

**M.Sc. CHEMISTRY
(FOUR SEMESTER COURSE) SCHEME OF EXAMINATION
M.Sc. (Previous)**

SEMESTER I

Paper Course No. Course Hrs Marks

Paper I MCH-401 Inorganic Chemistry I 60 50
Paper II MCH-402 Organic Chemistry I 60 50
Paper III MCH-403 Physical Chemistry I 60 50
Paper IV MCH-404 Group Theory & Spectroscopy I 60 50
Paper V MCH-405 a) Mathematics for Chemists* 60 50
b) Biology for Chemists** 60 50
Practical 270 100

Total Marks 350

* For student without Mathematics in B.Sc.

** For student without Biology in B.Sc.

SEMESTER II

Paper Course No. Course Hrs Marks

Paper VI MCH-406 Inorganic Chemistry II 60 50
Paper VII MCH-407 Organic Chemistry II 60 50
Paper VIII MCH-408 Physical Chemistry II 60 50
Paper IX MCH-409 Spectroscopy II 60 50
Paper X MCH-410 Computers for Chemists 60 50
Practical 270 100

Total Marks 350

M.Sc. (Final)

SEMESTER III Desertation

SEMESTER IV

Paper Course No. Course Hrs Marks

Paper XVI MCH-504 Applications of Spectroscopy
(Organic Chemistry) 60 50
Paper XVII MCH-505 Solid State Chemistry 60 50
Paper XVIII MCH-506 Environmental Chemistry 60 50
Paper XIX Elective Paper 60 50
Paper XX Elective Paper 60 50
Practical 270 100*

Total Marks 350

Grant Total Marks M.Sc. (Previous & Final) 1400

* Instead of laboratory work, student may performed Project work/Industrial Training.

The following elective papers are approved for M.Sc. II year course.

MCH-601: Organotransition Metal Chemistry.

MCH-602: Polymers

MCH-603: Organic Synthesis

MCH-604: Heterocyclic Chemistry

MCH-605: Chemistry of Natural Products

MCH-606: Analytical Chemistry

MCH-607: Physical Organic Chemistry

MCH-608: Electrochemistry

MCH-609: Medicinal Chemistry

SEMESTER I

Paper-I

MCH-401: INORGANIC CHEMISTRY I

Unit-I

Stereochemistry and Bonding in Main Group Compounds :

VSEPR, Walsh diagram (triatomic and penta-atomic molecules), $d\pi-p\pi$ bond, Bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules.

Unit-II

Metal-Ligand Equilibrium in Solution

Stepwise and overall formation constants and their interaction, trends in stepwise constant, 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 potentiometry and spectrophotometry.

Unit-III

Reaction Mechanism of Transition Metal Complexes

Energy profile of a reaction, reactivity of metal complex, inert and labile complexes, kinetic application of valence bond and crystal field theories, kinetics of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidences in favour of conjugate mechanism, anion reactions, reactions without metal ligand bond cleavage. Substitution reactions in square planar complexes, the trans effect, mechanism of the substitution reaction. Redox reaction, electron transfer reactions, mechanism of one electron transfer reactions, outer sphere type reactions, cross reactions and Marcus-Hush theory, inner sphere type reactions.

Unit-IV

Metal-Ligand bonding

Limitation of crystal field theory, molecular orbital theory for bonding in octahedral, tetrahedral and square planar complexes, π -bonding and molecular orbital theory.

Unit-V

HSAB Theory : Classification of acids and bases as hard and soft; HSAB principle, theoretical basis of hardness and softness; Lewis-acid base reactivity approximation; donor and acceptor numbers, E and C equation; applications of HSAB concept.

Books Suggested :

1. Advanced Inorganic Chemistry, F.A. 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.1. Carlin, Springer Verlag.
6. Comprehensive Coordination Chemistry eds., G. Wilkinson, R.D. Gillars and J.A. Mc Cleverty, Pergamon.

Paper-II

MCH-402: ORGANIC CHEMISTRY I

Unit-I

Nature of Bonding in Organic Molecules

Delocalized chemical bonding-conjugation, cross conjugation, resonance hyperconjugation, bonding in fullerenes, tautomerism. Aromaticity in benzenoid and non-benzoid compounds, alternate and non-alternate hydrocarbons. Huckel's rule, energy. Level of π -molecular orbitals, annulenes, anti-aromaticity, homo-aromaticity, PMO approach. Bonds weaker than covalent-addition compounds, crown ether complexes and cryptands, inclusion compounds, catenanes and rotaxanes.

Unit-II

Stereochemistry

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 spirane chirality due to helical shape. Stereochemistry of the compounds containing nitrogen, sulphur and phosphorus.

Unit III

Conformational analysis and linear free energy relationship

Conformational analysis of cycloalkanes, decalines, effect of conformation on reactivity, conformation of sugars. Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes. The Hammett equation and linear free energy relationship, substituents and reaction constants, Taft equation.

Unit-IV

Reaction Mechanism : Structure and Reactivity

Type 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, isotopes effects.

Unit-V

Aliphatic Nucleophilic Substitution

The SN₂, SN₁ mixed SN₁ and SN₂ and SET mechanism. The neighboring group mechanism, neighboring group participation by p and s bonds, anchimeric assistance. Classical and nonclassical carbocations, phenonium ions, norbornyl systems, common carbocation rearrangements. Application of NMR spectroscopy in the detection of carbocations. The SN₁ 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.

Book Suggested

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 & Professionals.
8. Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh, Macmillan.
9. Pericyclic Reactions, S.M. Mukherji, Macmillan, India
10. Stereochemistry of Organic Compounds, D.Nasipuri, New Age International.
11. Stereochemistry of Organic Compounds, P.S. Kalsi, New Age International.

Paper-III

MCH-403: PHYSICAL CHEMISTRY

Unit-I

Introduction to Exact Quantum Mechanical Results

Schrödinger equation and the postulates of quantum mechanics. Discussion of solutions of the Schrödinger equation to some model systems viz., particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom and helium atom.

Unit-II

Approximate Methods

The variation theorem, linear variation principle. Perturbation theory (First order and nondegenerate). Applications of variation method and perturbation theory to the Helium atom.

Molecular Orbital Theory

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

UNIT III

Angular Momentum

Ordinary angular momentum, generalized angular momentum, eigenfunctions for angular momentum, eigenvalues of angular momentum operator using ladder operators addition of angular momenta, spin, antisymmetry and Pauli exclusion principle.

Unit-IV

Classical Thermodynamics

Brief resume of concepts of laws of thermodynamics, free energy, chemical potential and entropies. Partial molar free energy, partial molar volume and partial molar heat content and their significance. Determinations of these quantities. Concept of fugacity and determination of fugacity. Non-ideal systems : Excess functions for non-ideal solutions.

Activity, activity coefficient, Debye Huckel theory for activity coefficient for electrolytic solutions; determination of activity and activity coefficients; ionic strength. Application of phase rule to three component systems; second order phase transitions.

Unit-V

Statistical Thermodynamics

Concept of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging. Canonical, grand canonical and micro-canonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers). Partition functions- translation, rotational, vibrational and electronic partition functions, Calculation of thermodynamic properties in terms of partition. Application of partition functions.

Fermi-Dirac Statistics, distribution law and applications to metal. Bose-Einstein statistics distribution Law and application to helium.

Books Suggested

1. Physical Chemistry, P.W. Atkins, ELBS.
2. Introduction to Quantum Chemistry, A.K. Chandra, Tata Mc Graw Hill.
3. Quantum Chemistry, Ira N. Levine, Prentice Hall.
4. Coulson's Valence, R. Mc Ween y, ELBS.
5. Chemical Kinetics. K.J. Laidler, McGraw-Hill.
6. Kinetics and Mechanism of Chemical Transformation J.Rajaraman and J. Kuriacose, Mc Millan.
7. Micelles, Theoretical and Applied Aspects, V. MOraoi, Plenum.
8. Modern Electrochemistry Vol. 1 and Vol II J.O.M. Bockris and A.K.N. Reddy, Planum.
9. Introduction to Polymer Science, V.R. Gowariker, N.V. Vishwanathan and J. Sridhar, Wiley Eastern.
10. Introduction to Quantum Chemistry-R.K. Prasad, New Age Publication.

Paper-IV

MCH-404: Group Theory & Spectroscopy I

Unit-I

Symmetry and Group theory in Chemistry

Symmetry elements and symmetry operation, definition of group, subgroup. Conjugacy relation and classes. Point symmetry group. Schonflies symbols, representations of groups by matrices (representation for the C_n , C_{nv} , C_{nh} , D_{nh} group to be worked out explicitly). Character of a representation. The great orthogonality theorem (without proof) and its importance. Character tables and their use; spectroscopy. Derivation of character table for C_{2v} and C_{3v} point group. Symmetry aspects of molecular vibrations of H_2O molecule.

Unit-II

Microwave Spectroscopy

Classification of molecules, rigid rotor model, effect of isotopic substitution on the transition frequencies, intensities, non-rigid rotor. Stark effect, nuclear and electron spin interaction and effect of external field. applications.

Unit-III

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.Q.R. branches, Breakdown of Oppenheimer approximation; vibrations of polyatomic 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.

Unit-IV

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).

Unit-V

Electronic Spectroscopy

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; radio-active and non-radioactive decay, internal conversion, spectra of transition metal complexes, charge-transfer spectra.

