H-1007 FIRST SEMESTER COURSE-I INORGANIC CHEMISTRY-I 60 hr

12 Hr

1. Stereochemistry and Bonding in Main Group Compounds

VSEPR, Walsh diagrams (tri atomic molecules).d pi-Ppi bonds, Bent rule and energetic of hybridization, some simple reactions of covalently bonded molecules.

2. Metal-Ligand Equilibria in Solution

8 Hr

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 Hr

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 reaction (such as Henry taube's classical reaction of (NH3)3Co3+- Cr2+, inner sphere type reaction), outer sphere type reaction, 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.

COURSE-II Organic chemistry -I H-1008

Nature of bonding in Organic Molecules

Delocalized chemical bonding,

Conjugation, hpyerconjucation, bonding in fullerenes, tautomerism.

Aromaticity in in benzenoid and non-benzenoid compounds, alternant and non-alternant hydrocarbons. Huckel's rule, energy level of n-molccular orbitals. annulenes, antiaromaticity.

W-aromaticity, homo-aromaticity. Bonds approach. PMO approach .Bonds weaker Than covalent-addition compounds, crown other and cryptands. complexes and cryptands inclusion compounds, cyclodextrins, catenanes and rotaxanes.

2.Stereochemistry

Conformational analysi 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. nantiotopic and diastereotopic atoms, groups and faces.

Stereospecific and stereoselcctive synthesis. Asymmetric synthesis. Optical activity in the absence of chiral carbon (biphenyls, al lenes 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, Hanmmond '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

The SN2, SNI. mixed SNI & SN2 and SET mechanisms. The rieighbouring group mechan ism, neighbouring group participation by t and o 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 nueleophile, leaving group and reaction medium. Phase transfer catalysis and ultrasound, ambident nucleophile, regioselectivity.

5. Aliphatic Electrophilic Substitution

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

COURSE-III H-1009 PHYSICAL CHEMISTRY-I I Quantum Chemistry

1. Introduction to Exact Quantum Mechanical Results The Schrodinger equation

- and the postulates of quantum mechanics. Discussion of solutions of the Schrodinge cquation to some model systems viz.. particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom.
- 2. Approximate Methods The variation theorem. lincar variation principle. Perturbation theory (first order and nondegenerate). Applications of variation method perturbation theory to the Helium atom.
- 3. Angular Momentum Ordinary angular momentum, generalized angular momentum, eigen functions for angular momentum, eigen values of angular mömentum, operator using ladder operators, addition of an gular 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 effect spin-orbit coupling and Zeeman splitting, introduction to the methods of self -consistet 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 cyclobutad iene etc. Introduction to extended Huckel theory.

II Thermodynamics

1. Classical Thermodynamies

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. Vectors and Matrix Algebra 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.

Course IV MATHEMATICS FOR CHEMISTS H-1010 Vector and Matrix Algebra A-vectors

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

B-Matrix Algebra Addiion and multiplicetion; inverse, adjoint and transpose of matrices. special matrices

(Symmetric, gkew-symmetric, Hermitian, skew-Hermitian, unit, diagonal, unitary etc.) and their properties Matrix equation homogeneous known homogeneous linear equation and condition for the solution linear dependence and independence introduction to vector space Matrix eigenvalues and eigenvectors diagonalization determinants example from huckle theory introduction to tensors polarizability and magnetic suscipitability as examples

II.Differential Calculus

functions continuity and differentiability rules for differentiation application of differential calculus including Maxima and minima (examples related to maximally populated rotational energy levels Bohr's radius and most profitable velocity from Maxwell's distribution etc) exact an inexact differential with their application to thermodynamics properties. integral calculus basic rule for integration integration by parts partial function and substitution reduction formula application of integral calculus function of several variable partial differentiation coordinate transformation(example cartesian of spherical polar) curve sketching III. elementary differential equation

variable separable and exact first order differential equations homogeneous exactly linear equation application to chemical kinetics secular equilibrium quantum chemistry etc solution of differential equations by the power series method Fourier series solution of harmony consolator and legendre equation etc. spherical harmonics second order differential equations and their solutions

IV. permutation and probability

permutation and combination, probability and probability theorems, probability curves, average, root mean square and most probable errors, example from the kinetic theory of gas etc, curve fitting

(including least square feet etc.)vacuum band with the general poly nominal fit.

