



M.Sc. Chemistry

2016 -2017

CORE COURSES				
I SEMESTER				
SUBJECT CODE	SUBJECT	THEORY	CCE	TOTAL
MCH 511	INORGANIC CHEMISTRY -I	80	20	100
MCH 512	ORGANIC CHEMISTRY-I	80	20	100
MCH 513	PHYSICAL CHEMISTRY-I	80	20	100
MCH 514	GROUP THEORY & VIBRATIONALSPECTROSCOPY	80	20	100
MCH 515	(a)MATHEMATICS FOR CHEMISTS	80	20	100
	(b) BIOLOGY FOR CHEMISTS			
MCH 516	PRACTICAL (LAB 1)	-	-	50
	TOTAL			550
SEMESTER: II				
MCH 521	INORGANIC CHEMISTRY - II	80	20	100
MCH 522	ORGANIC CHEMISTRY - II	80	20	100
MCH 523	PHYSICAL CHEMISTRY - II	80	20	100
MCH 524	MAGNETIC RESONANCE AND MÖSSBAUER SPECTROSCOPY	80	20	100
MCH 525	COMPUTATIONAL METHODS IN CHEMISTRY	80	20	100
MCH 526	PRACTICAL (Based on MCH 523 & MCH 524)	0	-	50
	TOTAL			550
SEMESTER III				
MCH 531	PHOTOCHEMISTRY	80	20	100
MCH 532	ENVIRONMENTAL CHEMISTRY	80	20	100
MCH 533	BIOINORGANIC CHEMISTRY	80	20	100
MCH 534	BASIC MEDICINAL CHEMISTRY	80	20	100
MCH 535	PHARMACEUTICAL BIOTECHNOLOGY	80	20	100
MCH 536	PRACTICAL (Based on MCH 535)	0	-	50
	TOTAL			550
SEMESTER IV				
MCH 541	ANALYTICAL CHEMISTRY	80	20	100
MCH 542	CHEMISTRY OF NATURAL PRODUCTS	80	20	100
MCH 543	RESEARCH METHODOLOGY	80	20	100
MCH 544	DISSERTATION			200
MCH 545	PRACTICAL(LAB 4)			50
	TOTAL			550
	GRAND TOTAL			2200

(Figures in parenthesis stand for number of hours of lecture , followed by number of hours of laboratory work, field work & total credit to be earned in the course respectively)

Note:1 hour of lecture=1 credit hour; 2 hours of lab=1 credit;3 to 4 sessions of field visit=1 credit

****15 LECTURE PER UNIT FOR EACH RESPECTIVE UNIT.**



SEMESTER I

**MCH-511: INORGANIC CHEMISTRY-
Unit-I**

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-II

Reaction Mechanism of Transition Metal Complexes I

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, anation reactions, reactions without metal ligand bond cleavage.

Unit-III

Reaction Mechanism of Transition Metal Complexes II

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, octahedral, tetrahedral and square planar complexes, p-bonding and molecular orbital theory. **Non-Aqueous Solvents** Ammonia and Sulphuric acid. Aprotic solvents: BrF_3 , POCl_3 . Molten salts and room temperature molten salts.

UNIT-V

HSBA Theory

Classification of HSAB, HSAB principle, uses of HSAB principle, theoretical basis of hardness and softness; Lewis acid base reactivity Approximation; donor acceptor number, symbiosis.

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...



MCH-512: ORGANIC CHEMISTRY-I

UNIT - I

Structure and reactivity:

Localised and delocalised covalent bond - Concept of resonance and aromaticity - Huckel's rule for aromaticity in benzenoid and non-benzenoid compounds, antiaromaticity and homoaromaticity. Nature of reaction energy and kinetic considerations - types of organic reactions - reagents - reactive intermediates. Their formation and stabilization - inductive and mesomeric effects.

Unit-II

Chirality;

Absolute and relative configuration, The terms chiral, achiral, stereogenic center (stereocenter), representations of three dimensional molecules, stereoisomerism resulting from more than one stereogenic unit, Pi-diastereoisomerism and torsional chirality in carbon-carbon double bonds, some stereochemical reactions near a stereocenter (formation of diastereomers) stereoselective and stereospecific reactions, stereoisomerism in compounds without a stereogenic carbon, optical activity due to stereoplane (planar chirality)- paracyclophanes and transcyclooctene, optical activity of compounds due to helicity, asymmetric synthesis.