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.

Books suggested

1. Modern Spectroscopy, J.M. Hollas, John Wiley.
2. Applied Electron Spectroscopy for chemical analysis d. H. Windawi and F.L. Ho, Wiley Interscience.
3. NMR, NQR, EPr and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Harwood.
4. Physical Methods in Chemistry, R.S. Drago, Saunders College.
5. Chemical Applications of Group Theory, F.A. Cotton.
6. Introduction to Molecular Spectroscopy, G.M. Barrow, Mc Graw Hill.
7. Basic Principles of Spectroscopy, R. Chang, Mc Graw Hill.
8. Theory and Application of UV Spectroscopy, H.H. Jaffe and M. Orchin, IBHOxford.
9. Introduction to Photoelectron Spectroscopy, P.K. Ghosh, John Wiley.
10. Introduction to Magnetic Resonance. A Carrington and A.D. Maclachalan, Harper& Row.

Paper-V

MCH-405 (a) : MATHEMATICS FOR CHEMISTS

(For students without Mathematics in B.Sc.)

Unit-I

Vectors

Vectors, dot, cross and triple products etc. gradient, divergence and curl, Vector Calculus.

Matrix Algebra

Addition and multiplication; inverse, adjoint and transpose of matrices.

Unit-II

Differential Calculus

Functions, continuity and differentiability, rules for differentiation, applications of differential calculus including maxima and minima (examples related to maximally populated rotational energy levels, Bohr's radius and most probable velocity from Maxwell's distribution etc.).

Unit-III

Integral calculus

Basic rules for integration, integration by parts, partial fractions and substitution. Reduction formulae, applications of integral calculus. Functions of several variables, partial differentiation, co-ordinate transformations (e.g. Cartesian to spherical polar).

Unit-IV

Elementary Differential equations

First-order and first degree differential equations, homogenous, exact and linear equations. Applications to chemical kinetics, secular equilibria, quantum chemistry etc. second order differential equation and their solutions.

Unit-V

Permutation and Probability

Permutations and combinations, probability and probability theorems average, variance root means square deviation examples from the kinetic theory of gases etc., fitting (including least squares fit etc with a general polynomial fit).

Book Suggested

1. The chemistry Mathematics Book, E.Steiner, Oxford University Press.
2. Mathematics for chemistry, Doggett and Suiclific, Logman.
3. Mathematical for Physical chemistry : F. Daniels, Mc. Graw Hill.
4. Chemical Mathematics D.M. Hirst, Longman.
5. Applied Mathematics for Physical Chemistry, J.R. Barante, Prentice Hall.
6. Basic Mathematics for Chemists, Tebbutt, Wiley.

Paper-V

CH-405 (b) BIOLOGY FOR CHEMISTS

(For students without Biology in B.Sc.)

Unit-I

Cell Structure and Functions

Structure prokaryotic and eukaryotic cells, intracellular organelles and their functions, comparison of plant and animal cells. Overview and their functions, comparison of plant and animal cells. Overview of metabolic processes- catabolism and anabolism. ATP - the biological energy currency. Origin of life-unique properties of carbon chemical evolution and rise of living systems. Introduction to bio-molecules, building blocks of biomacromolecules.

Unit-II

Carbohydrates

Conformation of monosaccharides, structure and functions of important derivatives of mono-saccharides like glycosides, deoxy sugars, myoinositol, amino sugars. N-acetylmuramic acid, sialic acid disaccharides and polysaccharides. Structural polysaccharides cellulose and chitin. Storage polysaccharides-starch and glycogen. Structure and biological function of glucosaminoglycans of mucopolysaccharides. Carbohydrates of glycoproteins and glycolipids. Role of sugars in biological recognition. Blood group substances. Ascorbic acid.

Unit-III

Lipid

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-oxidation of fatty acids.

Unit-IV

Amino-acids, Peptides and Proteins

Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing. Secondary structure of proteins. Force responsible for holding of secondary structures. α helix, β -sheets, super secondary structure, triple helix structure of collagen. Tertiary structure of protein-folding and domain structure. Quaternary structure. Amino acid metabolism-degradation and biosynthesis of

amino acids, sequence determination : chemical/enzymatic/mass spectral, racemization/detection. Chemistry of oxytocin and tryptophan releasing hormone (TRH).

Unit-V

Nucleic Acids

Purine and pyrimidine bases of nucleic acids, base pairing via Hbonding. Structure of ribonucleic acids (RNA) and deoxyribonucleic acid (DNA), double helix model of DNA and forces responsible for holding it. Chemical and enzymatic hydrolysis of nucleic acids. The chemical basis for heredity, an overview of replication of DNA, transcription, translation and genetic code. Chemical synthesis of mono and trinucleoside.

Book Suggested

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

PRACTICAL

(Duration: 6-8 hrs in each branch)

Practical examination shall be conducted separately for each branch.

Inorganic Chemistry

Quantitative and quantitative Analysis 8

Chromatography 8

Preparation 8

Record 4

Viva Voce 5

Qualitative and Quantitative Analysis

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

b. Insoluble- Oxides, sulphates and halides.

c. Separation and determination of two metal ions Cu-Ni, Ni-Zn, Cu-Fe etc. involving volumetric and gravimetric methods.

Chromatography Separation of cations and anions by Paper Chromatography.

Preparations

Preparation of selected inorganic compounds and their studies by I.R. electronic spectra,

Mossbauer, E.S.R. and magnetic susceptibility measurements. Handling of air and

moisture sensitive compounds.

1. $\text{VO}(\text{acac})_2$

2. $\text{TiO}(\text{C}_9\text{H}_8\text{NO})_2\text{H}_2\text{O}$

3. cis-K[Cr(C₂O₄)₂(H₂O)₂]
4. Na[Cr(NH₃)₂(SCN)₄]
5. Ni(acac)₂
6. K₃[Fe(C₂O₄)₃]
7. Prussian Blue, Turnbull's Blue.

Organic Chemistry

Qualitative Analysis 12

Organic Synthesis 12

Record 4

Viva Voce 5

Qualitative Analysis

Separation, purification and identification of compounds of ternary mixture (one liquid

and one solid) using TLC and columns chromatography, chemical tests. IR spectra to be

used for functional group identification

Organic Synthesis

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

chromatography. Oxidation : Adipic acid by chromic acid oxidation of cyclohexaneol

Grignard reaction : Synthesis of triphenylmethanol from benzoic acid The Products may

be Characterized by Spectral Techniques.

Physical Chemistry

Error Analysis and Statistical Data Analysis 8

Chemical Kinetics 9

Solution 8

Record 4

Viva Voce 5

Error Analysis and Statistical Data Analysis

Errors, types of errors, minimization of errors distribution curves precision, accuracy and

combination; statistical treatment for error analysis, student 't test, null hypothesis, rejection criteria. F & Q test; linear regression analysis, curve fitting. Calibration of

volumetric apparatus, burette, pipette and standard flask. Adsorption To study surface

tension-concentration relationship for solutions (Gibbs equation). Phase Equilibria

- i. Determination of congruent composition and temperature of a binary system (e.g. diphenylamine-benzophenone system).
- ii. Determination of glass transition temperature of given salt (e.g., CaCl_2) conductometrically.
- iii. To construct the phase diagram for three component system (e.g. chloroform-acetic acid-water).

Chemical Kinetics

- i. Determination of the effect of (a) Change of temperature (b) Change of concentration of reactant and catalyst and (c) Ionic strength of the media on the velocity constant of hydrolysis of an ester/ionic reaction.
- ii. Determination of the velocity constant of hydrolysis of an ester/ionic reaction in micellar media.
- iii. Determination of the velocity constant for the oxidation of iodide ions by hydrogen peroxide study the kinetics as an iodine clock reactions.
- iv. Flowing clock reactions (Ref : Experiments in Physical Chemistry by Showmaker)
- v. Determination of the primary salt effect on the kinetics of ionic reaction and testing of the Bronsted relationship (iodide ion is oxidised by persulphate ion).
- vi. Oscillatory reaction.

Solution

Determination of molecular weight of non-volatile and electrolyte/electrolyte by cryoscopic method and to determine the activity coefficient of an electrolyte. Determination of the degree of dissociation of weak electrolyte and to study the deviation from ideal behaviour that occurs with a strong electrolyte.

Books Suggested

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

SEMESTER II

Paper-VI

MCH-406: INORGANIC CHEMISTRY II

Unit-I

Electronic Spectral Studies of Transition Metal Complexes :

Spectroscopic ground states, correlation. Orgel and Tanabe-Sugano diagrams for transition metal complexes (d_1 - d_9 states), Selection rule for electronic spectroscopy. Intensity of various type electronic transitions. Calculations of $10Dq$, B and β parameters, charge transfer spectra.

Unit-II

Magnetic Properties of Transition Metal Complexes

Anomalous magnetic moments, Quenching of Orbital contribution. Orbital contribution to magnetic moment, magnetic exchange coupling and spin crossover.

Unit-III

Metal π -Complexes

Metal carbonyl, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls; preparation, bonding structure and important reaction of transition metal nitrosyl, dinitrogen and dioxygen complexes; tertiary phosphine as ligand.

Unit-IV

Metal Clusters

Higher boranes, carboranes, metalloboranes and metallo-carboranes compounds with metal metal multiple bonds.

