P.K.University
Shivpuri (M.P.)

Syllabus

For

M.Sc. CHEMISTRY

(I, II, III & IV Semester Course)

W.E.F. - Session 2023 - 2024

P.K.UNIVERSITY SHIVPURI (M.P.)

P.K.University
Shivpuri (M.P.)

M.Sc. Chemistry Examination Scheme (2023-24)

Semester	Course Code	Title of the Paper	Credit	L	T	P	T-CCE	T-UE	P-CCE	P-UE	Marks
First	MINORCH101	Inorganic Chemistry I	4	4	0	0	40	60	0	0	100
	MORGACH102	Organic Chemistry I	4	4	0	0	40	60	0	0	100
	MPHYSCH103	Physical Chemistry I	4	4	0	0	40	60	0	0	100
	MGROUCH104	Group Theory & Spectroscopy I	4	4	0	0	40	60	0	0	100
	MMATHCH105 MBIOLCH106	a) Mathematics for Chemists* b) Biology for Chemists**	4	4	0	0	40	60	0	0	100
	MLABCCH107	Lab course I	2	0	0	4	0	0	20	30	50
	MLABCCH108	Lab course II	2	0	0	4	0	0	20	30	50
		TOTAL	**24**				**200**	**300**	**40**	**60**	**600**
Second	MINORCH109	Inorganic Chemistry II	4	4	0	0	40	60	0	0	100
	MORGACH110	Organic Chemistry II	4	4	0	0	40	60	0	0	100
	MPHYSCH111	Physical Chemistry II	4	4	0	0	40	60	0	0	100
	MSPECCH112	Spectroscopy II	4	4	0	0	40	60	0	0	100
	MCOMPCH113	Computers for Chemists	4	4	0	0	40	60	0	0	100
	MLABCCH114	Lab course III	2	0	0	4	0	0	20	30	50
	MLABCCH115	Lab course IV	2	0	0	4	0	0	20	30	50
		TOTAL	**24**				**200**	**300**	**40**	**60**	**600**
Third	MAPPLCH201	Applications of Spectroscopy (Inorganic- Chemistry)	4	4	0	0	40	60	0	0	100
	MPHOTCH202	Photochemistry	4	4	0	0	40	60	0	0	100
	MBIOCCH203	Biochemistry	4	4	0	0	40	60	0	0	100
	MSOLICH204	Solid State Chemistry	4	4	0	0	40	60	0	0	100
	MLABCCH205	Lab course V	2	0	0	4	0	0	20	30	50
	MLABCCH206	Lab course VI	2	0	0	4	0	0	20	30	50
		TOTAL	**20**				**160**	**240**	**40**	**60**	**500**
Fourth	MAPPLCH207	Applications of Spectroscopy (Organic- Chemistry)	4	4	0	0	40	60	0	0	100
	MENVICH208	Environmental Chemistry	4	4	0	0	40	60	0	0	100
	MLABCCH209	Lab course VII	2	0	0	4	0	0	20	30	50
	MDISSCH210	Dissertation	10	0	0		0	0	0	250	250
		TOTAL	**20**				**80**	**120**	**20**	**280**	**500**
		Total marks of all semester	**84**				**640**	**960**	**140**	**460**	**2200**

L – Lecture T- Theory P- Practical CCE- Continuous comprehensive Exam UE- University Exam

SEMESTER I

Paper-I

MINORCH101: INORGANIC CHEMISTRY I

Unit-I

Stereochemistry and Bonding in Main Group Compounds :

VSEPR, Walsh diagram (triatomic and penta-**atomic molecules), dπ-pπ 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. Earnshow, Pergamon.
4. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
5. Magnetiochemistry, R.1. Carlin, Springer Verlag.
6. Comprehensive Coordiantion Chemistry eds., G. Wilkinson, R.D. Gillars and J.A. Mc Cleverty,Pergamon.

Paper-II
MORGACH102: ORGANIC CHEMISTRY I

Unit-I

Nature of Bonding in Organic Molecules

Delocalized chemical bonding-conjugation, cross conjugation, resonance hyperconjugation, bonding in fullerences, 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 complexs 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 ertythro 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 chirallity 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, phenomium ions, norborynl 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. 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 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.