Unit-III

Aromaticity:

Aromaticity, NMR spectroscopy and aromaticity, aromatic compounds, antiaromatic compounds, nonaromatic compounds, annulenes, ions, metallocenes Crown ether complexes and cryptates, phase transfer catalysis The Hammett equation- linear free energy relationship, Taft equation, steric effects, strain and Bredt rule.

Unit-IV

Aliphatic nucleophilic substitution:

S_N2 reaction as a stereospecific reaction, S_N1 Mechanism-Ion Pairs and other aspects, S_Ni and SET mechanisms, neighbouring group participation anchimeric assistance, non-classical carbocations Conformations and stereoisomerism of acyclic and cyclic systems, conformation and chemical Reactivity

Unit-V

Stereochemistry of elimination reactions: E1, E2 and E1cB mechanisms, elimination versus Substitution Free radical reactions, Structure, stability and geometry, properties of free radicals.

Books Suggested

1. J. March., Advanced Organic Chemistry: Reactions, Mechanisms and Structure, John Wiley
2. P. S. Kalsi. Stereochemistry, Conformation and Mechanism, New Age International
3. Peter Sykes, A guide book to mechanism in Organic chemistry, Orient-Longmans



MCH-513: PHYSICAL CHEMISTRY-I

Unit-I

Introduction to Exact Quantum Mechanical Results

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

Unit –II

Approximate Methods

Variational and perturbation methods. 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. Introduction to extended Huckel theory.

Unit-III

Chemical Thermodynamics

Partial molar Quantities: Partial molar free energy, partial molar volume and partial molar heat content, Non-ideal systems : Excess functions for non-ideal solutions. Activity, activity coefficient, Debye Huckel theory for activity coefficient forelectrolytic solutions; Determination of activity and activity coefficient; ionic strength. Application of phase rule to three component system; second order phase transitions.

UNIT-IV

Statistical Thermodynamics

Partition functions-translation, rotational, vibrational and electronic partition functions. Calculation of thermodynamic properties in terms of partitions. Heat capacity behaviour of solids-chemical equilibrium and equilibrium constant in terms of partition functions, Fermi-Dirac Statistics and Bose-Einstein statistics distribution law and application to helium.

UNIT-V

Macromolecules

Macromolecules: Molecular weight of a polymer (Number and mass average) Degree of polymerization and molecular weight, methods of determining molecular weights(Osmometry, viscometry, light scattering, diffusion and ultracentrifugation) Chemistry of polymerization. Mechanism of polymerization ,Free radical polymerization (Initiation,propagation and termination), kinetics of free radical polymerization, step growth polymerization (Polycondensation), kinetics of step polymerization, cationic and anionic polymerization.

Books Suggested

1. J. P. Lowe and K.Peterson, Quantum Chemistry Academic Press.
2. D. A. McQuarrie, Quantum Chemistry Viva Books Pvt. Ltd.: New Delhi.
3. R. G. Mortimer, Mathematics for Physical Chemistry Elsevier.
4. F. L. Pilar, Elementary Quantum Chemistry , Dover Publication Inc.: NewYork.



MCH-514: Group Theory & Vibrational Spectroscopy

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} , etc, 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 intercities, far IR region, metal ligand vibrations, normal co-ordinate analysis.

Unit-IV

Vibrational Spectroscopy

Symmetry, shapes and molecular vibrations of AB_2 , AB_3 , AB_4 , AB_5 and AB_6 , **Raman Spectroscopy** Classical and quantum theories of Raman effect. Pure rotational, vibrational and vibrationalrotationalRaman spectra, selection rules, mutual exclusion principle, Resonance aman spectroscopy, coherent anti stokes Raman spectroscopy (CARS).

Unit-V

Ultraviolet and Visible spectroscopy: Fundamentals, effect of solvent and extending conjugation 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

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.



MCH-515 (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

Permutations and Combinations

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 Suicliff, 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.



MCH-515 (b) BIOLOGY FOR CHEMISTS

(For students without Biology in B.Sc.)

Unit-I

Cell structure and functions

Structure of prokaryotic and eukaryotic cells, intercellular organelles and their function 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.