Unit-V

Optical Rotatory Dispersion and Circular Dichroism

Linearly and circularly polarized lights; optical rotatory power and circular birefringence, ellipticity and circular dichroism; ORD and Cotton effect, Faraday and Kerr effects; Assignment of electronic transitions; applications of ORD and CD for the determination of (i) absolute configuration of complexes and (ii) isomerism due to non-planarity of chelate rings.

Books Suggested :

7. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
8. Inorganic Chemistry, J.E. Huhey, Harpes & Row.
9. Chemistry of the Elements. N.N. Greenwood and A. Earnshaw, Pergamon.
10. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
11. Magnetochemistry, R.1. Carlin, Springer Verlag.
12. Comprehensive Coordination Chemistry eds., G. Wilkinson, R.D. Gillars and J.A. Mc Cleverty, Pergamon.

Paper-VII
MCH-407: ORGANIC CHEMISTRY II
Unit-I

Aromatic Electrophilic Substitution

The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles. Diazonium coupling, Vilsmeier reaction, Gatterman-Koch reaction

Aromatic Nucleophilic Substitution

The S_NAr SN1, benzyne and SN1 mechanism, Reactivity effect of substrate structure, leaving group and attacking nucleophile. The Von Richter. Sommelet-Hauser, and Smiles rearrangements.

Unit-II

Free Radical Reactions

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 halogenation (NBS), oxidation of aldehydes to carboxylic acids, autooxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts, Sandmeyer reaction. Free radical rearrangement. Hunsdiecker reaction.

Unit III

Addition Reactions

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.

Unit-IV

Addition to Carbon-Hetero Multiple bonds

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acid 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.

Elimination Reactions

The E2, E1 and E1cB 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.

Unit-V

Pericyclic Reactions

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions-conrotatory and disrotatory motions, $4n$ and $4n+2$ and allyl systems. Cycloadditions-antarafacial and suprafacial additions, $4n$ and $4n+2$ systems, $2+2$ addition of ketenes, 1,3 dipolar cycloadditions and cheletropic reactions. Sigmatropic rearrangements-suprafacial and antarafacial shifts of H, sigmatropic involving carbon moieties, 3,3- and 5,5 sigmatropic rearrangements. Claisen, Cope and aza-Cope rearrangements. Fluxional tautomerism. Ene reaction.

Book Suggested

12. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.
13. Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Plenum.
14. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
15. Structure and Mechanism in Organic Chemistry, C.K. Ingold, Cornell University Press.
16. Organic Chemistry, R.T. Morrison and R.N. Boyd, Prentice-Hall.
17. Modern Organic Reactions, H.O. House, Benjamin.
18. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic & Professional.
19. Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh, Macmillan.
20. Pericyclic Reactions, S.M. Mukherji, Macmillan, India
21. Stereochemistry of Organic Compounds, D.Nasipuri, New Age International.
22. Stereochemistry of Organic Compounds, P.S. Kalsi, New Age International.

Paper-VIII

MCH-408: PHYSICAL CHEMISTRY II

Unit-I

Chemical Dynamics

Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation and the activated complex theory; ionic reactions, kinetic salt effects, steady state kinetics, kinetic and thermodynamic control of reactions, treatment of unimolecular reactions. Dynamic chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of

ethane), photochemical (hydrogenbromine and hydrogen-chlorine reactions) and homogenous 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 unimolecular reactions (Lindemann Hinshelwood and Rice-Ramsperger-Kassel- Marcus (RRKM) theories for unimolecular reactions).

Unit-II

Surface Chemistry

Adsorption

Surface tension, capillary action, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, estimation of surface area (BET equation), Surface films on liquids (Electro-kinetic phenomenon).

Micelles

Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization-phase separation and mass action models, solubilization, micro emulsion, reverse micelles.

Unit-III

Macromolecules

Polymer-definition, types of polymers, electrically conducting, fire resistant, liquid crystal polymers, kinetics of polymerization, mechanism of polymerization. Molecular mass, number and mass average molecular mass, molecular mass determination (Osmometry, viscometry, diffusion and light scattering methods), sedimentation, chain configuration of macromolecules, calculation of average dimension of various chain structures.

Unit-IV

Non Equilibrium Thermodynamics

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

Unit-V

Electrochemistry

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. Overpotentials, exchange current density, derivation of Butler Volmer

equation, Tafel plot. Quantum aspects of charge transfer at electrodes-solution interfaces, quantization of charge transfer, tunneling. Semiconductor interfaces-theory of double layer at semiconductor, electrolyte solution interfaces, structure of double layer interfaces. Effect of light at semiconductor solution interface. Polarography theory, Ilkovic equation; half wave potential and its significance.

Books Suggested

11. Physical Chemistry, P.W. Atkins, ELBS.
12. Introduction to Quantum Chemistry, A.K. Chandra, Tata Mc Graw Hill.
13. Quantum Chemistry, Ira N. Levine, Prentice Hall.
14. Coulson's Valence, R. Mc Ween y, ELBS.
15. Chemical Kinetics. K.J. Laidler, McGraw-Hill.
16. Kinetics and Mechanism of Chemical Transformation J. Rajaraman and J. Kuriacose, Mc Millan.
17. Micelles, Theoretical and Applied Aspects, V. MOraoi, Plenum.
18. Modern Electrochemistry Vol. 1 and Vol II J.O.M. Bockris and A.K.N. Reddy, Plenum.
19. Introduction to Polymer Science, V.R. Gowarikar, N.V. Vishwanathan and J. Sridhar, Wiley Eastern.

Paper-IX

MCH-409: Spectroscopy II and Diffraction Methods

Unit-I

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 (AXB, AMX, ABC, A2B2 etc.). spin decoupling; basic ideas about instrument, NMR studies of nuclei other than protin-¹³C, ¹⁹F and ³¹P. FT NMR, advantages of FT NMR.

Unit II

Nuclear Quadrupole Resonance Spectroscopy

Quadrupole nuclei, quadrupole moments, electric field gradient, coupling constant, splitting. Applications.

Unit-III

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 Mc Connell relationship, measurement techniques, applications.

Unit-IV

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.

Unit-V

Electron Diffraction

Scattering intensity vs. scattering angle, Wierl equation, measurement technique, elucidation of structure of simple gas phase molecules. Low energy electron diffraction and structure of surfaces.

Neutron Diffraction Scattering of neutrons by solids measurement techniques, Elucidation of structure of magnetically ordered unit cells.

Books suggested

11. Modern Spectroscopy, J.M. Hollas, John Viley.
12. Applied Electron Spectroscopy for chemical analysis d. H. Windawi and F.L. Ho, Wiley Interscience.
13. NMR, NQR, EPr and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Harwood.
14. Physical Methods in Chemistry, R.S. Drago, Saunders College.
15. Chemical Applications of Group Theory, F.A. Cotton.
16. Introduction to Molecular Spectroscopy, G.M. Barrow, Mc Graw Hill.
17. Basic Principles of Spectroscopy, R. Chang, Mc Graw Hill.
18. Theory and Application of UV Spectroscopy, H.H. Jaffe and M. Orchin, IBHOxford.
19. Introduction to Photoelectron Spectroscopy, P.K. Ghosh, John Wiley.
20. Introduction to Magnetic Resonance. A Carrington and A.D. Maclachalan, harper & Row.

Paper-X

Ch-410 : COMPUTERS FOR CHEMISTS

This is a theory cum-laboratory co use with more emphasis on laboratory work.

Unit-I

Introduction to computers and Computing

Basic structure and functioning of computer with a PC as illustrative example.

Memory

I/O devices. Secondary storage Computer languages. Operating systems with DOS as an example Introduction to UNIX and WINDOWS. Principles of programming Alogrithms and flow-charts.

Unit-II

Computer Programming in FORTRAN/C/BASIC

(the language features are listed here with reference to FORTRAN. The instructor may choose another language such as BASIC or C the features may be replaced appropriately). Elements of the compute language. Constants and variables. Operations

and symbols Expressions. Arithmetic assignment statement. Input and output Format statement. Termination statements. Branching statements as IF or GO TO statement. LOGICAL variables. Double precision variables. Subscripted variables and DIMENSION. DO statement FUNCTION AND SUBROUTINE. COMMON and DATA statement (Student learn the programming logic and these language feature by hands on experience on a personal computer from the beginning of this topic.)

Unit-III

Programming in Chemistry

Developing of small computer codes using any one of the languages FORTRAN/C/BASIC involving simple formulae in Chemistry, such as Van der Waals equation. Chemical kinetics (determination of Rate constant) Radioactive decay (Half Life and Average Life). Determination Normality, Molarity and Molality of solutions. Evaluation Electronegativity of atom and Lattice Energy from experimental determination of molecular weight and percentage of element organic compounds using data from experimental metal representation of molecules in terms of elementary structural features such as bond lengths, bond angles.

Unit-IV

Use of Computer programmes

Operation of PC. Data Processing. Running of standard Programs and Packages such as MS WORD, MS EXCEL -special emphasis on calculations and chart formations. X-Y plot. Simpson's Numerical Integration method. Programmes with data preferably from physical chemistry laboratory.

Unit V

Internet

Application of Internet for Chemistry with search engines, various types of files like PDF, JPG, RTF and Bitmap. Scanning, OMR, Web camera.