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Paper-III
MPHYSCH103: 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, eigenfucntions 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 fo 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 Chemistyry, 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.

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Paper-IV
MGROUCH104: Group Theory & Spectroscopy I

Unit-I
Symmetry and Group theory in Chemistry

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

Unit-II
Microwave Spectroscopy

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

Unit-III
Infrared-Spectroscopy

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

Unit-IV
Raman Spectroscopy

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

Unit-V
Electronic Spectroscopy
Molecular Spectroscopy

Energy levels, molecular orbitals, vibronic transitions, vibrational progressions and geometry of the excited states, Franck-Condon principle, electronic spectra of polyatomic molecules. Emission spectra; radio-active and non-radioactive decay, internal conversion, spectra of transition metal complexes, charge-transfer spectra.

Photoelectron Spectroscopy

Basic principles; photo-electric effect, ionization process, Koopman's theorem.

Photoelectron spectra of simple molecules, ESCA, chemical information from ESCA. Auger electron spectroscopy-basic idea.

Books suggested

1. Modern Spectroscopy, J.M. Hollas, John Viley.
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, IBH-Oxford.
9. Introduction to Photoelectron Spectroscopy, P.K. Ghosh, John Wiley.
10. Introduction to Magnetic Resonance. A Carrington and A.D. Maclachalan, Harper & Row.

Paper-V
MMATHCH105 MATHEMATICS FOR CHEMISTS

(For students without Mathematics in B.Sc.)

Unit-I

Vectors

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

Matrix Algebra

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

Unit-II

Differential Calculus

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

Unit-III

Integral calculus

Basic rules for integration, integration by parts, partial fractions and substitution. Reduction formulae, applications of integral calculus.

Functions of several variables, partial differentiation, co-ordinate transformations (e.g. Cartesian to spherical polar).

Unit-IV

Elementary Differential equations

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

Unit-V

Permutation and Probability

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

Book Suggested

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

Paper-V
MBIOLCH106 BIOLOGY FOR CHEMISTS

(For students without Biology in B.Sc.)

Unit-I

Cell Structure and Functions

Structure prokaryotic and eukaryotic cells, intracellular organelles and their functions, comparison of plant and animal cells. Ove4rview and their functions, comparison of plant and animal cells. Overview of metabolic processes-catabolism and anabolism. ATP - the biological energy currency. Origin of life-unique properties of carbon chemical evolution and rise of living systems. Introduction to bio-molecules, building blocks of bio-macromolecules.

Unit-II

Carbohydrates

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

Unit-III

Lipid

Fatty acids, essential fatty acids, structure and function of triacylglycerols, glycerophospholipids, sphingolipids, cholesterol, bile acids, prostaglandins. Liproproteins-compositiion 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-b-oxidation of fatty acids.

Unit-IV

Amino-acids, Peptides and Proteins

Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing. Secondary structure of proteins. force responsible for holding of secondary structures. a-helix, -b-sheets, super secondary structure, triple helix structure of collagen. Tertiary structure of protein-folding and domina structure. Quaternary structure. Amino acid metabolism-degradation and biosynthesis of amino acids, sequence determination : chemical/enzymatic/mass spectral, racemization/detection. Chemistry of oxytocin and tryptophan releasing hormone (TRH).

Unit-V

Nucleic Acids

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

Book Suggested

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

PRACTICAL

(Duration: 6-8 hrs in each branch)
Practical examination shall be conducted separately for each branch.

Inorganic Chemistry

Quantitative and quantitative Analysis	10
Chromatography	10
Preparation	10
Record	10
Viva Voce	10

Qualitative and Quantitative Analysis

a. Less common metal ions : Ti, Mo, w, Ti, Zr, Th, V, U (two metal ions in cationic/anionic forms).
b. Insoluble- Oxides, sulphates and halides.
c. Separation and determination of two metal ions Cu-Ni, Ni-Zn, Cu-Fe etc. involving volumetric and gravimetric methods.

Chromatography

Separation of cations and anions by Paper Chromatography.