Unit-II

Carbohydrates

Structure and function of important derivatives of monosaccharides like glycosides deoxy sugars, yoinositol, amino sugars. N-acetylmuramic acid. Sialic acid. Structural polysaccharide: Cellulose and chitin, Storage polysaccharide: Starch and glycogen. Structural and biological functions of glucosaminoglycans or mucopolysaccharides. Carbohydrates of glycoprotein and glycolipids Role of sugars in biological recognition. Carbohydrate metabolism-Kreb's cycle, glycolysis, lycogenesis and glycogenolysis, gluconeogenesis, pentose phosphate pathway.

Unit-III

Lipids

Fatty acids, essential fatty acids, structure and function of triacylglycerols, glycerophospholipids sphingolipids, Lippoproteins: Composition and function, role in atherosclerosis. Properties of lipids aggregates-micelles, bilayers, liposomes and their possible biological functions. Lipid metabolism-• -oxidation of fatty acids.

Unit-IV

Amino acids, Proteins

Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing. Secondary structure of proteins, 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/enzymetic/mass spectral, recemization/detection. Chemistry of oxytocin and tryptophan releasing hormone (TRH).

Unit-V

Nucleic acid

Chemical and enzymatic hydrolysis of nucleic acids. Structure of ribonucleic acids (RNA) and deoxyribonucleic acids (DNA) double helix model of DNA and forces responsible for holding it. 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. Principles of Biochemistry, A.L. Lehninger, Worth Publishers.
2. Biochemistry, L. Stryer, W.H. Freeman.
3. Biochemistry, J.David Rwan, Nell Patterson.



**MCH-516: PRACTICAL
INORGANIC CHEMISTRY**

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.

Qualitative Analysis

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

ORGANIC CHEMISTRY

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.

Drug Analysis

PHYSICAL CHEMISTRY

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

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.

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.



SEMESTER II

MCH-521: INORGANIC CHEMISTRY- II

Unit-I

Electronic Spectra and Magnetic Properties of Transition Metal Complexes :

Spectroscopic ground states, correlation. Orgel and Tanabe-Sugano diagrams for transition metal complexes (d_1 - d_9 states), calculations of $10Dq$, B and β parameters, charge transfer spectra, anomalous magnetic moments, Orbital contribution to magnetic moment, magnetic exchange coupling and spin crossover.

Unit-II

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-III

Magnetic properties of transition metal complexes

Type of magnetic bodies, two sources of paramagnetism, orbital and spin effect, Curie equation and Curie-Weiss law, determination of magnetic susceptibility.

Unit-IV

Boranes

Classification, preparation, reactivity, bonding and topology of Boranes, carboranes, metalloboranes and metallocarboranes. Metal Clusters, Chains and Fullerenes Compounds with metal-metal multiple bonds. Isopoly and heteropoly acids and their salts. Fullerenes

Unit-V

Optical rotation dispersion and circular dichroism

Linearly and circularly polarized lights; optical rotation power and circular birefringence, ellipticity and circular dichroism; ORD and Cotton effect, Faraday and Kerr effects; assignment of electronic transitions; application of ORD and CD for the determination (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. Huheey, 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.I. Carlin, Springer Verlag.
6. Comprehensive Coordination Chemistry eds., G. Wilkinson, R.D. Gillars and J.A. Mc Cleverty, Pergamon.



MCH-522: ORGANIC CHEMISTRY-II

Unit-I

Common organic reactions:

Common organic reactions and their mechanisms base catalysed reactions, Stork Enamine reaction, acid catalysed reactions, reactions of carboxylic acids and their derivatives Reagents in organic synthesis and relevant name reactions, organotransition metal reagents, some transition metal organometallic reactions, phosphorus containing reagents, organosulphur compounds, silicon reagents, boron containing reagents.

Unit-II

Electrophilic aromatic substitution:

The arenium ion mechanism, orientation and reactivity, Ipsosubstitution, aromatic rearrangements Aromatic nucleophilic substitution- S_NAr mechanism, S_N1 mechanism, benzyne mechanism. Stereochemistry and mechanism of addition to carbon-carbon multiple bonds, addition reactions of alkenes and alkynes involving electrophiles, Birch reduction, epoxidation of alkenes Addition to carbon-hetero multiple bonds, addition to carbonyl compounds, metal hydride reduction, Meerwein-Ponndorf-Verley reduction, Wittig reaction.

Unit-III

Pericyclic reactions:

Pericyclic reactions: conservation of molecular orbital symmetry, electrocyclic reactions, cycloaddition, sigmatropic rearrangements, the ene reaction, Mobius – Huckel analysis (PMO approach), correlation diagram method. action, kolbe reaction and Hunsdiecker reaction.