Book Suggested :

Fundamentals of Computer : V. Rajaraman (Prentice Hall)

Computers in Chemistry : K.V. Raman (Tata Mc Graw Hill)

Computer Programming in FORTRAN IV-V Rajaraman (Prentice Hall)

PRACTICAL

(Duration: 6-8 hrs in each branch)

Practical examination shall be conducted separately for each branch.

Inorganic Chemistry

Chromatography 12

Preparation 12

Record 4

Viva Voce 5

Chromatography Separation of cations and anions by

Column Chromatography : Ion exchange.

Preparations

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

1. $[\text{Co}(\text{NH}_3)_6] [\text{Co}(\text{NO}_2)_6]$
2. cis- $[\text{Co}(\text{trien}) (\text{NO}_2)_2]\text{Cl}\cdot\text{H}_2\text{O}$
3. $\text{Hg}[\text{Co}(\text{SCN})_4]$
4. $[\text{Co}(\text{Py})_2\text{Cl}_2]$
5. $[\text{Ni}(\text{NH}_3)_6]\text{Cl}_2$
6. $\text{Ni}(\text{dmg})_2$
7. $[\text{Cu}(\text{NH}_3)_4]\text{SO}_4\cdot\text{H}_2\text{O}$

Organic Chemistry

Organic Synthesis 12

Quantitative Analysis 12

Record 4

Viva Voce 5

Organic Synthesis

Aldol condensation Dibenzal acetone from benzaldehyde. Sandmeyer reaction : p- Chlorotoluene from p-toluidine. Acetoacetic ester Condensation : Synthesis of ethyl-nbutylacetoacetate

by A.E.E. condensation. Connizzaro reaction : 4-Chlorobenzaldehyde as substrate. Friedel Crafts reaction : b-Benzoyl propionic acid from succinic anhydride and benzene. Aromatic electrophilic substitutions : Synthesis of p-nitroaniline and pbromoaniline.

The Products may be Characterized by Spectral Techniques.

Quantitative Analysis

Determination of the percentage or number of hydroxyl groups in an organic compound by acetylation method. Estimation of amines/phenols using bromate bromide solution/or acetylation method. Determination of iodine and Saponification values of an oil sample.

Determination of DO, COD and BOD of water sample.

Physical Chemistry

Conductometry 8

Potentiometry/pH metry 9

Polarimetry 8

Record 4

Viva Voce 5

Conductometry

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

ii. Determination of solubility and solubility product of sparingly soluble salts (e.g.

PbSO₄, BaSO₄) conductometrically.

- iii. Determination of the strength of strong and weak acid in a given mixture conductometrically.
- iv. to study of the effect of solvent on the conductance of AgNO₃/acetic acid and to determine the degree of dissociation and equilibrium constant in different solvents and in their mixtures (DMSO, DMF, dioxane, acetone, water) and to test the validity of Debye-Huckel-Onsager theory.
- v. Determination of the activity coefficient of zinc ions in the solution of 0.002 M zinc sulphate using Debye Huckel's limiting law.

Potentiometry/pH metry

1. Determination of strengths of halides in a mixture potentiometrically.
2. Determination of the valency of mercurous ions potentiometrically.
3. Determination of the strength of strong and weak acids in a given mixture using a potentiometer/pH meter.
4. Determination of temperature dependence of EMF of a cell.
5. Determination of the formation constant of silver-ammonia complex and stoichiometry of the complex potentiometrically.
6. Acid-base titration in a non-aqueous media using a pH meter.
7. Determination of activity and activity coefficient of electrolytes.
8. Determination of the dissociation constant of acetic acid in DMSO, DMF, acetone and dioxane by titrating it with KOH.
9. Determination of the dissociation constant of monobasic/dibasic acid by Albert-Sderjeant method.
10. Determination of thermodynamic constants, DG, DS, and DH for the reaction by e.m.f. method. $Zn + H_2SO_4 \rightarrow ZnSO_4 + 2 H$

1. Determination of rate constant for hydrolysis/inversion of sugar using a polarimeter.
2. Enzyme kinetics-inversion of sucrose.

Books Suggested

11. Vogel's Textbook of Quantitative Analysis, revised, J. Bassett, R.C. Denney, G.H. Jeffery and J. Mendham, ELBS.
12. Synthesis and Characterization of Inorganic Compounds, W.L. Jolly. Prentice Hall.
13. Experiments and Techniques in Organic Chemistry, D.P. Pasto, C. Johnson and M. Miller, Prentice Hall.
14. Macroscale and Microscale Organic Experiments, K.L. Williamson, D.C. Health.
15. Systematic Qualitative Organic Analysis, H. Middleton, Adward Arnold.
16. Handbook of Organic Analysis-qualitative and Quantitative. H. Clark, Adward Arnold.
17. Vogel's Textbook of Practical Organic Chemistry, A.R. Tatchell, John Wiley.
18. Practical Physical Chemistry, A.M. James and F.E. Prichard, Longman.

19. Findley's Practical Physical chemistry, B.P. Levitt, Longman.
20. Experimental Physical Chemistry, R.C. Das and B. Behera, Tata McGraw

SEMESTER IV

MCH-501 APPLICATION OF SPECTROSCOPY

(Inorganic & Organic Chemistry)

Compulsory

Unit - 1 Ultraviolet and Visible spectroscopy 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 compounds. Steric effect in biphenyls.

Electronic Spectroscopy:

Electronic Spectral Studies for $d_1 d_9$ systems in octahedral, tetrahedral and square planer complexes,

Unit - 2 Vibrational Spectroscopy Symmetry and shapes of AB_2 , AB_3 , AB_4 , AB_5 and AB_6 , mode

of bonding of ambidentate ligands, nitrosyl, ethylenediamine and diketonato complexes, application of resonance Raman spectroscopy and its applications.

Infrared Spectroscopy 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.

Unit - 3 Nuclear Magnetic Resonance Spectroscopy General introduction and definition, chemical shift, spin-spin interaction, shielding mechanism, mechanism of measurement, chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides & mercapto), chemical exchange, effect of deuteration, Stereochemistry, hindered rotation, Karplus curve-variation of coupling constant with disordered angle. NMR shift reagents, solvent effects. nuclear overhauser effect (NOE).

Nuclear Magnetic Resonance of Paramagnetic Substances in Solution The contact and Pseudo contact shifts, factors affecting nuclear relaxation, some applications including biochemical systems, an overview of NMR of metal nuclide with emphasis on ^{195}Pt and ^{119}Sn NMR.

Carbon-13 NMR Spectroscopy General considerations, chemical shift (aliphatic olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants. Two dimension NMR spectroscopy-COSY, NOESY, DEPT, HMBC and HMQC techniques.

Unit - 4 Mössbauer Spectroscopy 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 ML bond, coordination number, structure and (3) detection of oxidation state and inequivalent MB atoms.

Unit - 5 Mass Spectrometry Introduction ion production E1, C1 FD, ESI and FAB, factors affecting fragmentation, ion analysis, ion abundance Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak. Me Lafferty rearrangement. Nitrogen rule. High resolution mass spectrometry. Structure elucidation of simple molecules using UV – Visible, IR, NMR and mass spectral techniques.

Suggested Readings:

1. Physical Methods for Chemistry, R.S. Drago, Saunders Compnay.
2. Structural Methods in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H. Rankin and S. Cradock, ELBS.
3. Infrared and Raman Spectral : 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, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, .V. Parish, Ellis Haywood.
8. Practical NMR Spectroscopy, M.L. Martin. J.J. Deepish and G.J. Martin, Heyden.
9. Spectrometric Identification of Organic Compounds, R.M. Silverstein, G.C. Bassler adn 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.
12. Spectroscopic Methods in Organic Chemistry D.H. Williams, I. Fleming, Tata McGraw-Hill.
13. Structural Methods in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H. Rankin and S. Cradock, ELBS.
14. Introduction to NMR spectroscopy, R.J. Abraham, J. Fisher and P. Loftus, Wiley

MCH-502: PHOTOCHEMISTRY & SOLID STATE CHEMISTRY

Compulsory

Unit - 1 Photochemical Reactions Interaction of electromagnetic radiation with matter, types of excitations, fate of excited molecule, quantum yield, transfer of excitation energy, actinometry.

Determination of Reaction Mechanism Classification, rate constants and life times of reactive energy state 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. Photo chemical formation of smog, photochemistry of vision

Unit - 2 Photochemistry of Alkene Intramolecular reactions of the olefinic bond-geometrical isomerism, cyclisation reactions, rearrangement of 1,4- and 1,5-dienes.

Photochemistry of Aromatic Compounds Isomerisations, additions and substitutions.

Photochemistry of Carbonyl Compounds Intramolecular reactions of carbonyl compounds-saturated, cyclic and acyclic, b,g unsaturated and a, b unsaturated compounds, Intermolecular cycloaddition reactions-dimerisations and oxetane formation. Singlet molecular Oxygen reaction.

Unit - 3 Solid State Reactions General principles, experimental procedure, co-precipitation as a precursory to solid state reactions, kinetics of solid state reactions.

Crystal Defects and Non-Stoichiometry Perfect and imperfect crystals, intrinsic and extrinsic defects-point defects, line and plane defects, vacancies-Schottky defects and Frenkel defects. Thermodynamics of Schottky and Frenkel defect formation, colour centres, non-stoichiometry and defects.

