



2021-2022

PT. RAVISHANKAR SHUKLA UNIVERSITY
RAIPUR
CHHATTISGARH

SYLLABUS

CODE 321 & 322

M.Sc.CHEMISTRY

SEMESTER EXAMINATION



2021-2022

PT.RAVISHANKAR SHUKLA UNIVERSITY
RAIPUR-492010,CHHATTISGARH

EXAMINATION SCHEME

M.Sc. examination will be conducted in four SEMESTERS. Each semester exam shall consist of FOUR THEORY PAPERS AND TWO LAB COURSES.

SEMESTER –I (20 CREDIT)

THEORY (16 CREDIT)

PAPER Number and Paper Code	COURSE	CREDIT	DURATION	INTERNAL ASSESSMENT	THEORY MARKS	TOTAL MARKS
1 (CH–101)	GROUP THEORY AND CHEMISTRY OF METAL COMPLEXES	4	4 Hrs	20	80	100
2 (CH–102)	CONCEPTS IN ORGANIC CHEMISTRY	4	4 Hrs	20	80	100
3 (CH–103)	QUANTUM CHEMISTRY, THERMODYNAMICS AND CHEMICAL DYNAMICS - I	4	4 Hrs	20	80	100
4 (CH–104)	THEORY AND APPLICATIONS OF SPECTROSCOPY-I	4	4 Hrs	20	80	100

PRACTICAL (4 CREDIT)

PAPER Number and paper code	COURSE	CREDIT	DURATION	MARKS
5 (CH–105)	Lab Course - I	2	8 Hrs	100
6 (CH–106)	Lab Course - II	2	8 Hrs	100

SEMESTER –II (20 CREDIT)

THEORY (16 CREDIT)

PAPER Number and paper code	COURSE	CREDIT	DURATION	INTERNAL ASSESSMENT	THEORY MARKS	TOTAL MARKS
1 (CH–201)	TRANSITION METAL COMPLEXES	4	4 Hrs	20	80	100

2 (CH-202)	REACTION MECHANISMS	4	4 Hrs	20	80	100
3 (CH-203)	QUANTUM CHEMISTRY, THERMODYNAMICS AND CHEMICAL DYNAMICS - II	4	4 Hrs	20	80	100
4 (CH-204)	THEORY AND OF APPLICATIONS SPECTROSCOPY-II	4	4 Hrs	20	80	100

PRACTICAL (4 CREDIT)

PAPER Number and paper code	COURSE	CREDIT	DURATION	MARKS
5 (CH-205)	Lab Course - III	2	8 Hrs.	100
6 (CH-206)	Lab Course - IV	2	8 Hrs.	100

SEMESTER –III (20 CREDIT)**THEORY (16 CREDIT)**

PAPER Number and paper code	COURSE	CREDIT	DURATION	INTERNAL ASSESSMENT	THEORY MARKS	TOTAL MARKS
1 (CH-301)	RESONANCE SPECTROSCOPY, PHOTOCHEMISTRY AND ORGANOCATALYSIS	4	4 Hrs	20	80	100
2 (CH-302)	CHEMISTRY OF BIOMOLECULES	4	4 Hrs	20	80	100
3 (CH-303)	CATALYSIS, SOLID STATE AND SURFACE CHEMISTRY	4	4 Hrs	20	80	100
4 (CH-304)	ANALYTICAL TECHNIQUES AND DATA ANALYSIS	4	4 Hrs	20	80	100

PRACTICAL (4 CREDIT)

PAPER Number and paper code	COURSE	CREDIT	DURATION	MARKS
5 (CH-305)	Lab Course - V	2	8 Hrs.	100
6 (CH-306)	Lab Course - VI	2	8 Hrs.	100

SEMESTER –IV (20 CREDIT)**THEORY (16 CREDIT)**

PAPER Number and paper code	COURSE	CREDIT	DURATION	INTERNAL ASSESSMENT	THEORY MARKS	TOTAL MARKS
1 (CH- 401)	INSTRUMENTAL METHODS OF ANALYSIS	4	4 Hrs	20	80	100
2 (CH- 402)	NATURAL PRODUCTS AND MEDICINAL CHEMISTRY	4	4 Hrs	20	80	100
3 (CH- 403)	MATERIAL AND NUCLEAR CHEMISTRY	4	4 Hrs	20	80	100

4 (CH-404)	ENVIRONMENTAL & APPLIED CHEMICAL							
	ANALYSIS	4		4 Hrs	20	80		100.