UNIT-IV

Molecular orbital symmetry: frontier orbitals of ethylene, 1,3 Butadiene, 1,3,5- Hexatriene, allyl system, classification of pericyclic reactions FMO approach, Woodward- Hoffman correlation diagram method and perturbation of molecular (PMO) approach for the explanation of pericyclic reactions under thermal and photochemical conditions. Electrocyclic Reactions: Conrotatory and disrotatory motions ($4n$) and ($4n+2$), allyl systems and secondary effects. Cycloadditions: Antarafacial and suprafacial additions.

UNIT-V

FMO approach and perturbation of molecular (PMO) approach for the explanation of sigma tropic rearrangements under thermal and photochemical conditions. suprafacial and antarafacial shifts of H Sigmatropic shift involving carbon moieties, retention and inversion of configurations, (3.3) and (5.5) sigmatropic rearrangements detailed treatment of Claisen and Cope rearrangements fluxional tautomerism, aza-Cope rearrangements and Barton reaction.

Books Suggested

1. J. March., Advanced Organic Chemistry: Reactions, Mechanisms and Structure, John Wiley
2. P. S. Kalsi. Stereochemistry, Conformation and Mechanism, New Age International
3. Peter Sykes, A guide book to mechanism in Organic chemistry, Orient-Longmans
4. S. M. Mukherji and S. P. Singh, Reaction Mechanism in Organic Chemistry, Macmillan
5. F. A. Carey and R. J Sundberg, Advanced Organic Chemistry, Part A and B, Plenum



MCH-523: PHYSICAL CHEMISTRY-II

Unit-I

Chemical Dynamics

Chemical kinetics: Empirical rate laws, Arrhenius equation, theories of reaction rates, determination of reaction mechanisms. Kinetics of inorganic mechanisms : Hydrogen- Bromine reaction, Hydrogen- Chlorine Reaction. Decomposition of nitrogen pentaoxide, Decomposition of Ozone. Kinetics of organic Decompositions : Pyrolysis of acetaldehyde, decomposition of ethane.

Unit-II

Surface Chemistry and Catalysis

Adsorption :Gibbs adsorption isotherm, BET equation and estimation of surface area . Micelles:Surface active agents, classification of surface active agents, micellization, critical micellar concentration (CMC), factors affecting the CMC of surfactants, thermodynamics of micellization Concepts of catalysis: Homogenous catalysis, kinetics of enzyme reactions,

Unit –III

Complex and Fast Reaction

Complex Reactions: Opposing reactions, Complex reactions, Parallel reactions , kinetics of free radical polymerization Fast reactions: Experimental techniques for fast reactions viz., flow method, relaxation method, flash photolysis

Unit-IV

Applied Electrochemistry

Electrochemistry: Nernst equation, electrode kinetics, electrical double layer, Debye-Hückel theory. Voltammetry, Current voltage relationship, characteristics of DME, half-wave potential. Amperometric titrations.Corrosion: Introduction to corrosion, forms of corrosion, Corrosion monitoring and prevention Methods.

Unit-V

Non equilibrium thermodynamics

Thermodynamics criteria for non-equilibrium states, entropy production and entropy flow, entropy balance equation for different , irreversible processes (e.g., heat flow ,chemical reaction). Transformation of the generalized fluxes and forces , non equilibrium stationary states.

Books Suggested

1. P.W. Atkins , Physical Chemistry, ELBS.
2. A.K. Chandra, Introduction to Quantum Chemistry, Tata Mc Graw Hill.
3. Ira N. Levine, Quantum Chemistry, Prentice Hall.
4. K.J. Laidler, Chemical Kinetics. McGraw-Hill.



MCH-524: Magnetic Resonance and Mössbauer Spectroscopy

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.

Unit-II

Nuclear Quadrupole Resonance Spectroscopy

Quadrupole nuclei, quadrupole moments, electric field gradient, coupling constant, splitting. Applications. **Carbon-13 NMR Spectroscopy:** General considerations, chemical shift (aliphatic olefinic ,alkyne, aromatic, heteroaromatic and carboynl carbon), coupling constants. **Two dimensional NMR spectroscopy:** COSY, HETCOR, NOESY, DEPT, HMBC and HMQC techniques

Unit-III

Electron Spin Resonance Spectroscopy

Basic principles, Hyperfine coupling, Isotropic and anisotropic hyperfine coupling constnats, spin polarization for atoms and transition metal ions, spin-orbit coupling and significance of gtensors,factors affecting the 'g' value. Zero field splitting and Kramer's degeneracy.. spin Hamiltonian, spin densities and Mc Connell relationship. Applications.