Unit - 4 Electronic Properties and Band Theory Metal,s insulators and semiconductors,

Electronic structure of solidsband theory band structure of metals, insulators and semiconductors, Intrinsic and extrinsic semiconductors, doping semiconductors, p-n junctions, super conductors. Optical properties-Application of optical and electron microscopy. Magnetic Properties-Classification of materials : Effect of temperature calculation of magnetic moment, mechanism of ferro and anti ferromagnetic ordering super exchange.

Unit - 5 Organic Solids Electrically conducting solids. organic charge transfer complex, organic metals, new superconductors.

Liquid Crystals: Types of liquid crystals: Nematic, Smectic, Ferroelectric, Antiferroelectric, Various theories of LC, Liquid crystal display, New materials.

Suggested Readings:

1. Fundamentals of photochemistry, K.K. Rothagi-Mukheriji, Wiley-Eastern.
2. Essentials of Molecular Photochemistry, A Gilbert and J. Baggott, Blackwell Scientific Publication.

3. Molecular Photochemistry, N.J. Turro, W.A. Benjamin.
4. Introductory Photochemistry, A. Cox and t. Camp, McGraw Hill.
5. Photochemistry, R.P. Kundall and A. Gilbert. Thomson Nelson.
6. Organic Photochemistry, J. Coxon and B.halton, Cambridge University Press.
7. Solid state chemistry and its applications, A.R. West. Peenum.
8. Principles of the Solid State, H.V. Keer, Wiley Eastern.
9. Solid State Chemistry, N.B. Hannay.
10. Solid State Chemistry, D.K. Chakrabarty, New Wiley Eastern.

MCH-503 BIOCHEMISTRY & ENVIRONMENTAL CHEMISTRY

Compulsory

Unit - 1 Enzymes Introduction and historical perspective, chemical and biological catalysis, remarkable properties of enzymes like catalytic power, specificity and regulation. Nomenclature and classification, extraction and purification. Fischer's lock and key and Koshalnd'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, Michael's-Menten and Lineweaver Burk plots, reversible and irreversible inhibition.

Mechanism of Enzyme Action Transition-state theory, orientation and Steric effect, acidbase catalysis, covalent catalysis, strain or distortion. Examples of some typical enzyme mechanisms for chemotrypsin, ribonuclease, lysozyme and carboxypeptidase.

Kinds of Reactions Catalysed by Enzymes Nucleophilic displacement on a phosphorus atom, multiple displacement reactions and the coupling of ATP cleavage to endergonic processes. Transfer of sulphate, addition and elimination reactions, enolic intermediates in Isomerisations reactions, b-Cleavage and condensation, some isomerization and rearrangement reactions. Enzyme catalyzed carboxylation and decarboxylation.

Unit - 2 Co-Enzyme Chemistry Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD⁺, NADP⁺, FMN, FAD, lipoic acid, vitamin B12. Mechanisms of reactions catalyzed by the above cofactors.

Enzyme Models Host-guest chemistry, chiral recognition and catalysis, molecular recognition, molecular asymmetry and prochirality Biometric chemistry, crown ether, cryptates. Cyclodextrins, cyclodextrin-based enzyme models, clixarenes, ionospheres, micelles synthetic enzymes or synzymes.

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 cheese-making, syrups from cron starch, enzymes as targets for drug design. Clinical uses of enzymes, enzyme therapy, enzymes and recombinant DNA Technology.

Unit - 3 Metal Ions in Biological Systems Bulk and trace metals with special reference to Na, K, Mg, Ca, Fe, Cu, Zn, Co, and K⁺/Na⁺ pump.

Bioenergetics and ATP Cycle. DNA polymerisation, glucose storage, metal complexes in transmission of energy; chlorophyll's, photosystem I and photosystem II in cleavage of water.

Transport and Storage of Dioxygen Hem proteins and oxygen uptake structure and function of haemoglobin's, myoglobin, haemocyanins and hemerythrin, model synthetic complexes of iron, cobalt and copper.

Unit - 4 Environmental Toxicology

Toxic heavy metals : Mercury, lead, arsenic and cadmium. Causes of toxicity.

Bioaccumulation, sources of heavy metals. Chemical speciation of Hg, Pb, As, and Cd. Biochemical and damaging effects.

Toxic Organic Compound : Pesticides, classification, properties and uses of organochlorine and ionospheres pesticides detection and damaging effects.

Polychlorinated biphenyls : Properties, use and environmental continuation and effects.

Polynuclear Aromatic Hydrocarbons : Source, structures and as pollutants.

Unit - 5 Aquatic Chemistry and Water Pollution Redox chemistry in natural waters. Dissolved oxygen, biological oxygen demand, chemical oxygen demand, determination of DO, BOD and COD. Aerobic and anaerobic reactions of organic sulphure and nitrogen compounds in water acid-base chemistry of fresh water and sea water. Aluminum, nitrate and fluoride in water. Petrification. Sources of water pollution. Treatment of waste and sewage. Purification of drinking water, techniques of purification and disinfection.

Suggested Readings:

1. Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.

2. Bioinorganic Chemistry, 1. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, University Science Books.

3. Inorganic biochemistry vol. I and II ed. G.L. Eichhorn, Elsevier.

4. Progress in Inorganic Chemistry, Vol 18 and 38 ed J.J. Lippard, Wiley.

5. Bioorganic Chemistry : A chemical Approach to Enzyme Action, Hermann Dugas and C. Penny, Springer Verlag.

6. Understanding Enzymes, Trevor Palmer, Prentice Hall.

7. Enzyme Chemistry : Impact and applications, Ed. Collin J suckling, chemistry.

8. Enzyme Mechanisms Ed. M.I. Page and A Williams, Royal Society of Chemistry.

9. Fundamentals of Enzymology, N.C. Price and L. Stevens. Oxford University Press.

10. Immobilized Enzymes : An Introduction and Applications in Biotechnology, Michael ID.

Treva, Hohn Wiley.

11. Enzymatic Reaction Mechanisms. C. Walsh. W.H. Freeman.

12. Enzyme Structure and Mechanism, A Fersht, W.H. Freeman

13. Biochemistry : The Chemical Reactions of Living Cells, D.E. Metzler, Academic Press.
14. Environmental Chemistry, Colin Baird, W.H. Freeman Co. New York, 1998.
15. Chemistry of Atmospheres, R.P. Wayne, Oxford.
16. Environment Chemistry, A.K. De, Wiley Eastern, 2004.
17. Environmental Chemistry, S.E. Manahan, Lewis Publishers.
18. Introduction to atmospheric Chemistry, P.V. Hobbs, Cambridge.

MCH-601 Organotransition Metal Chemistry

Unit - 1 Alkyls and Aryls of Transition Metals

Types, routes of synthesis, stability and decomposition pathways organocopper in organic synthesis.

Compounds of Transition Metal-Carbon Multiple Bonds

Alkylidenes, alkylidyne, low valent carbenes and carbynes-synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions on the ligands, role in organic synthesis.

Unit - 2 Transition Metal π -Complexes

Transition metal π -Complexes with unsaturated organic molecules, alkenes, alkynes, allyl, diene, dienyl, arene and trienyl complexes, preparation, properties, nature of bonding and structural features. Important reactions relating to nucleophilic and electrophilic attack on ligands and to organic synthesis

Unit - 3 Transition metal compounds with bonds to hydrogen, boron, silicon :

Transition metal compounds with bonds to hydrogen, boron, silicon

Unit - 4 Homogeneous Catalysis

Stoichiometric reactions for catalysis, homogeneous catalytic hydrogenation, Zeigler-Natta polymerization of olefins, catalytic reactions involving carbon monoxide such as hydrocarbonylation of olefins (oxoreaction), explanation reactions, activation of C-H bond.

Unit - 5 Fluxional Organometallic Compounds

Flexionality and dynamic equilibrium in compounds such as η^2 -olefine, η^3 -allyl and dienyl complexes.

Suggested Readings:

1. Principles and Application of Organotransition Metal Chemistry, J.P. Collman, L.S. Hegsdus, J.R. Norton and R.G. Finke, University Science Books.
2. The Organometallic Chemistry of the Transition Metals, R.H. Crabtree. John Wiley.
3. Metallo-organic Chemistry, A.J. Pearson, Wiley.
4. Organometallic Chemistry, R.C. Mehrotra and A. Singh New Age International

M.Sc IV
Chemistry
MCH-602: Polymers
Optional

Unit - 1 Basics

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 copolymerization. Polymerization conditions and polymer reactions. Polymerization in homogeneous and heterogeneous systems.

Unit - 2 Polymer Characterization

Polydispersion-average molecular weight concept. Number, weight and viscosity average molecular weights. Polydispersity an molecular weight distribution. The practical significance of molecular weight. Measurement of molecular-weights. End-group, viscosity, light scattering, osmotic and ultracentrifugation methods.

Unit - 3 Analysis and testing of polymers

Chemical analysis of polymers, spectroscopic methods, X-ray diffraction study. Microscopy. Thermal analysis and physical testing-tensile strength. Fatigue, impact. Tear resistance, Hardness and abrasion resistance

Unit - 4 Inorganic Polymers

A general survey and scope of Inorganic Polymers special characteristics, classification, homo and hetero atomic polymers.