OR
OPTIONAL PAPERS

CH-404 a	MEDICINAL CHEMISTRY
404 b	CHEMISTRY OF SURFACTANTS
404 c	CHEMISTRY AND APPLICATION OF PESTICIDES
	MOLECULAR SYMMETRY, COORDINATION AND ORGANOMETALLIC 404 d CHEMISTRY
404 e	NANOCHEMISTRY
404 f	CHEMISTRY OF NATURAL PRODUCTS
404 g	POLYMERS
404 h	FORENSIC CHEMISTRY

PRACTICAL (4 CREDIT)

PAPER Number and paper code	COURSE	CREDIT	DURATION	MARKS
5 (CH-405)	Lab course VII or seminar	2	8 Hrs	100
6 (CH-406)	Lab course VIII	2	8 Hrs	100
Or				
7 (CH-407)	Project Work	2	-----	100
8 (CH-408)	Seminar	2	-----	100

SCHEME FOR LABORATORY EXPERIMENT EXAMINATION

EXPERIMENT	MARKS
Object-1	30
Object -2	30
Viva-voce	20
Sessional Marks	20
TOTAL MARKS	100

FIRST SEMESTER

PAPER NO 1. CH –101

GROUP THEORY AND CHEMISTRY OF METAL COMPLEXES

Max. Marks 80

UNIT - I

SYMMETRY AND GROUP THEORY IN CHEMISTRY: Symmetry elements and symmetry operation, definitions of group, subgroup, relation between orders of a finite group and its subgroup. Conjugacy relation and classes. Point symmetry group. Schoenflies

symbols, representations of groups by matrices (representation for the C_n , C_{nv} , C_{nh} , D_{nh} , etc. groups to be worked out explicitly). Character of a representation. The great orthogonality theorem (without proof) and its importance. Character tables and their use in spectroscopy.

UNIT - II

- A. **METAL-LIGAND BONDING:** Limitation of crystal field theory, molecular orbital theory, octahedral, tetrahedral and square planar complexes, bonding and molecular orbital theory.
- B. **METAL-COMPLEXES:** Metal carbonyls, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls; preparation, bonding, structure and important reactions of transition metal nitrosyl, dinitrogen and dioxygen complexes; tertiary phosphine as ligand.

UNIT –III

- A. **METAL-LIGAND EQUILIBRA IN SOLUTION:** Stepwise and overall formation constants and their interaction, trends in stepwise constants, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, chelate effect and its thermodynamic origin, determination of binary formation constants by pH-metry and spectrophotometry.
- B. **ISOPOLY ACID AND HETEROPOLYACID:** Isopoly and heteropoly acids of Mo and W. Preparation, properties and structure. Classification, Preparation, properties and structures of borides, carbides, nitrides and silicides. Silicates- classification and Structure, Silicones- preparation, properties and application.

UNIT – IV

- A. **METAL CLUSTERS:** Higher boranes, carboranes, metalloboranes and metallocarboranes. Metal carbonyl and halide cluster, compounds with metal-metal multiple bonds.
- B. **CHAINS:** catenation, heterocatenation, intercatenation.
- C. **RINGS:** Borazines, phosphazines.

BOOK SUGGESTED:

1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
2. Inorganic Chemistry, J.E. Huhey, Harpes and Row.
3. Chemistry of the Elements, N.N. Greenwood and A. Earnshaw, Pergamon.
4. Comprehensive Coordination Chemistry Eds. G. Wilkinson, R.D. Gillars and J.A. McCleverty, Pergamon.

CONCEPTS IN ORGANIC CHEMISTRY

Max. Marks 80

UNIT - I

- A. **NATURE OF BONDING IN ORGANIC MOLECULES:** Localized and Delocalized chemical bond, conjugation and cross-conjugation, Bonding in Fullerenes, Bonds weaker than covalent, addition compounds, Crown ether complexes and cryptands. Inclusion compounds, Cyclodextrins, Catenanes and Rotaxanes.
- B. **AROMATICITY:** Aromaticity in benzenoid and non-benzenoid compounds, Huckel anti-aromaticity, homo-aromaticity. PMO approach for Aromaticity, Annulenes.

UNIT - II

- A. **CONFORMATIONAL ANALYSIS:** Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity, conformation of sugars, steric strain due to unavoidable crowding.
- B. **STEREOCHEMISTRY:** Elements of symmetry, chirality, molecules with more than one chiral center, methods of resolution, optical purity, stereospecific and stereoselective synthesis. Asymmetric synthesis. Optical activity in the absence of chiral carbon - Biphenyls, allenes and spiranes, chirality due to helical shape.