Unit - IV

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 bondingand solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance

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.

Mass Spectrometry : Introduction, ion production EI, CI, FD, ESI and FAB, ion analysis, ion abundance, Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, Mc Lafferty rearrangement , Nitrogen rule, High resolution mass spectrometry.

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.



MCH-525: Computational Methods in Chemistry

This is a theory cum-laboratory course 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. Operating systems with DOS as an example Introduction to UNIX and WINDOWS.

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). 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.

Unit-III

Programming in Chemistry

Developing of small computer codes (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, dihedral angles, etc.

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. Use of Programs Chemcraft, Molden and PovRay.

Unit-V

Internet

Application of internet for chemistry with search engines like google. 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)



MCH-526: PRACTICAL

Inorganic chemistry

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.

Organic chemistry

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 p-bromoaniline. 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

- Determination of the velocity constant, order of the reaction and energy of activation for saponification of ethyl acetate by sodium hydroxide conductometrically.
- Determination of solubility and solubility product of sparingly soluble salts (e.g. $PbSO_4$, $BaSO_4$) conductometrically.
- Determination of the strength of strong and weak acid in a given mixture conductometrically.
- to study of the effect of solvent on the conductance of $AgNO_3$ /acetic acid and to determine the degree of dissociation and equilibrium constant in different solvents and in their mixtures (DMSO, DMF, dioxane, acetone, water) and to test the validity of Debye-Huckel-Onsager theory.

Potentiometry/pH metry

- Determination of the valency of mercurous ions potentiometrically.
- Determination of the strength of strong and weak acids in a given mixture using a potentiometer/pH meter.
- Determination of temperature dependence of EMF of a cell.
- Determination of the formation constant of silver-ammoniacomplex and stoichiometry of the complex potentiometrically.
- Acid-base titration in a non-aqueous media using a pH meter.
- Determination of activity and activity coefficient of electrolytes.

Polarimetry

- Determination of rate constant for hydrolysis/inversion of sugar using a polarimeter.



SEMESTER III
MCH-531: 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, 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 anilides, Photo-Fries rearrangement. Barton reaction. Singlet molecular oxygen reaction. Photochemical formation of smog. Photodegradation of polymers. Photochemistry of vision.

Books Suggested

1. K.K. Rothagi-Mukheriji, Fundamentals of photochemistry, Wiley-Eastern.
2. A Gilbert and J. Baggett, Essentials of Molecular Photochemistry, Blackwell Scientific Publication.
3. N.J. Turro, Molecular Photochemistry, Benjamin.
4. A. Cox and T. Camp, Introductory Photochemistry, McGraw Hill.



MCH-532: Environmental Chemistry

Unit I

Environment

Introduction. Composition of atmosphere, vertical temperature, temperature inversion, heat budget of the earth, atmospheric system, vertical stability atmosphere, Biochemical cycles of C, N, P, S and O. Biodistribution of elements.

Hydrosphere

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

Aquatic pollution – Inorganic, organic, pesticide, agriculture, industrial and sewage, detergents, oil spills and oil pollutants. Water quality parameters – dissolved oxygen, biochemical oxygen demand, solids, metals, content of chloride, sulphate, phosphate, nitrate and microorganisms.

Unit-II

Water quality standards

Analytical methods of measuring BOD, DO, COD, F, Oils, metals (As, Cd, Cr, Hg, Pb, Se etc.), residual chloride and chlorine demand. Purification and treatment of water.

Soils

Composition, micro and macro nutrients, pollution – fertilizers, pesticides, plastics and metals. Waste treatment.

Unit-III

Atmosphere

Chemical composition of atmosphere – particles, ions and radicals and their formation. Chemical and photochemical reactions in atmosphere, smog formation, oxides of N, C, S, O and their effect, pollution by chemicals, petroleum, minerals, chlorofluorohydrocarbons. Green house effect, acid rain, air pollution controls and their chemistry. Analytical methods for measuring air pollutants. Continuous monitoring instruments.