Structure, Properties and Applications of

- a. Polymers based on boron-borazines, boranes and carboranes.
- b. Polymers based on Silicon, silicone's polymetalloxanes and polymetallosiloxanes, silazanes.

Unit - 5 Structure, Properties and Application of

- a. Polymers based on Phosphorous-Phosphazenes, Polyphosphates
 - b. Polymers based on Sulphure-Tetrasulphur tetranitride and related compounds.
- Co-ordination and metal chelate polymers.

Suggested Readings:

1. Inorganic Chemistry, J.E. Huheey, Harper Row.
2. Developments in Inorganic polymer Chemistry, M.F. Lappert and G.J. Leigh.
3. Inorganic polymers- N.H. Ray.
4. Inorganic polymers, Graham and Stone.
5. Inorganic Rings and Cages : D.A. Armitage.
6. Textbook of Polymers Science, F.W. Billmeyer Jr. Wiley.
7. Contemporary Polymer Chemistry, H.R. Al cock and F.W. Lambe, Prentice Hall.

M.Sc IV
Chemistry
MCH-603: Organic Synthesis
Optional

Unit - 1 Disconnection Approach

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

Unit - 2 One Group C-C Disconnections

Alcohols and carbonyl compounds, regioselectivity, alkene synthesis, use of acetylenes and aliphatic Nitro compounds in organic synthesis.

Two Group C-C Disconnections

Diels-Alder Reaction, 1,3-difunctionalised compounds, a-b- unsaturated carbonyl compounds, control in carbonyl condensations, 1,5-difunctionalised compounds. Micheal addition and Robinson annelation.

Unit - 3 Oxidation

Introduction, Different oxidative processes. Hydrocarbons-alkenes, aromatic rings, saturated C-H groups (activated and unactivated) Alcohols, diols, aldehyde's, ketones, ketals and carboxylic acids. Amines, hydrazines, and sulphides. Oxidations with ruthenium tetraoxide, iodobenzene diacetate and thallium. (III) Nitrate. **Reduction**
Introduction, Different reductive processes. Alkanes, alkenes, alkynes, and aromatic rings. Carbonyl compounds-aldehydes, ketones, acids and their derivatives. Epoxides. Nitro, nitroso, azo and oxime groups. Expoxide, Nitro, Nitroso, azo and oxime groups. Hydrogenolysis

Unit - 4 Organometallic Reagents

Principle, preparations, properties and applications of the following in organic synthesis with mechanistic details. Group I and II metal organic compounds Li, Mg, Hg, Cd, Zn and Ce Compounds.

Unit - 5 Synthesis of some complex molecules:

Application of the above in the synthesis of following compounds:

Canphor, longifoline, cartisone, reserpine, vitamin D, juvabion, aphidicolin and fredericamycin. A

Suggested Readings:

1. Designing Organic Synthesis, S. Warren. Wiley.
2. Organic Synthesis-Concept, Methods and Starting Materials, J. Fuhrhop.
3. Some Modern Methods of Organic Synthesis. W. carruthers, Cambridge Univ. Press.
4. Modern Synthetic Reactions H.O. House, W.A Benjamin.
5. Advanced Organic Chemistry : Reactions, Mechanisms and Structure, J. March. Wiley.

6. Principles, of Organic Chemistry Part B. F.a. Carey and R.J. Sundberg, Plenum Press.

M.Sc IV

Chemistry

MCH-604: Heterocyclic Chemistry

Optional

Unit - 1 Nomenclature of Heterocycles

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

Aromatic Heterocycles

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

Unit - 2 Non-aromatic Heterocycles

Strain-bond angle and torsional strains and their consequences in small ring heterocycles. Conformation of six-membered heterocycles with reference to molecular geometry, barrier to ring inversion, pyramidal inversion and 1,3-diaxial interactions. Stereoelectronic effects anomeric and related effects, Attractive interactions-hydrogen bonding and intermolecular nucleophilic electrophilic interactions. Heterocyclic Synthesis Principles of heterocyclic synthesis involving cyclization reactions and cycloaddition reactions.

Unit - 3 Small Ring Heterocycles

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

Benzo-Fused Five-Membered Heterocycles

Synthesis and reactions including medicinal applications of benzopyrroles, bezofurans and benzothiophenes.

Unit - 4 Meso-ionic Heterocycles

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

Six-Membered Heterocycles with one Heteroatom

Synthesis and reactions of pyrylium salts and pyrones and their comparison with pyridinium & thiopyrylium salts and phridones. Synthesis and reactions of quionlizinium and benzopyrylium salts, coumarins and chromones.

Unit - 5 Six Membered Heterocycles with Two or More Heteroatoms Synthesis and reactions of diazoles, triazines, tetrazines and thiazines. Seven-and Large-Membered Heterocycles Synthesis and reactions of azepines, oxepines, thiepinines, diazepines thiazepines, azocines, diazocines, dioxocines and dithiocines.

Heterocyclic Systems Containing P, As, Sb and B

Heterocyclic rings containing phosphorus : Introduction, nomenclature, synthesis and

characteristics of 5- and 6-membered ring systems phosphorinaes, phosphorines, phospholanes and phospholes. Heterocyclic rings containing As and Sb : Introduction, synthesis and characteristics of 5- and 6-membered ring system. Heterocyclic rings containing B : Introduction, synthesis reactivity and spectral characteristics of 3- 5- and 6- membered ring system.

Suggested Readings:

1. Heterocyclic Chemistry Vol. 1-3, R.R. Gupta, M. Kumar and V.Gupta, Springer Verlag.
2. The Chemistry of Heterocycles, T. Eicher and S. Hauptmann, Thieme.
3. Heterocyclic chemistry J.A. Joule, K. Mills and G.F. Smith, Chapman and Hall.
4. Heterocyclic Chemistry, T.L. Gilchrist, Longman Scientific Technical.
5. Contemporary Heterocyclic Chemistry, G.R. Newkome and W.W. Paudler, Wiley-Inter Science.
6. An Introduction to the Heterocyclic Compounds, R.M. Acheson, John Wiley.
7. Comprehensive Heterocyclic Chemistry, A.R. Katritzky and C.W. Rees, eds. Pergamon Press.

M.Sc IV

Chemistry

MCH-605: Chemistry of Natural Products

Optional

Unit - 1 Terpenoids and Carotenoids

Calcifications, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Structure determination, stereochemistry, biosynthesis and synthesis of the following representative molecules : Citral, Geraniol a-Terpeneol, Menthol, Farnesol, Zingiberence, Santonin, Phytol, Abietic acid and b-Carotene.

Unit - 2 Alkaloids

Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, role of alkaloids in plants. Structure, stereochemistry, synthesis and biosynthesis of the following : Ephedrine , (+)- Coniine, Nicotine, Atropine, Quinine and Morphine.

Unit - 3 Steroids

Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry, Isolation, Structure determination and synthesis of Cholesterol, Bile acids, Androsterone, Testosterone, Estrone, Progesterone, Aldosterone, Biosynthesis of Steroids.

Unit - 4 Plant Pigments

Occurrence, nomenclature and general methods of structure determination. Isolation and synthesis of Apigenin, Luteolin Quercetin, Myrcetin, Quercetin 3-glucoside, Vitexin, Diadzein, Aureusin, Cyanidin-7arabinoside, Cyanidin, Hirsutidin, Biosynthesis of flavonoids: Acetate pathway and Shikimic acid pathway.

Prophyrins

Structure and synthesis of Haemoglobin and Chlorophyll.

Unit - 5 Prostaglandis

Occurrence, nomenclature, classification, biogenesis and physiological effects. Synthesis of PGE2 and PGF2a.

Pyrethroids and Rotenones

Synthesis and reactions of Pyrethroids and Rotenones. (For structure elucidation, emphasis is to be placed on the use of spectral parameters wherever possible).

Suggested Readings:

1. Natural Products : Chemistry and Biological Significance, J. Mann, R.S. Davidson, J.B. Hobbs, D.V. Bantrophe and J.B. Harborne, Longman, Essex.
2. Organic Chemistry : Vol. 2 1L. Finar, ELBS
3. Stereoselective Synthesis : A Practical Approach, M. Norgradi, VCH.
4. Rodd's Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier.
5. Chemistry, Biological and Pharmacological Properties of Medicinal Plants from the Americas, Ed. Kurt Hostettmann, M.P. Gupta and A. Marston. Harwood Academic Publishers.
6. Introduction to Flavonoids, B.A. Bohm. Harwood Academic Publishers.
7. New Trends in Natural Product chemistry, Ataur Rahman and M.L. Choudhary, Harwood Academic Publishers.
8. Insecticides of Natural Origin, Sukh Dev, Harwood Academic Publishers.

M.Sc IV

Chemistry

MCH-606: Analytical Chemistry

Optional

Unit - 1 Introduction

Role of analytical chemistry Classification of analytical methods classical and instrumental.

Types of instrumental analysis. Selecting an analytical method. Neatness and cleanliness. laboratory operations and practices. Analytical balance. Techniques of weighing, errors. Volumetric glassware cleaning and calibration of glassware. Sample Volumetric glassware cleaning and Calibration of glassware. Sample preparation-dissolution and decompositions.

Gravimetric techniques. Selecting and handling of reagents. Laboratory notebooks.