UNIT - III

- A. **REACTION INTERMEDIATES:** Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes. Sandmeyer reaction, Free radical rearrangement and Hunsdiecker reaction.
- B. **ELIMINATION REACTIONS:** The E₂, E₁ and E_{1cB} mechanisms. Orientation of the double bond. Reactivity, effects of substrate structures, attacking base, the leaving group and the medium.

UNIT - IV

PERICYCLIC REACTIONS: Classification of pericyclic reactions. Woodward-Hoffmann correlation 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 system, 2+2 addition of ketenes, 1,3 dipolar cycloadditions and cheletropic reactions. Sigmatropic rearrangements - suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 3,3- and 5,5- sigmatropic rearrangements. Claisen, Cope and Aza-Cope rearrangements. Ene reaction.

BOOKS SUGGESTED:

1. Advanced Organic Chemistry, F. A. Carey and R. J. Sundberg, Plenum.
2. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
3. Structures and Mechanism in Organic Chemistry, C. K. Ingold, Cornell University Press.
4. Organic Chemistry, R. T. Morrison and R. N. Boyd, Prentice-Hall.
5. Modern Organic Reactions, H. O. House, Benjamin.
6. Principles of Organic Synthesis, R. O. C. Norman and J. M. Coxon, Blackie Academic and Professional.
7. Pericyclic Reactions, S. M. Mukherji, Macmillan, India.
8. Reaction Mechanism in Organic Chemistry, S. M. Mukherji and S. P. Singh, Macmillan.
9. Stereochemistry of Organic Compounds, D. Nasipuri, New Age International.
10. Some Modern Methods of Organic Synthesis, W. Carruthers, Cambridge Univ. Press.
11. Rodd's Chemistry of Carbon Compounds, Ed. S. Coff
12. Organic Chemistry, Vol 2, I. L. Finar, ELBS.
13. Stereo selective Synthesis: A Practical Approach, M. Nogradi, and VCH.
14. Organic Chemistry, Paula Yurkanis Bruice, Pearson Education.

QUANTUM CHEMISTRY, THERMODYNAMICS AND CHEMICAL DYNAMICS - I

Max. Marks 80

UNIT - I

A. MATHEMATICAL CONCEPTS IN QUANTUM CHEMISTRY:

Vector quantities and their properties. Complex numbers and Coordinate transformation. Differential and Integral Calculus, Basic rules of differentiation and Integration applications.

- B.** The Schrodinger equation and 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 rotator, the hydrogen atom.

UNIT –II

BASICS OF THERMODYNAMICS: Maxwell's thermodynamic relations, Vant's Hoff hypothesis. Partial molar volume and partial molar heat content. Chemical potential, Gibbs-Duhem equation, variation of chemical potential with temperature and pressure. Chemical potential of ideal gases, pure solids, liquids and mixture of ideal gases. Activity and Fugacity, Determination of Fugacity, Variation of Fugacity with Temperature and Pressure.

UNIT –III

ELECTROCHEMISTRY–I: Electrochemistry of solution. Debye-Huckel Onsager treatment and its extension, ion solvent interactions. Debye-Huckel Limiting Law. Debye-Huckel theory for activity coefficient of electrolytic solutions. Determination of activity and activity coefficient, ionic strength, Thermodynamics of electrified interface equations. Derivation of electro-capillarity, Lippmann equation (surface excess), methods of determination.

UNIT –IV

CHEMICAL DYNAMICS –I: Methods of determining rate laws, consecutive reactions, collision theory of reaction rates, steric factor, Activated complex theory, kinetic salt effects, steady state kinetics, and thermodynamic and kinetic control of reactions. Dynamic chain (Hydrogen-bromine and Hydrogen-chlorine reactions) and Oscillatory reactions (Belousov-Zhabotinsky reaction etc.)