Preparations

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

1. $VO(acac)_2$
2. $TiO(C_9H_8NO)_2H_2O$
3. $cis\text{-}K[Cr(C_2O_4)_2(H_2O)_2]$
4. $Na[Cr(NH_3)_2(SCN)_4]$
5. $Ni(acac)_2$
6. $K_3[Fe(C_2O_4)_3]$
7. Prussian Blue, Turnbull's Blue.

Organic Chemistry

Qualitative Analysis	15
Organic Synthesis	15
Record	10
Viva Voce	10

Qualitative Analysis

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

Organic Synthesis

Acetylation : Acetylation of cholesterol and separation of cholesteryl acetate by column chromatography. Oxidation : Adipic acid by chromic acid oxidation of cyclothexaneol Grignard reaction : Synthesis of triphenylmethanol from benzoic acid The Products may be Characterized by Spectral Techniques.

Physical Chemistry

Error Analysis and Statistical Data Analysis	10
Chemical Kinetics	10
Solution	10
Record	10
Viva Voce	10

Error Analysis and Statistical Data Analysis

Errors, types of errors, minimization of errors distribution curves precision, accuracy and combination; statistical treatment for erro analysis, student 't test, null hypothesis, rejection criteria. F & Q test; linear regression analysis, curve fitting. Calibration of volumetric apparatus, burette, piette and standard flask. Adsorption To study surface tension-concentration relationship for solutions (Gibbs equation). Phase Equilibria

i. Determination of congruent composition and temperatur5e of a binary system (e.g. diphenylamine-benzophenone system).
ii. Determination of glass transition temperature of given salt (e.g., CaCl2) conductometrically.
iii. To construct the phase diagram for three component system (e.g. chloroform-acetic acid-water).

Chemical Kinetics

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

Solution

Determination of molecular weight of non-volatile and electrolyte/electrolyte by cryoscopic method and to determine the activity coefficient of an electrolyte.

Determination of the degree of dissociation of weak electrolyte and to study the deviation from ideal behaviour that occurs with a strong electrolyte.

Books Suggested

1. Vogel's Textbook of Quantitative Analysis, revised, J. Bassett, R.C. Denney, G.H. Jeffery and J. Mendham, ELBS.
2. Synthesis and Characterization of Inorganic Compounds, W.L. Jolly. Prentice Hall.

3. Experiments and Techniques in Organic Chemistry, D.P. Pasto, C. Johnson and M. Miller, Prentice Hall.
4. Macroscale and Microscale Organic Experiments, K.L. Williamson, D.C. Health.
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. Experimental Physical Chemistry, R.C. Das and B. Behera, Tata McGraw Hill.

SEMESTER II

Paper-VI
MINORCH109: 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 dioxgen 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, elipticity and circular dichroism; ORD and Cotton effect, Faraday and Kerr effects; Assignment of electronic transitions; applications of ORD and CD for the determination of (i) absolute configuration of complexes and (ii) isomerism due to non-planarity of chelate rings.

Books Suggested :

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

Paper-VII
MORGACH110: 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, Vilsmeir reactiion, Gatterman-Koch reaction.

Aromatic Nucleophilci Substitution

The SNAr SN1, benzyne and SN1 mechanism, Reactivity effect of substrate structure, leaving group and attacking nucleophile. The Von Richte. 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 carboyxlic acids, auto-oxidation, 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 bounds, 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 usaturated carbonyl compounds. Witting 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 E1 cB mechanisms and their spectrum. Orientation of the double bond. Reactitivty-effects of substrate structures, attacking base, the leavign group and the medium. Mechanism and orientation in pyrolytic elimination.

Unit-V

Pericyelic Reactions

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of periycyclic 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 cheleotrpic 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

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

Paper-VIII
MPHYSCH111: 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. Dyamic chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogen-bromine and hydrogen-chlorine reactions) and homogenous catalysis, kinetics of enzyme reactions, general features fo fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis and the nuclear magnetic resonance method, dynamics of unimolecular reactiosn (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, solublization, 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 Theromodynamics

Thermodynamic criteria for non-equilibrium states, entropy production and entropy flow, entropy balance equations for different irreversible processes (e.g., heat flow, chemical reaction etc.) transformations of the generalized fluxes and forces, non

equilibrium stationary states, phenomenological equations, microscopic reversibility and Onsager's reciprocity relations, electrokinetic phenomena, diffusion, electric conduction.