Biology for Chemists H-1011

I. cell structure and function

Structure of prokaryotic and eukaryotic cells, intercellular organelles and their functions, comparison of plant and animal cells. Overview of metabolic processes catabolism and anabolism. ATP the biological energy currency.

II. Carbohydrates

Confirmation of monosaccharides, structure and functions of important derivatives of monosaccharides like glycosides, deoxy sugars, myoinositol amino sugar, N-acetylmuramic acid, sailoc acid, disaccharides and polysaccharides structure polysaccharides cellulose and chitin. Stories polysaccharides starch and glycogen structure and biological functions of glucosaminoglycanes or mucopolysaccharides carbohydrates of glycoproteins and glycolipids role of sugar in biological recognition ascorbic acid. God but I did metabolic Krebs cycle glycolysis. Glycogenesis and glycogenolysis gluconeogenesis, pantos phosphate pathway,

III.Lipids

Fatty acids, essential fatty acids, structure and function of dry acyl glycos glycerol, glycerol phospholipids, sphinogolipids cholesterol, buy lessons, protostoglandins.Lipoproteins composition and functions, role in antherosclerosis. Properties of lipid aggregates micelles, bilayers, liposomas and their possible biological functions. Biological membranes, Fluid mosaic model of membrane structure. pid metabolism-ß-oxidation of fatty acids,

IV. Amino-acids, Peptides and Proteins

Chemical and enzynmatic hydrolysis of proteins to peptides. Sccondary structure of proteins, forces responsible for holding of secondary structures. a-helix. Pseets, Super secondary structure, triplec 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, racemiation/detection.

V. Nucleic Acids

5 Hrs.

Purine and pyrimidine bases of nucleic acids. & their syntheiss 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 transcriptiop translation and genetic code. Chemical synthesis of mono and trinucleoside.

COURSE-IV

COMPUTERS FOR CHEMISTS H-1012

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 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

The language feature are listed here with reference to 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.

3. Programming in Chemistry

LOGICAL variables, Double Precision variables. Subscripted variables and DIMENSIONS. DO statements. FUNCTION and SUBROUTINE. COMMON and DATA statements. Decision control structure. case4 contròl structure, functions, introduction to arrays. programmes based on above.

4. Use of Computer Programmes

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 latice energy and ionic radii from experimental data. Lincar 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 dattabase such as Cambridge database.

4. Use of computer Programmes

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 Ofice (MS Word, MS Excel, MS PowerPoint), Lab sessions based on MS Office package, Introduction to IInternet Explorer.

PRACTICAL SYLLABUS - I-SEMESTER 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 CH,COOH solution by titrating it against N/10 NaOH using pH meter.
- 3. To find out the strength of HCl and CH,COOH in a mixture of both by titrating it against N/I0 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 KMnO, 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 (I) Dibydrate.
- 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
- Nitration Oxime formation
- Hydrolysis Bromination
- Benzoin condensation reaction etc.
- Hoffmann Bromide reaction
- 4. To determine the iodine value of the, given fat sample.
- 5. To determine the saponification value of the given fat sample.

SECOND SEMESTER

COURSE-I

INORGANIC CHEMISTRY-II

H-2007

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 B 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 - pi 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 an dioxygen cómplexes; tertiary phosphine as Ligand

3. Metal Clusters

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

4. Nuclear Chemistry

Radioactive decay & cquilibrium. Nuclear Reactions, Q-Valuc crosS-Sections, types or reactions, Chemical effects of nuclear transformations Fission & Pusion, FiSsion produçt, & fission yields. Radioactive techniques, tracer techniques.

Course-II

ORGANIC CHEMISTRY-II

H-2008

1. Aromatic Electrophilic Substitution

The arenium ion mechanism. orientation and reactivity, energy profile diagrams. Th

ortho/para ratio. ipso attack, orientation in other ring systems. Quantitative treatmex of reactivity in substrates and electrophilés. Diazonium coupling, Vilsmeir reaction, Gattermann-Koch reaction.