Unit-IV

Industrial Pollution

Cement, sugar, distillery, drug, paper and pulp, thermal power plants, nuclear power plants, metallurgy. Polymers, drugs etc.

Environmental disasters – Chernobyl, Three mile island, Seveso and minamata disasters, Japan tsunami

Unit-V

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.

Books Suggested

1. Environmental Chemistry, S.E. Mahan, Lewis Publishers.
2. Environmental Chemistry, Sharma & Kaur, Krishna Publishers.
3. Environmental Chemistry, A.K. De, Wiley Eastern
4. Environmental Pollution Analysis, S.M. Khopkar, Wiley Eastern



MCH-533: Bioinorganic Chemistry

Unit I

Electron Transfer in Biology

Structure and function of metal of proteins in electron transport processes cytochrome's and ionsulphureproteins, synthetic models. Biological nitrogen fixation, and its mechanism, nitrogenase, Chemical nitrogen fixation.

Unit II

Metalloporphyrins

Structure and optical spectra; heme proteins: magnetic susceptibility, epr and electronic spectra; hemoglobin and myoglobin: molecular structures, thermodynamics and kinetics of oxygenation, electronic and spatial structures, synthetic oxygen carriers, model systems; iron enzymes, peroxidase, catalase and cytochrome P-450.

Unit III

Metalloenzymes

Copper enzymes, superoxide dismutase, cytochrome oxidase and ceruloplasmin; Coenzymes; Molybdenum enzyme: xanthine oxidase; Zinc enzymes: carbonic anhydrase, Vitamin B12 and B12 coenzymes; Iron storage, transport, biomineralization and siderophores, ferritin and transferrins.. **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.

Unit-IV

Enzymes: Introduction, Nomenclature and classification, concept and identification of active site by use of inhibitors, reversible & irreversible inhibition.

Mechanism of Enzyme action: Transition state theory, Orientation and steric effect, acid-base catalysis, covalent catalysis.

Co-Enzyme Chemistry: Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes, Structure and biological functions of coenzyme A.

Enzyme Models : Host guest chemistry, Chiral recognition and catalysis, molecular recognition, crown ethers, micelles synthetic enzyme or synzymes.

Unit-V

Biotechnological Application of enzymes: Large scale production and purification of enzymes, techniques and methods of immobilization of enzyme activity, application of immobilized enzymes, effect of immobilization on Enzyme activity, application of immobilized enzymes. Clinical uses of enzymes, enzyme therapy, enzymes and recombinant DNA technology.

Text Books

1. S. J. Lippard & J. M. Berg. *Principles of Bioorganic Chemistry*, Panima Publ. Corpn. (2005).
2. E.-I. Ochiai. *Bioinorganic Chemistry – An Introduction*, Allyn and Bacon Inc. (1977).
3. M. N. Hughes. *The Inorganic Chemistry of Biological Processes*, Wiley (1981).
4. R.P. Hanzlik. *Inorganic Aspects of Biological and Organic Chemistry*, Academic Press



MCH-534: Basic Medicinal Chemistry

Unit –I

Basic consideration of drugs:-

Classification, nomenclature and metabolism. Development of drugs: Sources, Genesis of drugsmolecularmodification general and special processes: prodrugs (prolongation of action, shortening of action, drug localisation, transport regulation, adjunct to pharmaceutical formulation).Theoretical aspects of drug action: Structure-activity, Physico-chemical parameters andpharmacological activity; drug receptors; mechanism of drug action.

Unit-II

Drugs affecting the central nervous system:-

Sedatives and Hypnotics- Barbiturates (structure-activity-relationship and metabolism); benzodiazepines (structure-activity-relationship and metabolism); miscellaneous compounds. Synthesis of Phenobarbital, hexobarbital nitrazepam and oxazepam.

Unit-III

Anesthetics:- General anesthetics; local anesthetics- Mode of action, structure-activity relationships. Synthesis of methohexital and chloro-procaine.

Analgesics:- Synthetic analgesics, structure-activity-relationships, Antipyretic analgesics, Antinflammatory analgesics, metabolism and mode of action. Opioid analgesics and antagonists.

Unit -IV

Cardiovascular Drugs

Introduction, cardiovascular diseases, drug inhibitors of peripheral sympathetic function central intervention of cardiovascular output, direct acting arteriolar dilators, Synthesis of Amylnitrate, Sorbitrate, Quinidine, Verapamil, Methyldopa, Atenolol, Oxyproprenolol.