Unit-V

Electrochemistry

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

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

Books Suggested

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

Paper-IX

MSPECCH112: Spectroscopy II and Diffraction Methods

Unit-I

Nuclear Magnetic Resonance Spectroscopy

Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurements, factors, influencing chemical shift, deshielding, spin -spin interactions, factors influencing coupling constant "j" Classification (AXB, AMX, ABC, A2B2 etc.). spin decoupling; basic ideas about instrument, NMR studies of nuclei other than protin-13C, 19F and 31P. FT NMR, advantages of FT NMR.

Unit II

Nuclear Quadrupole Resonance Spectroscopy

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

Unit-III

Electron Spin Resonance Spectroscopy

Basic principles, zero field splitting and Kramer's degeneracy, factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densities and Mc Connell relationship, measurement techniques, applications.

Unit-IV

X-ray Diffraction

Bragg condition, Miller indices, Laue Method, Bragg method, Debye Scherrer method of X-ray structural analysis of crystals, index reflections, identification of unit cells from systematic absences in diffraction pattern, Structure of simple lattices and X-ray intensities, structure factor and its relation to intensity and electron density, phase problem. Description of the procedure for an X-ray structure analysis, absolute configuration of molecules.

Unit-V

Electron Diffraction

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

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

Books suggested

11. Modern Spectroscopy, J.M. Hollas, John Viley.
12. Applied Electron Spectroscopy for chemical analysis d. H. Windawi and F.L. Ho, Wiley Interscience.

13. NMR, NQR, EPr and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Harwood.
14. Physical Methods in Chemistry, R.S. Drago, Saunders College.
15. Chemical Applications of Group Theory, F.A. Cotton.
16. Introduction to Molecular Spectroscopy, G.M. Barrow, Mc Graw Hill.
17. Basic Principles of Spectroscopy, R. Chang, Mc Graw Hill.
18. Theory and Application of UV Spectroscopy, H.H. Jaffe and M. Orchin, IBH-Oxford.
19. Introduction to Photoelectron Spectroscopy, P.K. Ghosh, John Wiley.
20. Introduction to Magnetic Resonance. A Carrington and A.D. Maclachalan, harper & Row.

Paper-X

MCOMPCH113: COMPUTERS FOR CHEMISTS

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

Unit-I

Introduction to computers and Computing

Basic structure and functioning of computer with a PC as illustrative example. Memory I/O devices. Secondary storage Computer languages. Operating systems with DOS as an example Introduction to UNIX and WINDOWS. Principles of programming Alogrithms and flow-charts.

Unit-II

Computer Programming in FORTRAN/C/BASIC

(the language features are listed here with reference to FORTRAN. The instructor may choose another language such as BASIC or C the features may be replaced appropriately). Elements of the computer language. Constants and variables. Operations and symbols Expressions. Arithmetic assignment statement. Input and output Format statement. Termination statements. Branching statements as IF or GO TO statement. LOGICAL variables. Double precession variables. Subscripted variables and DIMENSION. DO statement FUNCTION AND SUBROUTINE. COMMON and DATA statement (Student learn the programming logic and these language feature by hands on experience on a personal computer from the beginning of this topic.)

Unit-III

Programming in Chemistry

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

Unit-IV

Use of Computer programmes

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

Unit V

Internet

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

Book Suggested :

Fundamentals of Computer : V. Rajaraman (Prentice Hall)
Computers in Chemistry : K.V. Raman (Tata Mc Graw Hill)
Computer Programming in FORTRAN IV-V Rajaraman (Prentice Hall)

PRACTICAL

(Duration: 6-8 hrs in each branch)
Practical examination shall be conducted separately for each branch.

Inorganic Chemistry

Chromatography	15
Preparation	15
Record	10
Viva Voce	10

Chromatography Separation of cations and anions by

Column Chromatography : Ion exchange.

