Chemistry, C. Baird, W. H. Freeman.

CH-402 Organic Synthesis (PG-331)

60Hrs

1. Organometallic Reagents:

15 Hrs

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

Group I & 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.

2. Oxidation: 11 Hrs

Introduction. Different oxidative processes.

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

Alcohols, diols, aldehydes, ketones, ketals and carboxylic acids.

Amines, Hydrazines and sulphides.

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

3. Reduction: 11 Hrs

Introduction. Different reductive processes.

Hydrocarbons- alkanes, alkenes, alkynes and aromatic rings.

Carbonyl Compounds- aldehydes, ketones, acids and their derivatives. Epoxides, nitro, nitroso, azo and oxime groups.

4. Rearrangements:

15 Hrs

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

A detailed study of the following rearrangements:

Pinacol-Pinnacolone, Wagner-Meerwin, Demjanov, benzyl-Benzilic acid, Favorskii, Arndt-Eistern synthesis, Neber, Beckmann, Hoffman, Curtius, Schmidt, Baeyer Villiger, Shaprio reaction, Barton, Chichibaben, Hoffman-Lofler Freytag reaction, Wittig reaction.

5. Metallocenes, Nonbenzenoid Aromatic and Polycyclic Aromatic Compounds:

8 Hrs

General considerations, synthesis and reactions of Ferrocene, Chrysene, Azulene.

- 1. Modern Synthetic reactions, H. O. House, W.A. Benjamin.
- 2. Some Modern Methods of Organic Synthesis, W. Carruthers, Cambridge Univ. Press.
- 3. Advanced Organic Chemistry, Reaction Mechanisms and Structure, J. March, John Wiley.
- 4. Principles of Organic Synthesis, R.O.C. Norman and J. M. Coxoxn, Blackie Academic and Professional.
- 5. Advanced Organic Chemistry Part B, F.A. Carey and R. j. Sundberg, Plenum Press.
- 6. Rodd's Chemistry of carbon compounds, Ed. S. Coffey, Elsevier.

60Hrs

1. Introduction to Medicinal Chemistry:

2 Hrs

Introduction to important functional groups in medicinal chemistry, a century of drug research.

2. Drug design: 6 Hrs

Strategies for drug research including various targets, lead generation/ sources for drugs, receptor and drug receptor interactions; enzymes and design of inhibitors; concept of Prodrugs, hard and soft drugs.

3. Combinatorial Chemistry:

7 Hrs

Introduction; solid support and linkers; combinatorial synthesis of compounds on solid phase, split and mix method, premix method, spatially addressable parallel chemical synthesis, multiple synthesis; Identification of active compounds from combinatorial libraries; Analytical methods for characterization of combinatorial libraries; Application of combinatorial libraries using solid phase chemistry.

4. Computational approaches:

7 Hrs

Structure activity relationship, concept of QSAR, physicochemical parameters-lipopilicity, partition coefficient, electronic-ionization constants, H-bonding, steric parameters, Hammett equation. Isosterism, bioisosterism.

5. Biodisposition and implications:

10 Hrs

Pharmacokinetics; concepts including absorption, distribution, metabolism and excretion of the drug, pharmacokinetic parameters; drug metabolism including phase I and phase II biotransformatins; mention of the uses of pharmacokinetics in drug development process. Molecular toxicology, avoidance of toxic intermediates,

6. Neuroactive agents:

10 Hrs

The chemotherapy of the mind: Introduction, neurotransmitters, CNS depressant, General anaesthetics, mode of action of hypnotics, sedatives, antianxiety agents, bezodiazepines, buspirone, neurochemistry of mental diseases. Antipsychotic drugsthe neuroleptics, antidepressants, butyrophenone, serendipity and drug development, stereochemical aspects of neuroactive drugs. Synthesis of Diazepam, Oxazepam, Chlorazepam, barbiturates.

7. Cardiovascular agents:

5 Hrs

Introduction, cardiovascular diseases, drug inhibitors of theperipheral sympathetic function, central intervention of the cardiovascular output, direct acting arteriolar dilators, synthesis of amyl nitrate, sorbitrate, diltiazam, quinidine, verapamil, methyldopa, atenolol, oxeprenolol.

