

AWADHESH PRATAP SINGH UNIVERSITY, REWA (M.P.)



SYLLABUS FOR M.Sc. CHEMISTRY FOUR SEMESTERS (TWO YEAR COURSE)

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

SEMESTER –I

Paper	Course No.	Course	Marks (Theory + CCE)
Paper I	MCH-401	Inorganic Chemistry I	100(75+25)
Paper II	MCH-402	Organic Chemistry I	100(75+25)
Paper III	MCH-403	Physical Chemistry I	100(75+25)
Paper IV	MCH-404	Group Theory , Mathematics for Chemists & Biology for Chemists	100(75+25)
Practical *			
Total Marks			400

* Practical Examinations will be held in second semester.

SEMESTER –II

Paper	Course No.	Course	Marks
Paper V	MCH-405	Inorganic Chemistry II	100(75+25)
Paper VI	MCH-406	Organic Chemistry II	100(75+25)
Paper VII	MCH-407	Physical Chemistry II	100(75+25)
Paper VIII	MCH-408	Spectroscopy II and Diffraction Methods	100(75+25)
Practical		Inorganic + Organic + Physical	300
Total Marks			700

M.Sc. (Final)**SEMESTER– III**

Paper	Paper Code	Course	Marks
Paper-I	MCH-501	Applications of Spectroscopy I	100(75+25)
Paper-II	MCH-502	Photochemistry	100(75+25)
Paper-III	MCH-503	Polymer Chemistry	100(75+25)
Paper-IV	MCH-504	Heterocyclic Chemistry	100(75+25)
Practical*			
Total Marks			400

* Practical Examinations will be held in fourth semester.

SEMESTER– IV

Paper	Course No.	Course	Copm / Opt	Marks (Theory + CCE)
Paper V	MCH-505	Applications of Spectroscopy II	Compulsory	100(75+25)
Paper VI	MCH-506	Solid State Chemistry	Compulsory	100(75+25)
Paper VII	MCH-507	Natural Products	Compulsory	100(75+25)
Paper VIII	MCH-508-512	Optional Paper*	Optional	100(75+25)
Practical		Inorganic + Organic + Physical		300
	Project Work			150
Total Marks				850

Optional Paper*

MCH - 508: Organic Synthesis

MCH - 509: Organotransition Metal Chemistry

MCH - 510: Analytical Chemistry

MCH - 511: Electrochemistry

MCH - 512: Medicinal Chemistry

Grant Total Marks M.Sc. (Previous & Final) 1100 + 1250 = 2350

* Minimum passing marks in theory is 25 marks.

* Minimum passing marks in CCE is 10 marks.

* Instead of laboratory work, student may performed Project work.

(Sample for Question Papers)

M.Sc. I / II/ III / IV

Chemistry

Paper: MCH-

Time allowed: Three hours

Maximum Marks: 75

Minimum Passing Marks: 25

Note:- This paper is divided into two Sections (A and B). Marks are indicated against each sections. Read the instruction of each sections carefully and answer accordingly.

Section - A

(Short Answer type Questions)

Note:- All questions are compulsory.

7 x 5 =35

Unit - I

Q.1

Or

Q.2

Unit -II

Q.3

Or

Q.4

Unit-III

Q.5

Or

Q. 6

Unit- IV

Q.7

Or

Q. 8

Unit -V

Q.9

Or

Q.10

Section B

(Long answer type questions)

Note:- Attempt any two Questions.

20 x 2 = 40

(One question from each Unit should be given)

Q.11

Q.12

Q.13

Q.14

Q.15

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. McCleverty, Pergamon.

SEMESTER-I
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, Curtir-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, Comell 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 & Professionsl.
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. Stereochemisty of Organic Compounds, P.S. Kalsi, New Age International.

SEMESTER –I
Paper-III
MCH-403: PHYSICAL CHEMISTRY I

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 function s 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. Gowarikar, N.V. Vishwanathan and J. Sridhar, Wiley Eastern.
10. Introduction to Quantum Chemistry-R.K. Prasad, New Age Publication.

SEMESTER- I**Paper-IV****MCH-404: Group Theory, Mathematics for Chemists and Biology for Chemists****Unit-I****Symmetry and Group theory in Chemistry**

Symmetry elements and symmetry operation, definition of group, subgroup. Conjugacy relation and classes. Point symmetry group. Schoenflies 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**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.

Or**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**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.).

Or**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-IV**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). First-order and first degree differential equations, Applications to chemical kinetics,

Or**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 -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.

Or**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.