Preparations

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

1. $[Co(NH_3)_6]\ [Co(NO_2)_6]$
2. cis-$[Co(trien)\ (NO_2)_2]Cl.H_2O$
3. $Hg[Co(SCN)_4]$
4. $[Co(Py)_2Cl_2]$
5. $[Ni(NH_3)_6]Cl_2$
6. $Ni(dmg)_2$
7. $[Cu(NH_3)_4]SO_4H_2O$

Organic Chemistry

Organic Synthesis	15
Quantitative Analysis	15
Record	10
Viva Voce	10

Organic Synthesis

Aldol condensation Dibenzal acetone from benzaldehyde. Sandmeyer reactuion : p-Chlorotoluene from p-toluidine. Acetoacetic ester Condensation : Synthesis of ethyl-n-butylacetoacetate 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 sustitutions : 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.

Conductometry	10
Potentiometry/pH metry	10
Polarimetry	10
Record	10
Viva Voce	10

Determination of DO, COD and BOD of water sample.

Physical Chemistry

Conductometry

i. Determination of the velocity constant, order of the reaction and energy of activation for saponification of ethyl acetate by sodium hydroxide conductometrically.
ii. Determination of solubility and solubility product of sparingly soluble salts (e.g. $PbSO_4$, $BaSO_4$) conductometrically.
iii. Determination of the strength of strong and weak acid in a given mixture conductometrically.
iv. to study of the effect of solvent on the conductance of $AgNO_3$/acetic acid and to determine the degree of dissociation and equilibirum constant in different solvents and in their mixtures (DMSO, DMF, dioxane, acetone, water) and to test the validity of Debye-Huckel-Onsager theory.
v. Determination of the activity coefficient of zinc ions in the solution of 0.002 M zinc sulphate using Debye Huckel's limiting law.

Potentiometry/pH metry

1. Determination of strengths of halides in a mixture potentiometrically.
2. Determination of the valency of mercurous ions potentiometrically.
3. Determination of the strength of strong and weak acids in a given mixture using a potentiometer/pH meter.
4. Determination of temperature dependence of EMF of a cell.
5. Determination of the formation constant of silver-ammonia complex and stoichiometry of the complex potentiometrically.
6. Acid-base titration in a non-aqueous media using a pH meter.
7. Determination of activity and activity coefficient of electrolytes.
8.

9. Determination of the dissociation constant of acetic acid in DMSO. DMF, acetone and dioxane by titrating it with KOH.
10. Determination of the dissociation constant of monobasic/dibasic acid by Albert-Sderjeant method.
11. Determination of thermodynamic constants, DG, DS, and DH for the reaction by e.m.f. method. Zn + H2SO4 -> ZnSO4 + 2 H

Polarimetry

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

Books Suggested

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

SEMESTER III

Paper-XI
MAPPLCH201: APPLICATION OF SPECTROSCOPY
(Inorganic Chemistry)

Unit-I

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 particularly for the study of active sites of metalloproteins.

Unit II

Electron Spin Resonance Spectroscopy

Hyperfine coupling, spin polarization for atoms and transition metal ions, spin-orbit coupling and significance of g-tensors, application to transition metal complexes (having one unpaired electron) including biological systems and to inorganic free radicals.

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

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 inequivalent MB atoms.

Unit V

Electronic Spectroscopy:

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

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.

Paper XII
MPHOTCH202: 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, b,g unsaturated and a, b unsaturated compounds, cyclohexadienones. Intermolecular cyloaddition reactions-dimerisations and oxetane formation.

Unit V

Miscellaneous Photochemical Reactions.

Photo-Fries reactions of annelid's, Photo-Fries rearrangement. Barton reaction. Singlet molecular Oxygen reaction. Photochemical formation of smog. Photodegration 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.

Paper-XIII
MBIOCCH203: BIOCHEMISTRY

Unit I

Metal Ions in Biological Systems

Bulk and trace metals with special reference to Na, K, Mg, Ca, Fe, Cu, Zn, Co, and K+/Na+ pump.

Bioenergetics and ATP Cycle.

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

Transport and Storage of Dioxygen

Heam proteins and oxygen uptake structure and function of haemoglobin's, mygolobin, haemocyanms and hemerythrin, model synthetic complexes of iron, cobalt and copper.