Unit-V

Local antiinfective drugs

Introduction and general mode of actions Furazolidone, Nalidixic acid, Ciprofloxacin, Norfloxacin, Dapsone, Aminosalicyclicacid,Isoniazid, Ethambutal, Ethionamide, Fluconazole, Econazole.

Sulpha Drugs:

Classification, structure-activity-relationship, Mode of action. Synthesis: Sulphadiazine, Sulphaisoxazole, Sulphadimethoxine.

Books recommended

1. Robert F.dorge Wilson and Gisvod. Textbook of organic Medicinal and Pharmaceutical Chemistry.
2. Ed. M.E. Wolff, John wiley. Berger's Medicinal Chemistry and drug discovery, Vol-I.
3. J.Faprhop and G.Penzillin. Organic synthesis-concept, method and starting material.
4. Eds.Korolkovas and Burkhattar J.H. John Wiley & sons. Essentials of medicinal Chemistry.
6. Goodman and Gilman's Pharmacological Basis of Therapeutics, McGraw-Hill.
7. Wilson and Gisvold's Text Book of Organic Medicinal and Pharmaceutical Chemistry,



MCH-535: Pharmaceutical Biotechnology

Unit -I

Immunology -Basic Immunology, innate-acquired immunity, antibody structure, immune response against bacterial, viral and parasitic infections, vaccines (classical and modern).

Unit-II

Molecular Biology-DNA, RNA, Basic techniques in genetic engineering, Recombinant DNA methods, restriction enzymes, gene identification and isolation, cloning, screening expression of clone genes using plasmid and phage vector systems, use of recombinant DNA technology, Chemical synthesis of DNA, polymerase chain Reaction (PCR).

Unit-III

Introduction to Nanotechnology: Characteristic scale for quantum phenomena, nanoparticles, nano-clusters, nano-tubes, nanowires and nanodots. Electronic structure: quantum dots, quantum wires and quantum wells, confinement of electrons energy quantization Semiconductor nanocrystals, carbon nanotubes, Nanofluidics and surfaces: liquid structure near solid-liquid interfaces (simple liquids; layering electrolytes: Poisson-Boltzmann equation; Debye Hückel approx.)

Unit -IV

Genomics and Bioinformatics- Introduction, sequencing of genomics, Comparative genomics, gene prediction and Counting, Functional genomics, Bioinformatics- DNA sequencing, Data base and search tools.

Enzymes Technology- Introduction, enzyme activity, enzyme kinetics (Michaelis-Menten equation), immobilized enzymes: methods of immobilization, types of matrices, application and advantages of immobilized enzymes, Bio-sensors, basic principle and their applications.

Unit -V

Fermentation Technology - Detailed aspects of fermentation technology, isolation and screening of microorganism, screening for new products, identification of new metabolites, maintenance of strains, inoculum development, culture media, batch culture, continuous culture, kinetics of culture methods, sterilization, scale up, Downstream processing (DSP), Fermenters, Production of Antibiotics using fermentation technology.

Books Suggested

- 1 S. P. Vyas, Advances in Pharmaceutical Biotechnology, Cbs Publishers & Distributors Pvt. Ltd.
2. S. K. Singh, Biotechnology Campus Books International
3. H.D. Kumar, Modern Concepts of Biotechnology, Vikas Publication House Pvt Ltd .
4. Smith E. John, Biotechnology, Cambridge
5. P. K. Gupta, Biotechnology and Genomics, Rastogi publication.



MPC-536: Practical

(A) Interpretations of Electronic, Infra-red, NMR, ESR, Mössbauer, Mass and XPS spectra

(B) Electronic Spectroscopy

- i. Determination of k_{Pa} 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. Electronic spectral studies for transition metal complexes.

(B) Separation method based on chromatography



SEMESTER-IV

MCH-541: Analytical Chemistry

Unit -I

Statistical tests and Error Analysis:

Accuracy, precision, classification of errors, significant figures and computation, mean deviation and standard deviation, Least square methods, regression coefficient, F-test, t-test and Chi-test.

Sampling and Sample Treatment: Factors involved in effective sampling, good samples; Representative and homogeneous, samples of mixtures.

Unit -II

Spectrochemical

Spectrophotometry: Quantities principles of absorption, instrumentation, single beam, double beam, determination of pKa value of an indicator, detectors, applications.