2. Aromatic Nucleophilic Substitution

The SNAr, SN 1, benzyne and SRN I 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 abridgehead. Reactivity in the attacking radicals. The effect of solvents on reactivity. Allylic halogenations (NBS), oxidation of aldehydes to carboxylic acid. autooxidation, coupling ofalkynes and arylation ofaromatic compounds by diazonium salts. Sandmeyer reaction. Free radical rearrangement. Hunsdiecker reaction.

4. Addition to Carbon-Carbon Multiple Bonds

Mechanistic and stercochemical 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

Mechanism of metal hydride reduction of saturated and unsaturated carbonvl 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.

6. Elimination Reactions

The E2. El and El CB mechanisms and their spectrum. Orientation of the double hon. 5 Hrs

Reactivity - effects of substrate structures, attacking hase, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination.

7. Pericyclic Reactions

Molecutar orbital symmetry, Frontier orbitals of ethylene, 1,3- butadiene, 1,3.5- hexatriene and allyl system. Classification of pericyclic reactions. Woodward Hoffimann correlation diagrams. FMO and PMO approach. Electrocyclic reactions -

conrotatory and disrotatory motions, 4n, 4nt2 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.

COURSE-III

PHYSICAL CHEMISTRY -II

H-2009

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 unimolocilar reactions.

Dynamic chain (hydrogen-bromine reaction, pyrolysis ofacctaldehyde, decomposition of ethanc). photochemical (hydrogen-bromine and hydrogen-chlorinc 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 ofmolecular 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 equátion), 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 CMCof surfactants, counter ion binding to micelles, thermodynamics of micellization, solubilization, miero 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 configuratiomof macromolecules, calculation of average dimensions of various chain structures.

3. Electrochemistry

Electrochemistry of solutions. Debye-Huckel - Onsager treatment and its extension. ion' solvent interactions. Debye-Huckel-Jerum mode. Thermodynamics of electrified interface equations. Derivátion of electro-capillarity, Lippmann equations (surface excess), methods of determination. Structure of electrified interfaces, Guoy -Chapman. Stern.

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 laver al Semiconductor. electro lyte solution interfaces, structure of houble layer interfaces. Electrocatalysis' - influence of various parameters: Hydrogen electrode. Bioclectrochemistry, Polarography theory, Ilkovic equation, half wave potential and its significance.

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

GROUP THEORY, SPECTROSCOPY & DIFFRACTION METHODS & SOLID STATE H-2010

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 subroup. Conjugacy relation and classes. Point symmetry group. Schonflies symbols, representations of groups by matrices (representation for the Cn, Cny, Cnh. Dnh ctc. 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

Electromagnetic radiation, interaction of electromagnetic radiation with matter absorption, emission, ransmission, 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

- **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. Photoélectron Spectroscopy Basic principles; photo-electric effect, ionization process, Koopman's theorem. Photoelectron spectra of simple molecules, ESCA, chemical information from ESCA. Auger clectron 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

constantJ'. 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 spliting 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

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.

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 CH,COOH, C,H,OH, n-Hexane at room temperature and hence calculate the atomic parachors of C, H, andO.
- 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 HCI solution by titrating it against N/10 NaOH using conductometer.
- 7. To find out the strength of given NH,OH by titrating it against HCl solution using conductometer.
- 8. To find the velocity constant of the hydrolysis of methyl acetate catalyzed by i.HCl.
- 9. Determine the relative strengths of two acids i.e. HCI & H,SO, 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 Níckel in a given solution,

ORGANIC PRACTICAL

- 1. Analysis of binary organic mixturés
- Separartion with NaHCO3 separation with NaOH separation with HCI

2.Two step preparations

To prepare Anthranilic Acid from Phthaic Anhydride, To prepare o- Chlorobenzojc Acid from Phthalamide. • To prepare Benzil from Benzaldehyde. • To prepare Benzanilide from Benzophenone.

Third Semester

Paper-1 Photochemistry (Compulsory far all branches) H- 3007

1-Basic of Photochemistry

Absorption, excitation, photochemical laws, quantum yield, electronically excited states-life times-measurements of the times. Flash photolysis, stopped Flow techniques, Energy dissipation by radiative and non-radiative processes, absorption spectra, Franck-Condon principle, photochemical stages-primary and secondary processes.