Unit II

Electron Transfer in Biology

Structure and function of metal of proteins in electron transport processes cytochrome's and ion-sulphure proteins, synthetic models.

Nitrogen fixation

Biological nitrogen fixation, and its mechanism, nitrogenase, Chemical nitrogen fixation.

Unit III

Enzymes

Introduction and historical perspective, chemical and biological catalysis, remarkable properties of enzymes like catalytic power, specificity and regulation. Nomenclature and classification, extraction and purification. Fischer's lock and key and Koshalnd's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site-directed mutagenesis. Enzyme kinetics, Michael's-Menten and Lineweaver Burk plots, reversible and irreversible inhibition.

Mechanism of Enzyme Action

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

Kinds of Reactions Catalysed by Enzymes

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

Unit IV

Co-Enzyme Chemistry

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

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

Biotechnological Applications of Enzymes

large-scale prodcution and purification of enzymes, techniques and methods of immobilization of enzymes, effect of immobilization on enzyme activity, application of immobilized enzymes, use of enzymes in food and drink industry-brewing and cheese-making, syrups from cron starch, enzymes as targets for drug design. Clinical uses of enzymes, enzyme therapy, enzymes and recombinant DNA Technology.

Unit V

Biological Cell and its Constituents

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

Bioenergetics

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

Biopolymer Interactions

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

Cell Membrane and Transport of Ions

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

Book Suggested

1. Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.
2. Bioinorganic Chemistry, 1. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, University Science Books.
3. Inorganic biochemistry vol. I and II ed. G.L. Eichhorn, Elsever.
4. Progress in Inorganic Chemistry, Vol 18 and 38 ed J.J. Lippard, Wiley.
5. Bioorganic Chemistry : A chemical Approach to Enzyme Action, Hermann Dugas and C. Penny, Springer Verlag.
6. Understanding Enzymes, Trevor Palmer, Prentice Hall.
7. Enzyme Chemistry : Impact and applications, Ed. Collin J suckling, chemistry.
8. Enzyme Mechanisms Ed. M.I. Page and A Williams, Royal Society of Chemistry.
9. Fundamentals of Enzymology, N.C. Price and L. Stevens. Oxford University Press.
10. Immobilized Enzymes : An Introduction and Applications in Biotechnology, Michael ID. Trevan, Hohn Wiley.
11. Enzymatic Reaction Mechanisms. C. Walsh. W.H. Freeman.
12. Enzyme Structure and Mechanism, A Fersht, W.H. Freeman
13. Biochemistry : The Chemical Reactions of Living Cells, D.E. Metzler, Academic Press.

Paper XIV
MSOLICH204: SOLID STATE CHEMISTRY

Unit I

Solid State Reactions

General principles, experimental procedure, co-precipitation as a precursory 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 detects and Frenkel defects. Thermodynamics of Schottky and Frenkel defect formation, colour centres, non-stoichiometry and defects.

Unit III

Electronic Properties and Band Theory

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

Unit 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.

Practical

(Duration: 6-8 hrs in each branch)

Practical examination shall be conducted separately for each branch.

Inorganic Chemistry

Quantitative determinations of a three component mixture	15
Chromatographic Separations	15
Record	10
Viva Voice	10

Quantitative determinations of a three component mixture :

One Volumetrically and two gravimetrically

a. Cu+2, Ni+2, Zn+2
b. Cu+2, Ni+2, Ng+2

Chromatographic Separations

a. Cadmium and zinc
b. Zinc and magnesium.
c. Thin-layer chromatography-separation of nickel, manganese, cobalt and zinc. Determination of Rf values.

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

Multi-step Synthesis of Organic Compounds

The exercise should illustrate the use of organic reagents and may involve purification of the products by chromatographic techniques. Photochemical reaction Benzophenone -> Benzpinacol _> Benzpinacolone Beckmann rearrangement : Benzanilide from benzene Benzene -> Benzophenone -> Benzphenone 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 (+) ehtyl-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.

Paper Chromatography

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

Spectroscopy

i. Determination of PKa of an indicator (e.g. methyl red) in (a) aqueous and (b) micellar media.

ii. Determination of stoichiometry and stability constant of Ferricisothicoyanation complex ion in solution.
iii. Determination of rate constant of alkaline bleaching of Malachite green and effect of ionic strength on the rate of reaction.