Books suggested

1. Physical Methods in Chemistry, R.S. Drago, Saunders College.
2. Chemical Applications of Group Theory, F.A. Cotton.
3. The chemistry Mathematics Book, E.Steiner, Oxford University Press.
4. Mathematical for Physical chemistry : F. Daniels, Mc. Graw Hill.
5. Applied Mathematics for Physical Chemistry, J.R. Barante, Prentice Hall.
6. Chemical Mathematics D.M. Hirst, Longman.
7. Principles of Biochemistry, A.L. Lehninger, Worth Publishers.
8. Biochemistry, L. Stryer, W.H. Freeman.
9. Biochemistry, J. David Rawan, Neil Patterson.
10. Biochemistry, Voet and Voet, John Wiley.

SEMESTER –II
Paper-V
MCH-405: 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 :

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.

SEMESTER –II
Paper-VI
MCH-406: 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, S_N1, benzyne and S_N2 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 E_{1cB} mechanisms and their spectrum. Orientation of the double bond. Reactivity-effects of substrate structures, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination.

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 correlatino diagrams. FMO and PMO approach. Electrocyclic reactions-conrotatory and disrotatory motions, $4n$ $4n+2$ and allyl systems. Cycloadditions-antarafacial and suprafacial additions, $4n$ and $4n+2$ systems, $2+2$ addition of ketenes, 1,3 dipolar cycloadditions and cheleotrpc reactions. Sigmatropic rearrangements-suprafacial and antarafacial shifts of H, sigmatropic involving carbon moieties, 3,3- and 5,5 sigmatropic rearrangements. Claise n, Cope and aza-Cope rearrangements. Fluxional tautomerism. Ene reaction.

Book Suggested

1. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry, F.A. Carey and R.J. Sunderg, Plenum.
3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
4. Structure and Mechanism in Organic Chemistry, C.K. Ingold, Comell 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.
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. Stereochemisty of Organic Compounds, P.S. Kalsi, New Age International.

SEMESTER-II
Paper-VII
MCH-407: 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

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. Kineties 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. Gowarikar, N.V. Vishwanathan and J. Sridhar, Wiley Eastern.

SEMESTER –II**Paper-VIII****MCH-408: 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

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.

PRACTICAL**(Duration: 6-8 hrs in each branch)****Practical examination shall be conducted separately for each branch in Second semester (M.Sc. 1st Year)****Inorganic Chemistry**

Separation and estimation of two metal ions.	35
Preparation and synthesis of metal complexes	20
Paper chromatography	20
Record	10
Viva Voce	15
Total	100

1. Separation and estimation of two metal ions:

- (i) Estimation of copper and nickel both by gravimetric method.
- (ii) Estimation of barium gravetrically and copper volumetrically methods.
- (iii) Estimation of copper and zinc in a mixed solution of both by gravimetric methods.
- (iv) Estimation of nickel and zinc in a mixed solution of both by gravimetric methods.

2. Preparation and synthesis of metal complexes

- (i) $\text{VO}(\text{acac})_2$
- (ii) $\text{Ni}(\text{acac})_2$
- (iii) $\text{K}_3[\text{Fe}(\text{C}_2\text{O}_4)_3]$
- (iv) Prussian Blue, Turnbull's Blue.
- (v) $\text{Co}(\text{NH}_3)_6$ $[\text{Co}(\text{NO}_2)_6]$
- (vi) $\text{Hg}[\text{Co}(\text{SCN})_4]$
- (vii) $[\text{Cu}(\text{NH}_3)_4]\text{SO}_4\text{H}_2\text{O}$
- (viii) $[\text{Ni}(\text{NH}_3)_6]\text{Cl}_2$
- (ix) $\text{Ni}(\text{dmg})_2$

3. Paper chromatography:

Separation of cations by Paper Chromatography of following cations:

- (i) Ag(I), Pb(II) and Hg₂(II)
- (ii) Hg(II), Cu(II) and Pb(II)
- (iii) Ni(II), Co(II) and Zn(II)
- (iv) Ni(II), Co(II) and Cu(II)

Physical Chemistry

Chemical Kinetics (determination of rate constant for hydrolysis of esters)	35
Determination of composition of a mixture of weak and strong acids by conductometric titration	20
Determination of composition of a mixture of weak and strong acids by pH metric titration	20
Record	10
Viva Voce	15
Total	100

1. Chemical Kinetics

- (i) Determination of velocity constant of the hydrolysis of methyl acetate catalysed by an acid (say HCl, H₂SO₄, etc.).
- (ii) Determination of velocity constant of saponification of ethyl acetate with sodium hydroxide.
- (iii) Determination of velocity of the reaction between potassium persulphate and potassium iodide.