2-Photochemical Reactions

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

3-Properties of Excited States

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

4-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-photo-dissociation, gas-phase photolysis.

5- Photochemistry of Alkenes

Intromolecular reactions of the olefinic bond-geometrical isomerism, cyclisat ion reactions, rearrangement of 1,4 and 1,5-dienes,

6- Photochemistry of Carbonyl compounds

Intramolecular reactions of carbonyl compounds-saturated, cyclic and acyclic, , - unsaturated and , unsaturated compounds, Cyclohexadienones. Intermolecular ..buchi Reaction.

7- Photochemistry of Aromatic Compounds

Isomerisations, additions and substitutions.

8- 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.

Paper-II Spectroscopy (Compulsory for all branches) H-3008

1- Ultraviolet Visible Spectroscopy

Various electronic transitions (185-800 nm), Beer-Lambert law, effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes. Fieser-Woodward rules for conjugated dienes and carbonyl compounds ultraviolet spectra of aromatic and heterocyclic compounds Steric effect in biphenyls.

2- Infrared Spectroscopy Instrumentation and sample handling.

Characteristic vibrational frequencies of alkanes, 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. Symmetry and shapes of AB, A2, AB2, AB3, AB4, AB5, and AB6, mode of bonding of ambidentate ligand, ethylenediamine and diketonato complexes, application of resonance

3- Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD)

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

4- Nuclear Magnetic Resonance Spectroscopy

General introduction and definition, chemical shift, spin-spin interaction, shielding mechanism, mechanism, of measurement chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides & mercapto), Intensity of NMR regnals, chemical exchange, effect of deuteration, complex spin-spin interaction between two, three, four and five nuclei (first order spectra) virtual coupling, stereochemistry hindered rotation, karlus curve variation of coupling constant with dihedral angle. Simplification of complex spectra, nuclear magnetic double resonance, contact shift reagents, solvent effects. Fourier transforms technique, Nuclear Overhauser Effect (NOE) Resonance of other nuclei-F, P. Some applications including biochemical systems.

5- Carbon-13 NMR Spectroscopy

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

6- 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 pH4, F2- and (BH3).

7- Mossbauer spectrocopy

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) Sn2+ and Sn4+

compounds –nature of M-L bond, coordination number, structure and (3) detection of oxidation state and in equivalent MB atoms.

Book suggested-

- 1- Inorganic Electronic Spectroscopy, A.P.B. Lever, Elsevier.
- 2- Physical Methods for Chemistry, R.S. Drago, Saunders Company.
- 3- Structural Methods in Inorganic chemistry, E.A.V. Ebsworth, D.W.H. Rankin and S. Cradock. ELBS.
- 4- Infrared and Raman Spectra: Inorganic and Coordination compounds,
- K. Nakamoto. Wiley.
- 5- Progress in Inorganic Chemistry vol., 8. ed, F.A. cotton, vol., 15, ed.
- S.J. Lippard, wiley.
- 6- Transition Metal Chemistry ed, R.L. Carlin vol. 3 Dekker.
- 7- Inorganic Electronic Spectroscopy, A.P.B. Lever, Elsevier.
- 8- NMR, NOR, EPR and Mossbauer spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis.
- 9- Horwood. Practical NMR Spectroscopy, M.L. Martin, J.J. Delpeugh and G.J. NBrtin. Heyden.
- 10- Introduction to NMR Spectroscopy, R.J. Abraham, J. Fisher and P. Loftus. Wiley.

Paper-III Analytical Chemistry (Compulsory for all branches) 60Hrs. H-3009

1- Introduction

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

2- Errors and Evaluation:

Definition of terms of mean and median, precision-standard deviation, relative standard deviation, accuracy, absolute 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:

Elementary working, Principles of Geiger Muller, lionization, proportional and -ray counters. Neutron radiation sources, radio tracer techniques. Nautron 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:

Introduction of different thermal methods, Thermogravimetry- TGA & DTA, static thermogravimetry, quasithermogravimetry and dynamic thermogravimetry, Instrumental and balances, X-Y recorder,thermogram, factors affecting thermograms. Application of thermogravimetry. Differential Scanning Calorimetry (DSC): Introduction, instrumentation, DSC-curves, factors affecting DSC curves and applications.