Safety

in the analytical laboratory.

Errors and Evaluation Definition of terms in mean and median. Precision-standard deviation, relative standard deviation. Accuracy-absolute error, relative error. Types of error

in experimental data determinate (systematic), indeterminate (or random) and gross.

Sources of error and the effects upon the analytical results. Methods for reporting analytical

data. Statistical evaluation of data-indeterminate errors. The uses of statistics.

Unit - 2 Food analysis

Moisture, ash, crude protein, fat crude fiber, carbohydrates, calcium, potassium, sodium and

phosphate. Food adulteration-common adulterants in food, contamination of foods stuffs. Microscopic examination of foods for adulterants. Pesticide analysis in food products. Extraction and purification of sample. HPLC. Gas chromatography for organophosphates. Thin-layer chromatography for identification of chlorinated pesticides in food products.

Unit - 3 Analysis of Water Pollution

Origin of Waste water, types, water pollutants and their effects. Sources of water pollution-domestic,

industrial, agricultural soil and radioactive wastes as sources of pollution.

Objectives of analysis-parameter for analysis-colour, turbidity, total solids, conductivity, acidity, alkalinity, hardness, chloride, sulphate, fluoride, silica, phosphates and different forms of nitrogen, Heavy metal pollution-public health significance of cadmium, chromium,

copper, lead, zinc, manganese, mercury and arsenic. General survey of instrumental technique for the analysis of heavy metals in aqueous systems. Measurements of DO, BOD,

and COD. Pesticides as water pollutants and analysis. Water pollution laws and standards.

Unit - 4 Analysis of soil, Fuel, Body Fluids and Drugs

(a) Analysis of Soil, moisture pH total nitrogen, phosphorus, silica, lime, magnesia, manganese, sulphur and alkali salts.

Fuel analysis : liquid and gas. Ultimate and proximate analysis-heating values-grading of coal. Liquid fuels-flash point, aniline point, octane number and carbon residue. Gaseous fuels-produced gas and water gas-calorific value.

Unit - 5 (a) Clinical Chemistry : Composition of blood-collection and preservation of samples.

Clinical analysis. Serum electrolytes, blood glucose, blood urea nitrogen, uric acid, albumin,

globulins, barbiturates, acid and alkaline phosphates. Immunoassay : principles of radio immunoassay (RIA) and applications. The blood gas analysis trace elements in the body

(b) **Drug analysis** : Narcotics and dangerous drug. Classification of drugs. Screening by gas

and thin-layer chromatography and spectrophotometric measurements.

Suggested Readings:

1. Analytical Chemistry, G.D. Christian, J.Wiley.
2. Fundamentals of analytical Chemistry. D.A. Skoog. D.M. West and F.J. Hooler, W.B. Saunders.
3. Analytical Chemistry-Principles. J.H. Kennedy. W.B. Saunders.
4. Analytical Chemistry-Principles and Techniques. L.G. Hargis. Prentice Hall.
5. Principles of Instrumental analysis D.A. Skoog and J.L. Loary, W.B. Saunders.
6. Principles of Instrumental Analysis D.A. Skoog W.B. Saunders.
7. Quantitative Analysis, R.A. Day, Jr. and A.L. Underwood, Prentice Hall.
8. Environmental Solution, S.M. Khopkar, Wiley Eastern.
9. Basic Concepts of Analysis Chemistry, S.M. Khopkar, Wiley Eastern.
10. Handbook of Instrumental Techniques for Analytical Chemistry, F. Settle, Prentice Hall.

M.Sc IV

Chemistry
MCH-607: Physical Organic Chemistry
Optional

Unit - 1 Concepts in Molecular Orbital (MO) and Valence Bond (VB) Theory

Introduction to Huckel molecular orbital (MO) method as a mean to explain modern theoretical methods. Advanced techniques in PMO and FMO theory. Molecular mechanics, semi empirical methods and ab initio and density functional methods. Scope and limitations of several computational programmes.

Unit - 2 Quantitative MO theory : Huckel molecular orbital (HMO - method as applied to ethene, allyl and butadiene. Qualitative MO theory ionisation potential. Electron affinities. MO energy levels. Orbital symmetry. Orbital interaction diagrams. MO of simple organic systems such as ethene, allyl, butadiene, methane and methyl group. Conjugation and hyper-conjugation. Aromaticity. Valence bond (B) configuration mixing diagrams. Relationship between VB configuration mixing and resonance theory. Reaction profiles. Potential energy diagrams. Curve-crossing model-nature of activation barrier in chemical reactions.

Unit - 3 Principles of Reactivity Mechanistic significance of entropy, enthalpy and Gibb's free energy. Arrhenius equation. Transition state theory. Uses of activation parameters, Hammond's postulate, Bell-Evans-Polanyi Principle. Potential energy surface model. Marcus theory of electron transfer. Reactivity and selectivity principles.

Kinetic Isotope Effect

Theory of isotope effects. Primary and secondary kinetic isotope effects. Heavy atom isotope effects. Tunneling effect. Solvent effects.

Structural Effects on Reactivity

Linear free energy relationships (LFER). The Hammett equation, substituent constants, theories of substituent effects. Interpretation of ρ -values. Reaction constants. Deviations from Hammett equation. Dualparameter correlations, inductive substituent constant. The Taft model, σ_1 and σ_R scales.

Unit - 4 Acids, Bases, Electrophiles, Nucleophiles and Catalysis

Acid-base dissociation, Electronic and structural effects, acidity and basicity. Acidity functions and their applications. Hard and soft acids and bases. Nucleophilicity scales. Nucleofugacity. The α -effect. Ambivalent nucleophiles. Acid-base catalysis-specific and general catalysis. Bronsted catalysis, Nucleophilic and electrophilic catalysis. Catalysis by noncovalent binding-micellar catalysis.

Steric and Conformation Properties

Various type of steric strain and their influence on reactivity. Steric acceleration. Molecular measurements of steric effects upon rates. Steric LFET, Conformational barrier to bond rotation-spectroscopic detection of individual conformers. Acyclic and monocyclic systems. Rotation around partial double bonds. Winstein-Holness and Curtin-Hammett principle.

Unit - 5 Nucleophilic and Electrophilic Reactivity

Structural and electronic effects on SN1 and SN2 reactivity. Solvent effect Kinetic isotope effects. Intramolecular assistance. Electron transfer nature of SN2 reaction.

Nucleophilicity and SN2 reactivity based on curved crossing mode. Relationship between polar and electron transfer reactions SRN1 mechanism. Electrophilic reactivity, general mechanism. Kinetic of SE2 Ar reaction. Structural effects on rates and selectivity. Curve-crossing approach to electrophilic reactivity.

Supramolecular Chemistry

Properties of covalent bonds-bond length, inter-bond angles, force constant, bond and molecular dipole moments. Molecular and bond polarizability, bond dissociation enthalpy, entropy. intermolecular forces, hydrophobic effects. Electrostatic, induction, dispersion and resonance energy, magnetic interactions, magnitude of interaction energy, forces between macroscopic bodies, medium effects. Hydrogen bond.

Suggested Readings:

1. Molecular Mechanics, U. Burkert and N.L. Allinger, ACS Monograph 177, 1982.
2. Organic Chemists, Book of Orbitals : L. Salem and W.L. Jorgensen, Academic Press.
3. Mechanism and Theory in Organic chemistry, T.H. Lowry and K.C. Richardson, Harper and Row.
4. Introduction to Theoretical Organic Chemistry and Molecular Modeling.
5. Physical Organic Chemistry : N.S. Isaacs, ELBS/Longman.
6. Supramolecular Chemistry : Concepts and Perspective, J.M. Lehn, VCH.
7. The Physical Basis of Organic Chemistry : H. Maskill, Oxford University Press

M.Sc IV

Chemistry

MCH-608: Electrochemistry

Optional

Unit - 1 1. Conversion and Storage of Electrochemical Energy Present status of energy

consumption : Pollution problem. History of fuel cells, Direct energy conversion by electrochemical means. Maximum intrinsic efficiency of an electrochemical converter. Physical interpretation of the Carnot efficiency factor in electrochemical energy converters.

Power outputs.electrochemical Generators (Fuel Cells) : Hydrogen oxygen cells, Hydrogen Air cell, Hydrocarbon air cell, Alkane fuel cell, Phosphoric and fuel cell, direct NaOH fuel cells, applications of fuel cells.

Electrochemical Energy Storage :

Properties of Electrochemical energy storage : Measure of battery performance, Charging and discharging of a battery, Storage Density, Energy Density. Classical Batteries : (i) Lead

Acid (ii) Nickel-Cadmium, (iii) Zinc manganese dioxide. Modern Batteries : (i) Zinc-Air (ii) Nickel-Metal Hydride, (iii) Lithium Battery, Future Electricity storers : Storage in (i) Hydrogen, (ii) Alkali Metals, (iii) Non aqueous solutions.

Unit - 2 Corrosion and Stability of Metals :

Civilization and Surface mechanism of the corrosion of the metals; Thermodynamics and

the stability of metals, Potential -pH (or Pourbaix) Diagrams; uses and abuses, Corrosion

current and corrosion potential -Evans diagrams. Measurement of corrosion rate : (i) Weight Loss method, (ii) Electrochemical Method.