2. Determination of composition of a mixture of weak and strong acids by conductor metric titration of following acids:

- (i) HCl and CH₃COOH
- (ii) HNO₃ and CH₃COOH
- (iii) H₂SO₄ and CH₃COOH

3. Determination of composition of a mixture of weak and strong acids by pH metric titration of followings acids:

- (i) HCl and CH₃COOH
- (ii) HNO₃ and CH₃COOH
- (iii) H₂SO₄ and CH₃COOH

Organic Chemistry

Qualitative Analysis	35
Organic Synthesis	20
Quantitative analysis	20
Record	10
Viva Voce	15
Total	100

1. 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.

2. 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
Aromatic electrophilic substitutions : Synthesis of p-nitroaniline and pbromoaniline.
Aldol condensation Dibenzal acetone from benzaldehyde. Synthesis of different Schiff bases using salicylaldehyde and amines, Synthesis of different dithiocarbamates. The Products may be characterized by Spectral Techniques

3. 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.

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, Adward Arnold.
6. Handbook of Organic Analysis-qualitative and Quantitative. H. Clark, Adward Arnold.
7. Vogel's Textbook of Practical Organic Chemistry, A.R. Tatchell, John Wiley.
8. Practical Physical Chemistry, A.M. James and F.E. Prichard, Longman.
9. Findley's Practical Physical chemistry, B.P. Levitt, Longman.
10. Advanced Physical Chemistry by Gurtu and Gurtu, Pragati Prakashan.
11. Experimental Physical Chemistry, R.C. Das and B. Behera, Tata McGraw Hill.

SEMESTER –III**Paper-I****MCH-501: APPLICATION OF SPECTROSCOPY - I****Unit - I****Electronic Spectroscopy:**

Electronic Spectral Studies for d^1 - d^9 systems in octahedral, tetrahedral and square planer complexes,

Unit - II**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.

Unit -III**Nuclear Magnetic Resonance Spectroscopy – I**

General introduction and definition, Chemical shift, spin – spin interaction, shielding and deshielding mechanism, mechanism of measurement of chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, and amides & mercapto).

Unit-IV**Nuclear Magnetic Resonance Spectroscopy – II**

Chemical exchange, effect of deuteration, Complex spin – spin interaction between two, three, four and five nuclei (1 order spectra) Stereochemistry, hindered rotation, Karplus curve-variation of coupling constant with disordered angle, NMR shift reagents, solvent effects, Nuclear overhauser effect (NOE).

Unit-V**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 M-L bond, coordination number, structure and (3) detection of oxidation state and in equivalent MB atoms.

Book Suggested

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. Craddock, 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.

SEMESTER –III
Paper II
MCH-502: PHOTOCHEMISTRY

Unit-I

Photochemical Reactions

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

Unit -II

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.

Unit -III

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.

Unit -IV

Photochemistry of Carbonyl Compounds

Intramolecular reactions of carbonyl compounds-saturated, cyclic and acyclic, α , β , γ unsaturated and α , β , unsaturated compounds, cyclohexadienones, Intermolecular cycloaddition reactions-dimerisations and oxetane formation.

Unit-V

Miscellaneous Photochemical Reactions.

Photo-Fries reactions of annelids, Photo-Fries rearrangement, Barton reaction, Singlet molecular oxygen and its reactions, Photochemical formation of smog, Photodegradation of polymers, Photochemistry of vision.

Books Suggested

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.

SEMESTER –III
Paper III
MCH-503: Polymer Chemistry

Unit-I
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-II
Polymer Characterization

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

Unit-III
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-IV
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 V
Structure, Properties and Application of

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

Books Suggested

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. Alcock and F.W. Lambe, Prentice Hall.

SEMESTER –III
Paper IV
MCH-504: Heterocyclic Chemistry

Unit-I**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-II**Non-aromatic Heterocycles**

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

Unit-III**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-IV**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-V

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, thiepines, 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.

Books Suggested :

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 Scietific Techinal.
5. Contemporary Hetrocyclic Chemistry, G,.R. Newkome and W.W. Paudler, Wiley-Inter Science.
6. An Introductiion to the Heterocyclic Compounds, R.M. Acheson, Johnwiely.
7. Comprehensive Heterocyclic Chemistry, A.R. Katrizky and C.W. Rees, eds. Pergamon Press.

SEMESTER –IV
Paper V
MCH-505: APPLICATION OF SPECTROSCOPY

Unit-I**Ultraviolet and Visible spectroscopy**

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

Unit-II**Infrared Spectroscopy**

Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ether's, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (ketone's, aldehyde's, esters, amides, acids, anhydride's, lactones, lactams and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and fermi resonance.