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

5- Chromatographic Techniques:

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

6- Electroanalytical Techniques:

A- Voltametry:

General introduction, Principle, Instrumentation, types of Voltammetry Paleography (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 Selective Electrodes:

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 electode. Applications of ion selective electrode in determination of some toxic metal and some anions (F-, CI- Br, I-, and NO3).

Paper-IV Bioorganic Chemistry Elective 1 H-3011

1. Introduction:

Chemistry of amino acids proteins and their derivatives; methods of isolation and identification; Primary, secondary, tertiary and quaternary structures of proteins; determination and biochemical applications of the structures proteins; Nomenclature of nucleosides and nucleotides; Effects of acid and alkali on hydrolysis of nucleic acids; Structure of DNA and RNA; prokaryotic versus eukaryotic organisms.

2. 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. Fisher'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, Michaelismeten and Lineweaver-Burk Plots, reversible and irreversible inhibition.

3. Mechanism of Enzyme Action

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

4. 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, intermediates in isomerization reactions, cleavage and condensation, some isomerization and rearrangement reactions. Enzyme catalyzed carboxylation and decarboxylation.

5. Co-Enzyme Chemistry

Co-Factors as derived from vitamins, co-enzymes, prosthetic groups, apoenzymes. Structure and biological functions of co-enzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD+, NADP+, FMN, FAD, lipoic acid, vitamin B12 Mechanisms of reactions catalyzed by the above co-factors.

6. Enzyme Models

Host-guest chemistry, chiral recognition and catalysis, molecular recognition, molecular asymmetry and prochirality. Biomimetic chemistry, crown ethers. Cyptates. Cyclodextrins, cyclodextrin-based enzyme models, calixarenes, ionophores, micelles, synthetic enzyme of synzymes.

7. Biotechnological Applications of Enzymes

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 chesse-making, syrups from corn starch, enzymes as targets for drug design. Clinical uses of enzymes, enzyme therapy.enzymes and recombinant DNA technology. Application of enzymes in organic synthesis.

III SEMESTER

ANALYTICAL PRACTICAL

- 1. To verify Lambert's Beer's Law with the help of U.V. visible spectrophotometer.
- a. To determine max of a given sample.
- b. 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. Tg, Tm of unknown sample with the help of DSC.
- 6. To determine kinematic viscosity of plasticizer with the help of Redwood viscometer.
- 7. To determine the dynamic viscosity of polymeric plastcizer at different temperature with the help of Brook field viscometer.
- 8. To separate the chlorophyll pigments with the help of TLC.
- 9. Apply paper chromatography to separate.
- a. The chlorophyll pigments.
- b. Lead anions and cations.
- 10. To separate the amino acids with the help of TLC.
- 11. To determine formation constant of Fe SCN-2 compounds by conductometry.
- 12. To determine rate constants & formation constants of intermediate complex in the reaction of Cerium (IV) ammonium nitrate and hypo phosphoric acid in avid medium.

BIOCHEMISTRY PRACTICAL

- 1. To make a phosphate buffer of pH.
- 2. Qualitative test for carbohydrates.

Molish's Iodine, Scliwanhoff, Benediet, Anthrone, Barfoed, Fehling, Bial's Test

3. Qualitati ve test for lipids.

Acrolien test for presence of FA, Test for unsaturation of FA.

- 4. Determination of acid value of fats and oils.
- 5. Determination of saponification value of fats and oils.
- 6. Determination of lodine no. of a fat sample.
- 7. Qualitative test for Amino acid and protein.

Ninhydrin, Million's, Sakaguchi, Xanthoproteic, Biuret.

- 8. To detect Ketone bodies in urine sample.
- 9. Separation of plant pigmen by TLC.
- 10. Estimation of amylase activity in saliva.
- 11. To Know blood group 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.

M. Sc. IV Chemistry Syllabus FOURTH SEMESTER

ENVIRONMENTAL CHEMISTRY H-4007

1.Environment

Introduction. Composition of atmosphere, vertical termperature. heat budget of the carth atmospheric system, vertical stability atmosphere. Biogeochemical cycles of C. N,P. S and O. Biodistribution of elements.