8. Antineoplastic agents:

7 Hrs

Introduction, cancer chemotherapy, role of alkylating agents and antimetabolites in the treatement of cancer. Mention of carcinolytic antibiotics and mitotic inhibitors; synthesis of mechlorethamine, cyclophosphamide, melphalan, uracil, mustards, 6-mercaptopurine. Recent development in cancer chemotherapy, the hormones and natural products.

9. Local anti-infective drugs:

6 Hrs

Introduction and general mode of action, synthesis of sulphonamide, furazolidone, naxilidic acid, eiprofloxacin, dapsone, aminosalicylic acid, isoniazid, ethionamide, ethambutol, fluconazole, econozole, gresiofulvin, chloroquin, primaquin.

- 1. Comprehensive Medicinal Chemistry, Vols. 1-6, Corvin Hansch (editor) 1990.
- 2. Burger's Medicinal Chemistry, 4th edition, 3 parts; M.E. Wolff, Ed. (RS 403.B8-1979-pt. 1,2 &3).
- 3. Principles of Medicinal Chemistry, W.O. Foye (editor), 4th edition, 1995.
- 4. Molecular Mechanism of Drug Action, C. J. Coulson, 1998.
- 5. Medicinal Chemistry: A Biochemical Approach, Thomas Nogrady, 2nd edition, 1998.
- 6. Wilson and Gisvold's Textbook of Organic, Medicinal and Pharmaceutical Chemistry, J.N. delago and W.A. Remers (editors) 9th edition 1991.
- 7. Organic Chemistry of Drug Synthesis, Vol. I, Daniel Lednicer and Lester A., Mitscher (RS 403.L38-Vols. 1,2 and 3).
- 8. The Pharmacological Basis of Therapeutics, Louis S. Goodman and Alfred Gilman (RM 101.G63-1970).

60Hrs

1. Basics 8 Hrs

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 reaction. Polymerization in homogeneous and heterogeneous systems.

2. Polymer characterization

14 Hrs

Polydispersion-average molecular weight concept. Number, Weight and Viscosity average molecular weight. Polydispersity and molecular weight distribution. The practical significance of molecular weight. Measurement of molecular weight. End group, viscosity light scattering, osmotic and ultracentrifugation methods. Analysis and testing of polymers and chemical analysis of polymers, spectroscopic methods, physical testing – tensile strength, fatigue, impact. Tear resistance. Hardness and abrasion resistance.

3. Structure and Properties

14 Hrs

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 & Tg, effects of molecular weight, diluents, chemical structure, chain topology, branching and cross linking. Property requirements and polymer utilization.

4. Polymer Processing

12 Hrs

Plastics, elastomers and fibers. Compounding. Processing techniques: Calendering, die casting, rotational casting, film casting, injection moulding, blow moulding, extrusion moulding, thermoforming, foaming, reinforcing and fiber spinning.

5. Properties of Commercial Polymers

12 Hrs

Polyethylene, Polyvinyl chloride, polyamides, polyesters, phenolic resins, epoxy resins and silicon polymers. Functional Polymers- Fire retarding polymers and electrically conducting polymers. Biomedical polymers- contact lens, dental polymers, artificial heart, kidney, skin and blood cells.

- 1. Text Book of Polymer Science, F.W. Billmeyer Jr, Willey.
- 2. Polymer Science, V.R. Gowariker, N.V. Viswanathan and J. Sreedhar, Wiley-Eastern
- 3. Functional Monomers and Polymers, K. Takemoto, Y. Inaki and RM. Ottanbrite.
- 4. Contemporary Polymer Chemistry, H.R. Alcock and F.W. Lambe, Prentice Hall.
- 5. Physics and Chemistry of Polymers, J. M. G Cowie, Blackie Academic and Professional.

PRACTICAL SYLLABUS <u>IV- SEMESTER</u>

ORGANIC PRACTICAL

- 1. Analysis of ternary organic mixtures.
 - Separation with NaHCO3 and water
 - Separation with NaOH and water.
 - Separation with HCl and water
 - Separation with organic solvents.
- 2. Three step organic preparations.
 - TO prepare O-chlorobenzoic acid from phthalic anhydride.
 - To prepare benzilic acid from benzaldehyde.
 - To prepare dibenzil from benzaldehyde.
 - To prepare benzoic acid from benzophenone.
- 3. To determine the strength of the given aniline solution (estimation of aniline).
- 4. To determine the percentage of sulphur in the given organic compound by messenger's method.