Unit-III**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.

Unit-IV**Carbon-13 NMR Spectroscopy**

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

Unit V**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.

Book Suggested

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.

SEMESTER –IV
Paper-VI
MCH-506: SOLID STATE CHEMISTRY

Unit-I

Solid State Reactions

General principles, experimental procedure, co-precipitation as a precursor to solid state reactions, kinetics of solid state reactions.

Unit-II

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 defects.

Unit-III

Electronic Properties and Band Theory

Metals insulators and semiconductors, electronic structure of solid band 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-IV

Organic Solids

Electrically conducting solids. organic charge transfer complex, organic metals, new superconductors.

Unit-V

Liquid Crystals:

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

Books Suggested.

1. Solid state chemistry and its applications, A.R. West. Peenum.
2. Principles of the Solid State, H.V. Keer, Wiley Eastern.
3. Solid State Chemistry, N.B. Hannay.
4. Solid State Chemistry, D.K. Chakrabarty, New Wiley Eastern.

SEMESTER –IV**Paper VII****MCH-507: Chemistry of Natural Products****Unit-I****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 α -Terpeneol, Menthol, Farnesol, Zingiberence, Santonin, Phytol, Abietic acid and β -Carotene.

Unit-II**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-III**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-IV**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 V**Prostaglandis**

Occurrence, nomenclature, classification, biogenesis and physiological effects. Synthesis of PGE₂ and PGF_{2a}.

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).

Books Suggested

1. Natural Products : Chemistry and Biological Significance, J. Mann, R.S. Davidson, J.B. Hobbs, D.V. Banthrope adn J.B. Harbome, Longman, Esses.
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.

**SEMESTER –IV
PAPERS IV (OPTIONAL)**

Out of the following select any one paper each of marks 100 (75 + 25)

- | | |
|---------------|----------------------------------|
| OPT – MCH-508 | Organic Synthesis |
| OPT – MCH-509 | Organotransition Metal Chemistry |
| OPT – MCH-510 | Analytical Chemistry |
| OPT – MCH-511 | Electrochemistry |
| OPT – MCH-512 | Medicinal Chemistry |

SEMESTER –IV
Optional–1
MCH-508: Organic Synthesis

Unit-I**Disconnection Approach**

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

Unit-II**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-III**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 tetroxide, 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 IV**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 V**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

Books Suggested

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.

SEMESTER –III
Optional–2
MCH-509: Organotransition Metal Chemistry

Unit -I

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 -II

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 -III

Transition organometallic compounds:

Transition metal compounds with bonds to hydrogen, boron, silicon

Unit -IV

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 -V

Flexional Organometallic Compounds

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

Books Suggested

1. Principles and Application of Organotransition Metal Chemistry, J.P. Collman, L.S. Heagsdus, 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.

SEMESTER –IV
Optional-3
MCH-510: Analytical Chemistry

Unit-I**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 or 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-II**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-III**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-IV**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.
- (b) 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-V

- (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.

Book Suggested

1. Analytical Chemistry, G.D. Christian, J.Wicy.
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. LG. 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.

SEMESTER –IV
Optional-4
MCH-511: Electrochemistry

Unit-I**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-II**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) Diaphragms; 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 changing 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-III**Bioelectrochemistry:**

bioelectrodics, 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) and Transfer coefficient (a), Exchange Current.

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

Unit-IV

Methods of determining kinetic parameters for quasi-rversible and irreversible waves: Koutecky's methods, Meits 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-V

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.

Books Suggested

1. Modern Electrochemistry Vol. I, Ila, 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)

SEMESTER –IV
Optional–5
MCH-512: Medicinal Chemistry

Unit-I**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-II**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-III**Antibiotics and antibacterials:**

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

Unit-IV**Antifungal**

Polyenes, Antibacterial - Ciprofloxacin, Norfloxacin, Antiviral . Acyclovir

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

Unit-V**Non-steroidal Anti-inflammatory Drugs:**

Diclofenac Sodium, Ibuprofen and Netopam

Antihistaminic and antiasthmatic agents:

Terfenadine, Cinnarizine, Salbutamol and Beclomethasone dipropionate.