Chemical Kinetics

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

Books Suggested

1. Inorganic Experimens, 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 Nostrad.
4. The systematic Identification of Organic Compounds, R.L. Shriner and D.Y. curlin.

SEMESTER IV

Paper-XVII
MAPPLCH207: APPLICATION OF SPECTROSCOPY
(Organic Chemistry)

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.

Optical Rotatory Dispersion (ORD) and Circular Dichromium (CD)

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

Unit-III

Nuclear Magnetic Resonance Spectroscopy

General introduction and definition, chemical shift, spin-spin interaction, shielding mechanism, mechanism of measurement, chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides & mercapto), chemical exchange, effect of deuteration, complex spinspin interaction between two, three, four and five nuclei (first order spectra), Stereochemistry, hindered rotation, Karplus curve-variation of coupling constant with disordered angle. Simplification of complex spectranuclear magnetic double resonance, NMR shift reagents, solvent effects. Fourier transform technique, nuclear overhauser effect (NOE).

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, IONEPT, APT and INADEQUATE 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. Example of mass spectral fragmentation of organic compounds with respect to their structure determination.

Book Suggested

13. Physical Methods for Chemistry, R.S. Drago, Saunders Compnay.
14. Structural Methods in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H. Rankin and S. Cradock, ELBS.
15. Infrared and Raman Spectral : Inorganic and Coordination Compounds K. Nakamoto, Wiley.
16. Progress in Inorganic Chemistry vol., 8, ed., F.A. Cotton, vol., 15 ed. S.J. Lippard, Wiley.
17. Transition Metal Chemistry ed. R.L. Carlin vol. 3 dekker.
18. Inorganic Electronic Spectroscopy, A.P.B. Lever, Elsevier.
19. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, .V. Parish, Ellis Haywood.
20. Practical NMR Spectroscopy, M.L. Martin. J.J. Deepish and G.J. Martin, Heyden.
21. Spectrometric Identification of Organic Compounds, R.M. Silverstein, G.C. Bassler adn T.C. Morrill, John Wiley.
22. Introduction to NMR spectroscopy, R.J. Abraham, J. Fisher and P. Loftus, Wiley.
23. Application of Spectroscopy of Organic Compounds, J.R. Dyer Prentice Hall.
24. Spectroscopic Methods in Organic Chemistry D.H. Williams, I. Fleming, Tata McGraw-Hill.

Paper XVIII
MENVICH208: ENVIRONMENTAL CHEMISTRY

Unit-I

Atmosphere

Atmospheric layers, Vertical temperature profile, heat/radiation budget of the earth atmosphere systems. Properties of troposphere, thermodynamic derivation of lapse rate. Temperature inversion. Calculation of Global mean temperature of the atmosphere. Pressure variation in atmosphere and scale height. Biogeochemical cycles of carbon, nitrogen, sulphure, phosphorus oxygen. Residence times.

Atmospheric Chemistry

Sources of trace atmospheric constituents : nitrogen oxides, sulphure dioxide and other sulphure compounds, carbon oxides, chlorofluorocarbons and other halogen compounds, methane and other hydrocarbons.

Tropospheric Photochemistry

Mechanism of Photochemical decomposition of NO2 and formation of ozone. Formation of oxygen atoms, hydroxyl, hydroperoxy and organic radicals and hydrogen peroxide. Reactions of hydroxyl radicals with methane and other organic compounds. Reaction of OH radicals with SO2 and NO2. Formation of Nitrate radical and its reactions.

Photochemical smog meteorological conditions and chemistry of its formation.

Unit-II

Air Pollution

Air pollutants and their classifications. Aerosols-sources, size distribution and effect on visibility, climate and health.

Acid Rain

Definition, Acid rain precursors and their aqueous and gas phase atmospheric Oxidation reactions. Damaging effects on aquatic life, plants, buildings and health. Monitoring of SO2 and NOx. Acid rain control strategies.

Stratospheric Ozone Depletion

Mechanism of Ozone formation, Mechanism of catalytic Ozone depletion, Discovery of Antarctic Ozone hole and Role of chemistry and meteorology. Control Strategies.