2. Hydrosphere

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-organ isms. 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

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

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. S. O and their effect. pol fution 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

5. Industrial Pollution

- Cement. sugar, distillery, drug. paper and pulp. thermal power plants, nuclear pewr plants. metallurgy. Polymers, drugs etc. Radionuclide analysis. Disposal of wastes and their imanagement.

6. Environmental Toxicology

Chemical solutions to environmental problems, biodégradability, principles of decomposition: better industrial processes. Bhopal gas tragedy, Chernobyl, Three Mile Island, SewalD.and Minamata disasters.

ORGANIC CHEMISTRY SPECIAL I (Organic Synthesis) H-4013

1. Organometallic Reagents:

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

Group | & 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:

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

3.Reduction:

Introduction. Different reductive processes.

Aiydrocarbons- alkanes, alkenes, alkynes and aromatic rings.

Aarbonyl Compounds- aldehydes, ketones, acidş and their derivatives.

Epoxides, nitro. nitroso, azo and oxime groups.

4. Rearrangements:

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, BaeyerVilliger, Shaprio reaction. Barton,

Chichibaben, Hoffiman-Lofler Freytag reaction, Wittig reaction.

5. METALLOCENES, NONBENZĒNOID AROMATIC AND POLYCYCLIC AROMATIC COMPOUNDS:

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

ORGANIC CHEMISTRY SPECIAL III

Polymers H-4015

1. Basics

Importance of polymers. Basic concepts: Monomers, repeat units, degree of polymerization. Linear, branched and nctwork polymers. Classification of polymers. Polymerization: condensation, addition, radicat chain-ionic and co-ordination and copolymerization. Polymerization conditions and polymer reaction. Polymerization in homogeneous and heterogeneous systems.

2. Polymer characterization

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

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

4. Polymer Processing

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

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.

ORGANIC CHEMISTRY SPECIAL IV (Chemistry of Natural Products) H-4016

- **1.Terpenoids and Carotenoids**: Classification, nomenclature, occurrence, isolation. genera' nethods of structure, determination, isoprene rule, Structure determination. stereochemistry biosynthesis and synthesis of the following representative molecules: Citral, Geraniol, termpencol Menthol, Farnesol, Zingiberen.
- **2. Alkaloids**: Definition, nomenclature and physiological action, occurrence, isolation. general methods or structure elucidation, degradation, classification based on nitrogen heterocyclic rings, role of alkalords in plants, Structure, stereochemistry, synthesis and biosynthesis of the following: Ephedrine, (+) Coniline, Nicoline, Atropine, Quinine and Morphine.
- **3. Steroids**: Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation, Structure determination and synthesis of Cholestrol. Bile acids. Androsterone, Testosteronc, Estronc, Progestrone, Aldosterone, Biosynthesis of steroids.
- **4.Plant Pigments**: Occurrence, nomenclature and general methods of structure

determination, Isolation and synthesis of Apigenin, Luteolin, Quercetin, mytcelin. Ouercetin-3-glucoside, Vitexin, Diadzein, Butein, Aureusin, Cyanidin-7- arabinoside, Cyanidin, Hirsutidin. Biosynthesis of flavonoids: Acetate pathway and Shikimic acid pathway.

5.Prophyrins:

Structure and synthesis of Haemoglobin and Chlorophyll.

6. Prostaglandins: Occurrence, biogenesis and physiological effects Synthesis of PGE2, and PGF2a,

ORGANIC CHEMISTRY PRACTICALS

- 1. Duration of examination: Three days, six hours daily
- 2. One internal examiner from college and one external examiner from other university are to be appointed.
- 3. Total section-4

Total practicals to be conducted in he exam-4 (One from each section)

4. Marks distribution:

Total marks=100

Mixture=30 marks

Preparation=15marks
Estimation of aniline=10marks
Estimation of sulphur=20marks
Viva=10marks
Record=10marks
2

Each section is to be covered in practice.

- 1. Analysis of ternary organic mixtures.
- Separation with NaIHCO, and water
- Separation with HCI and water
- Separation with NaOH 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/phenol solution (estimation of Aniline phenol).
- 4, To determine the percentage of sulphur in the given organic compound by messenger's