Books Suggested:

1. Introduction to medicinal chemistry, A. Gringuage, Wiley-VCH.
2. Wilson and Gisvold's Text Book of Organic Medicinal and Pharmaceutial Chemistry, Ed. Robert F. Dorge.
3. An Introduction to Drug Design, S.S. Pandeya and J. R. Dimmock, New Age International.
4. Burger's Medicinal Chemistry and Drug Discovery, Vol-I (Chapter 9 and Chapter 14), Ed. M.E. Wolff, John Wiley.
5. Goodman and Gilman's Pharmacoloical Basis of Therapeutics, Mc-GRaw- Hill.
6. The organic Chemistry of Drug Design and Drug Action, R.B. Silverman, Academic Press.
7. Strategies for Organic Drug Synthesis and Design, D.Ledinicer, John Wiley.
8. Principals of Medicinal Chemistry W.O. Foye.
9. Medicinal Chemistry; The role of organic chemist in Drug Research, S.M. Roberts and B. J. Pricer.

PRACTICAL
(Duration: 6-8 hrs in each branch)

Practical examination shall be conducted separately for each branch in Second semester (M.Sc. 2nd Year)

Inorganic Chemistry

Quantative determtions of a three component mixture	35
Synthesis and characterization of metal complexes	20
Chromatography Separations	20
Record	10
Viva Voce	15
Total	100

1. Quantitative determinations of a three component mixture :

One Volumetrically and two gravimetrically

- (i) Cu^{2+} , Ni^{2+} , Zn^{2+}
- (ii) Cu^{2+} , Ni^{2+} , Ag^{2+}
- (iii) Cu^{2+} , Ni^{2+} , Ba^{2+}

2. Synthesis and characterization of following metal complexes:

- (i) Sodium tetrathionate $\text{Na}_2\text{S}_4\text{O}_6$.
- (ii) Metal complex of dimethyl sulfoxide : $\text{CuCl}_2 \cdot 2\text{DMSO}$
- (iii) Synthesis of metal acetylacetonate
- (iv) Synthesis of copper and nickel Schiff base complexes.
- (v) Synthesis of copper and nickel dithiocarbamates

3. Chromatographic Separations

- (i) Cadmium and zinc
- (ii) Zinc and magnesium.
- (iii) Thin-layer / Paper chromatography-separation of nickel, manganese, cobalt and zinc. Determination of R_f values.

Physical Chemistry

Chemical Kinetics (determination of strength of two acids)	35
Determination of Equivalence conductance of strong electrolyte and polarography	20
Spectroscopy and study of adsorption	20
Record	10
Viva Voce	15
Total	100

1. Chemical Kinetics (determination of strength of two acids)

- (i) Determination of relative strengths of HCl and H₂SO₄ (k_1 / k_2) for the hydrolysis of methyl acetate.
- (ii) Determination of relative strengths of HNO₃ and H₂SO₄ (k_1 / k_2) for the hydrolysis of methyl acetate.

2. Determination of Equivalence conductance of following strong electrolyte:**(a) Equivalence conductance**

- (i) KCl
- (ii) NaCl
- (iii) AgNO₃
- (iv) HCl
- (v) KNO₃

(b) 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).

3. Spectroscopy and adsorption**(a) 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 Ferric isothiocyanate ion complex ion in solution.

(b) Adsorption

To study the adsorption of oxalic acid on activated charcoal and test the validity of Freundlich's adsorption isotherm.

Organic Chemistry

Multistep of organic compounds	35
Isolation	20
Paper Chromatography	20
Record	10
Viva Voce	15
Total	100

1. 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. Prepreparation in steps: Benzophenone →Benzpinacol→Benzpinacolone Beckmann rearrangement : Benzanilide from benzene, Benzene →Benzophenone →Benzophenone oxime→ Benzanilide, Benzilic acid rearrangement : Benzilic acid from benzoin, Benzoin→Benzil→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.

2. Isolation

1. Isolation of caffeine from tea leaves.
2. Isolation of casein from milk (the students are required to try some typical colour reactions of proteins).
3. Isolation of lactose from milk (purity of sugar should be checked by LC and PC and R_F values reported).
4. Isolation of nicotine dipicrate from tobacco.
5. Isolation of piperine from black pepper.
6. Isolation of lycopene from tomatoes.
7. Isolation of b-carotene from carrots.
8. Isolation of eugenol from clove.
9. Isolation of (+) limonine from citrus rind.

3. Paper Chromatography

Separation and identification of the sugars present in the given mixture of glucose, fructose and sucrose by paper chromatography and determination of R_F values/

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.
5. A Practical text book by Singh and Yadav, Pragati prakashan.
6. Findley's Practical Physical chemistry, B.P. Levitt, Longman.
7. Advanced Physical Chemistry by Gurtu and Gurtu, Pragati Prakashan.
8. Experimental Physical Chemistry, R.C. Das and B. Behera, Tata McGraw Hill.