Inhibiting Corrosion :

Cathodic and Anodic Protection. (i) Inhibition by addition of substrates to the electrolyte environment, (ii) by charging the corroding method from external source, anodic Protection,

Organic inhibitors, The fuller Story Green inhibitors.

Passivation :

Structure of Passivation films, Mechanism of Passivation, Spontaneous Passivation Nature's

method for stabilizing surfaces.

Unit - 3 Bioelectrochemistry :

bioelectrodes, Membrane Potentials, Simplistic theory, Modern theory, Electrical conductance in biological organism: Electronic, Protonic electrochemical mechanism of nervous systems, enzymes as electrodes.

Kinetic of Electrode Process :

Essentials of Electrode reaction. Current Density, Overpotential, Tafel Equation, Butler Volmer equation. Standard rate constant (K_0) and Transfer coefficient (α), Exchange Current.

Irreversible Electrode processes : Criteria of irreversibility, information from irreversible wave.

Unit - 4 Methods of determining kinetic parameters for quasi-reversible and irreversible waves

: Koutecky's methods, Meites Israel Method, Gellings method

Electrocatalysis :

Chemical catalysts and Electrochemical catalysts with special reference to porphyrins, porphyrin oxides of rare earths. Electrocatalysis in simple redox reactions, in reaction involving adsorbed species. Influence of various parameters.

Unit - 5 Potential Sweep Method :

Linear sweep Voltammetry, Cyclic Voltammetry, theory and applications. Diagnostic criteria of cyclic voltammetry. Controlled current microelectrode techniques : comparison with controlled potentials methods, chronopotentiometry, theory and applications.

Bulk Electrolysis Methods :

Controlled potential coulometry, Controlled Coulometry, Electroorganic synthesis and its important applications. Stripping analysis : anodic and Cathodic modes, Pre electrolysis and Stripping steps, applications of Stripping Analysis.

Suggested Readings:

1. Modern Electrochemistry Vol. I, IIA, Vol. IIB J'OM Bockris and A.K.N. Reddy, Plenum Publication, New York.
2. Polarographic Techniques by L. Meites, Interscience.
3. "Fuel Cells : Their electrochemistry". McGraw Hill Book Company, New York.

4. Modern Polarographic Methods by A.M. Bond, Marcell Dekker.
5. Polarography and allied techniques by K. Zutshi, New age International publicatin. New Delhi.
6. "Electroanalytical Chemistry by Basil H. Vessor & Galen W. ; Wiley Interscience.
7. Electroanalytical Chemistry by Basil H. Vessor & alen w. ; Wiley Interscience.
8. Topics in pure and Applied Chemistry, Ed. S. K. Rangrajan, SAEST Publication, Karaikudi (India)

M.Sc IV
Chemistry
MCH-609: Medicinal Chemistry
Optional

Unit - 1 Structure and activity : Relationship between chemical structure and biological activity

(SAR). Receptor Site Theory. Approaches to drug design. Introduction to combinatorial synthesis in drug discovery. Factors affecting bioactivity. QSAR-Free-Wilson analysis, Hansch analysis, relationship between Free-Wilson analysis and Hansch analysis.

Unit - 2 Pharmacodynamics:

Introduction, elementary treatment of enzymes stimulation, enzyme inhibition, sulfonamides, membrane active drugs, drug metabolism, xenobiotics, biotransformation, significance of drug metabolism in medicinal chemistry.

Unit - 3 Antibiotics and antibacterials

Introduction, Antibiotic β -Lactam type - Penicillins, Cephalosporins, Antitubercular – Streptomycin, Broad spectrum antibiotics – Tetracyclines, Anticancer - Dactinomycin (Actinomycin D)

Unit - 4 Antifungal –

polyenes, Antibacterial – Ciprofloxacin, Norfloxacin, Antiviral – Acyclovir

Antimalarials : Chemotherapy of malaria. SAR. Chloroquine, Chloroguanide and Mefloquine

Unit - 5 Non-steroidal Anti-inflammatory Drugs :

Diclofenac Sodium, Ibuprofen and Netopam

Antihistaminic and antiasthmatic agents :

Terfenadine, Cinnarizine, Salbutamol and Beclomethasone dipropionate.

M.Sc. Semester IV

Practical

(Duration: 6-8 hrs in each branch)

Practical examination shall be conducted separately for each branch.

Inorganic Chemistry Max Marks - 33

Preparation 12

Spectrophotometric Determinations

Flame Photometric Determinations 12

Record 04

Viva Voice 05

Preparation

Preparation of selected inorganic compounds and their study by IR, electronic spectra, and magnetic

susceptibility measurements. Handling of air and moisture sensitive compounds involving vacuum lines.

Selection can be made from the following :

1. Sodium amide. Inorg. Synth., 1946, 2, 128.
2. Atomic absorption analysis of Mg and Ca.
3. Synthesis of trichlorodiphenylantimony (V) hydrate. Inorg. Synths., 1985, 23, 194
4. Sodium tetrathionate $\text{Na}_2\text{S}_4\text{O}_6$.
5. Metal complex of dimethyl sulfoxide : $\text{CuCl}_2 \cdot 2\text{DMSO}$ J.Chem. Educ., 1982, 59, 57.
6. Synthesis of metal acetylacetonate : Inorg. Synths, 1957, 5, 130, 1963, 1, 183.
7. Cis and Trns $[\text{Co}(\text{en})_2\text{Cl}_2]^+$.
8. Determination of Cr (III) complex. $[\text{Cr}(\text{H}_2\text{O})_6]\text{NO}_3 \cdot 3\text{H}_2\text{O}$,. Inorg. synths., 1972, 13, 184.
9. Preparation and use of Ferrocene. J. Chem. Edu. 1966, 43, 73; 1976, 53, 730.
10. Preparation of $[\text{Co}(\text{phenanthroline-5,6 quinone})]$.

Spectrophotometric Determinations

- a. Manganese/Chromium in steel sample.
- b. Nickel by extractive spectrophotometric method.
- c. Fluoride/nitrite/phosphate.
- d. Copper-Ethylene diamine complex : Slope-ratio method.

Flame Photometric Determinations

- a. Sodium and potassium when present together.
- b. Lithium/calcium/barium/strontium.
- c. Cadmium and magnesium in tap water.

Organic Chemistry Max Marks - 33

Multi-step Synthesis of Organic Compounds 12

Spectroscopy/Spectrophotometric Determinations 12

Record 04

Viva Voice 05

Multi-step Synthesis of Organic Compounds

The exercise should illustrate the use of organic reagents and may involve purification of the products by chromatographic techniques. Photochemical reaction Benzophenone \rightarrow Benzpinacol \rightarrow Benzpinacolone Beckmann rearrangement : Benzanilide from benzene Benzene \rightarrow Benzophenone \rightarrow Benzophenone oxime \rightarrow Benzanilide Benzilic acid rearrangement : Benzilic acid from benzoin Benzoin \rightarrow Benzil \rightarrow Benzilic acid Synthesis of heterocyclic compounds Skraup synthesis : Preparation of quinoline from aniline Fisher Indole synthesis : Preparation of 2-phenylindole from phenylhydrazine.

Enzymatic synthesis Enzymatic synthesis Enzymatic reduction : reduction of ethyl acetoacetate using

Baker's yeast to yield enantiomeric excess of S (+) ethyl-3-hydroxybutanoate and determine its optical

purity. Biosynthesis of ethanol from sucrose. Synthesis using microwave Alkylation of diethyl malonate

with benzyl chloride. Synthesis using phase transfer catalyst. Alkylation of diethyl malonate or ethyl

acetoacetate with an alkylhalide.

Spectroscopy

Identification of organic compounds by the analysis of their spectral data (UV, IR, PMR, CMR & MS)

Spectrophotometric (UV/VIS) Estimations of the following (any one compound)

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

Physical Chemistry Max Marks - 34

Experiment No. 1 13

Experiment No. 2 12

Record 04

Viva Voice 05

Spectroscopy

- i. Determination of PK_a of an indicator (e.g. methyl red) in (a) aqueous and (b) micellar media.
- ii. Determination of stoichiometry and stability constant of Ferricisothiocyanation complex ion in solution.
- iii. Determination of rate constant of alkaline bleaching of Malachite green and effect of ionic strength on the rate of reaction.

Chemical Kinetics

- i. Determination of rate constant and formation constant of an intermediate complex in the reaction of Ce(IV) and Hypophosphorous acid at ambient temperature.
- ii. Determination of energy and enthalpy of activation in the reaction of KMnO₄ and benzyl alcohol in acid medium.
- iii. Determination of energy of activation of and entropy of activation from a single kinetic run.
- iv. Kinetics of an enzyme catalyzed reaction.

Thermodynamics

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

Polarography

- i. Identification and estimation of metal ions such as Cd²⁺, Pb²⁺, Zn²⁺, and i²⁺ etc. polarographically.
- ii. Study of a metal ligand complex polarographically (using Lingane's Method).

Books Suggested

1. Inorganic Experiments, J. Derek Woolings, VCH.
2. Microscale Inorganic Chemistry, Z. Szafran, R.M. Pike and M.M. Singh, Wiley.
3. Practical Inorganic Chemistry, G. Marr and B. W. Rockett, Van Nostrand.
4. The systematic Identification of Organic Compounds, R.L. Shriner and D.Y. Curtin.