Green House Effect

Terrestrial and solar radiation Spectra, Major green house gases and their sources and Global warming potentials. Climate change and consequences.

Urban Air Pollution

Exhaust emissions, damaging effects of carbon monoxide. Monitoring of CO. Control strategies.

Unit-III

Aquatic Chemistry and Water Pollution

Redox chemistry in natural waters. Dissolved oxygen, biological oxygen demand, chemical oxygen demand, determination of DO, BOD and COD. Aerobic and anaerobic reactions of organic sulphure and nitrogen compounds in water acid-base chemistry of fresh water and sea water. Aluminum, nitrate and fluoride in water. Petrification.

Sources of water pollution. Treatment of waste and sewage. Purification of drinking water, techniques of purification and disinfection.

Unit IV

Environmental Toxicology

Toxic heavy metals : Mercury, lead, arsenic and cadmium. Causes of toxicity. Bioaccumulation, sources of heavy metals. Chemical speciation of Hg, Pb, As, and Cd. Biochemical and damaging effects.

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

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

Polynuclear Aromatic Hydrocarbons : Source, structures and as pollutants.

Unit-V

Soil and Environmental Disasters

Soil composition, micro and macronutrients, soil pollution by fertilizers, plastic an metals. Methods of re-mediation of soil. Bhopal gas tragedy, Chernobyl, three mile island, Minimtata Disease, Sevoso (Italy), London smog.

Books Suggested

1. Environmental Chemistry, Colin Baird, W.H. Freeman Co. New York, 1998.
2. Chemistry of Atmospheres, R.P. Wayne, Oxford.
3. Environment Chemistry, A.K. De, Wiley Eastern, 2004.
4. Environmental Chemistry, S.E. Manahan, Lewis Publishers.
5. Introduction to atmospheric Chemistry, P.V. Hobbs, Cambridge.

PRACTICAL

Preparation

Preparation of selected inorganic compounds and their study by IR, electronic spectra, and magnetic susceptibility measurements. Handling of air and moisture sensitive compounds involving vacuum lines. Selection can be made from the following :

1. Sodium amide. Inorg. Synth., 1946, 2, 128.
2. Atomic absorption analysis of Mg and Ca.
3. Synthesis of trichlorodiphenylantimony (V) hydrate. Inorg. Synths., 1985, 23, 194
4. Sodium tetrathionate $Na_2S_4O_6$.
5. Metal complex of dimethyl sulfoxide : $CuCl_2.2DMSO$ J.Chem. Educ., 1982, 59, 57.
6. Synthesis of metal acethylacetonate : Inorg. Synths, 1957, 5, 130, 1963, 1, 183.
7. Cis and Trns $[Co(en)_2CI_2]^+$.
8. Determination of Cr (III) complex. $[Cr(H_2O)_6]NO_3.3HO$,. Inorg. synths., 1972, 13, 184.
9. Preparation and use of Ferrocene. J. Chem. Edu. 1966, 43, 73; 1976, 53, 730.
10. Preparation of [Co(phenathroline-5,6 quinone)].

Spectrophotometric Determinations

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

Flame Photometric Determinations

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

Extraction of Organic Compounds from Natural Sources

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 Rf 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.

Spectroscopy

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

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

Thermodynamics

i. Determination of partial molar volume of solute (e.g. KCl) and solvent in a binary mixture.

ii. Determination of the temperature dependence of the solubility of a compound in two solvents having similar intromolecular in tetractions (benzoic acid in water and in DMSO water mixture and calculate the partial molar heat of solution.

Polarography

i. Identification and estimation of metal ions such as Cd+2, Pb+2, Zn+2, and i+2 etc. polarographically.
ii. Study of a metal ligand complex polarographically (using Lingane's Method).

Books Suggested

5. Inorganic Experimens, J. Derek Woolings, VCH.
6. Microscale Inorganic Chemistry, Z. Szafran, R.M, Pike and M.M. Singh, Wiley.
7. Practical Inorganic Chemistry, G. Marr and B. W. Rockett, Van Nostrad.
8. The systematic Identification of Organic Compounds, R.L. Shriner and D.Y. curlin.