Atomic spectroscopy: Principles of emissions, atomic emission spectroscopy and flame emission

Unit -III

Electroanalytical Methods:

Theory of electrogravimetric analysis, electrode reactions, over potential, Cyclic voltammetry, Linear-scan voltammetry, Pulse voltammetric methods, stripping methods.

Coulometry : Coulometric titrations and controlled- potential electrolysis.

Unit - IV

Chromatography Techniques :

Classification of chromatographic separations. Theory of chromatography. Applications of chromatographic methods: Adsorption and partition chromatography. Ion exchange chromatography, LC, HPLC and GC, Column matrices, Detectors. Affinity and chiral columns(all type of chromatography)

Unit - V

Separation Techniques :

Principles of analytical separations, liquid-liquid extraction : Distribution coefficient, distribution ratio, solvent extraction of metals, analytical separations, multiple batch extractions, countercurrent distribution., multiple extractions.

Thermal Methods :

Thermal methods of analysis: Principles and instrumentation of TG and DTA. Complementary nature of TG and DTA. Differential scanning calorimeter (DSC). Applications of thermal methods in analytical chemistry.

Books Suggested

1. Gary D.Christian, Analytical Chemistry, John-Wiley
2. H.A.Willard, L.L.Meritt, and J.A.Dean, Instrumental Methods of Analysis, Van Nostrand, New York, 1986.
3. D.A.Skoog & D.M.West Principles of Instrumental Analysis. Holt Rinehart Winston, New York, 1988.
4. K A Robinsons Chemical Analysis, Harper Collins Publishers, New York.
5. A.J. Bard and L. R. Faulkner, Electrochemical Methods: Fundamentals and Applications, John Wiley & Sons: New York.



MCH-542: Chemistry of Natural Products

Unit – I

Terpenoids

Structure determination, stereochemistry, biosynthesis and synthesis of some common terpenoids Citral, α -Terpeneol, Farnesol, Zingiberence, Santonin, Phytol and Abietic acid.

Unit –II

Alkaloids

Structure, stereochemistry, synthesis and biosynthesis of some common alkaloids Ephedrine, Nicotine, Atropine, (+) Conin ,Quinine and Morphine.

Unit –III

[a] Steroids: Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry, Isolation, Structure determination and synthesis of: Cholesterol, Bile acids. Harmons: Androsterone, Testosterone, Ostrone, Progesterone, Aldosterone, Biosynthesis of Steroids.

[B] Prostaglandis

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

Unit -IV

Plant Pigments

Occurrence, nomenclature and general methods of structure determination. Isolation and synthesis of Apigenin, Luteolin Quercetin, Myrcetin, Vitexin, Diadzein, Aureusin, Cyanidn, Hirsutidin, Biosynthesis of flavonoids: Acetate pathway and Shikimic acid pathway. Prophyryns: Structure and synthesis of Haemoglobin and Chlorophyll.

Unit –V

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 Books:

1. Organic Chemistry : Vol. 1 and 2, I. L. Finar, ELBS
2. Organic Chemistry of Natural Products Vol. I and Vol. II, Gurdeep R. Chatwal, Himalaya Publishing House
3. Stereoselective Synthesis: A Practical Approach, M. Norgradi, VCH.
4. Rodd's Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier.
5. Introduction to Flavonoids, B.A. Bohm. Harwood Academic Publishers.
6. New Trends in Natural Product chemistry, Ataur Rahman and M.L. Choudhary, Harwood Academic Publishers.
7. Insecticides of Natural Origin, Sukh Dev, Harwood Academic Publishers.



MCH-543 Research Methodology AND PROJECT WORK

Research methodology-

Types of research (descriptive vs. analytical, fundamental vs. applied, qualitative vs. quantitative, conceptual vs. empirical, empirical vs. simulation based, conclusion oriented vs. decision-oriented, historical vs. a-historical, etc.).Methods of sampling: samples size. Techniques of sampling.

Errors, Determinant, constant and indeterminate. Accuracy and precisionDistribution of random errors. the nature of problem and appropriate methodology, macro-level vs. micro level research, mass observation, questionnaires, personal interviews, group interviews, case studies , small group study.

Statistical Methods :Statistical analysis,data compilation & interpretation, Significance figures and computation rules.Mean, Median and Mode, Standard deviation, Chi- square,t,f and z Test.