BOOKS SUGGESTED :

1. Physical Chemistry, P.W. Atkins, ELBS.
2. Coulson's Valence, R. McWeeny, ELBS.
3. Chemical Kinetics, K. J. Laidler, Pearson.
4. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman and J. Kuriacose, McMillan.
5. Modern Electrochemistry Vol. I and Vol. II, J.O.M. Bockris and A.K.N. Reddy, Plenum.
6. Thermodynamics for Chemists, S. Glasstone EWP.
7. An Introduction to Electrochemistry S. Glasstone EWP.
8. Organic Chemist's Book of Orbitals. L. Salem and W.L. Jorgensen, Academic Press
9. The Physical Basis of Organic Chemistry, H. Maskill, Oxford University Press

THEORY AND APPLICATIONS OF SPECTROSCOPY- I

Max. Marks 80

UNIT - I

UNIFYING PRINCIPLES:

Electromagnetic radiation, interaction of electromagnetic radiation with matter-absorption, emission transmission, reflection, dispersion, polarization and scattering, Uncertainty relation and natural line width and natural line broadening, transition probability, selection rules, intensity of spectral lines, Born-Oppenheimer approximation, rotational, vibrational and electronic energy levels. Region of spectrum, representation of spectra, F.T. spectroscopy, computer averaging, lasers.

UNIT- II

MICROWAVE SPECTROSCOPY:

Classification of molecules in term of their internal rotation mechanism, determination of rotation energy of diatomic and polyatomic molecules, intensities of rotational spectral lines, effect of isotopic substitution on diatomic and polyatomic molecules, intensities of rotational spectral lines and parameters of rotational energy of linear and the transition frequencies, non-rigid rotators, spectral lines and parameters of rotational energy of linear and symmetric top polyatomic molecules. Application in determination of bond length.

UNIT- III

INFRA RED SPECTROSCOPY:

Introduction, simple and anharmonic oscillators in vibrational spectroscopy, diatomic-vibrating rotator, Modes of vibration in polyatomic molecules, vibration-coupling, Fourier Transform IR spectroscopy: instrumentation, interferometric spectrophotometer, sample handling, Factors influencing vibrational frequencies, Application of IR spectroscopy: Interpretation of IR spectra of normal alkanes, aromatic hydrocarbons, alcohols, phenols, aldehydes, ketones, ethers, esters, carboxylic acids, amines and amides.

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), Instrumentation , Application of Raman effect in molecular structures, Raman activity of molecular vibration, structure of CO₂, H₂O, N₂O, SO₂, NO₃⁻, ClF₃.

BOOKS SUGGESTED

1. Modern Spectroscopy, J.M. Hollas, John Wiley.
2. Fundamentals of Molecular Spectroscopy, C.N. Banwell.
3. Spectroscopy, B.K. Sharma, Goel Publication.
4. Organic Spectroscopy: Principles and Applications, Jag Mohan, Narosa Publication.
5. Spectroscopy Methods in Organic Chemistry, D.H. Williams & I. Fleming, Tata Mcgraw-Hill Publication.
6. Spectrophotometric Identification of Organic Compounds, R.M. Silversteion & F. X. Webster, John Wiley Publication.

PAPER NO 5. CH - 105

LABORATORY COURSE-I

Max. Marks 100

1. QUALITATIVE ANALYSIS OF MIXTURE CONTAINING EIGHT RADICALS INCLUDING TWO LESS COMMON METAL FROM AMONG THE FOLLOWING BY SEMI MICRO METHOD.

1) *Basic Radicals* :

Ag, Pb, Hg, Bi, Cu, Cd, As, Sb, Sn, Fe, Al, Cr, Zn, Mn, Co, Ni, Ba, Sr, Ca, Mg, Na, K, Ce, Th, Zr, W, Te, Ti, Mo, U, V, Be, Li, Au, Pt.

2) *Acid Radicals* :

Carbonate, Sulphite, Sulphide, Nitrite, Nitrate, Acetate, Fluoride. Chloride, Bromide, Iodide, Sulphate, Borate, Oxalate, Phosphate, Silicate, Thiosulphate, Ferrocyanide, Ferricyanide, Sulphocyanide, Chromate, Arsenate and Permanganate.

2. QUANTITATIVE ANALYSIS:

Involving separation of two of the following in ores, alloys, or mixtures in solution, one by volumetric and the other by gravimetric methods.

3. ESTIMATION OF:

- 1) Phosphoric acid in commercial orthophosphoric acid.
- 2) Boric acid in borax.
- 3) Ammonia in ammonium salts.
- 4) Manganese dioxide in pyrolusite.
- 5) Available chlorine in bleaching powder.
- 6) Hydrogen peroxide in commercial samples.

4. PREPARATIONS:-

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

- (1) VO (acac)₂
- (2) TiO(C₉H₈NO)₂ · 2H₂O
- (3) cis-K [Cr(C₂O₄)₂ (H₂O)₂]
- (4) Na [Cr (NH₃)₂ (SCN)₄]
- (5) Mn (acac)₃
- (6) K₂[Fe(C₂O₄)₃]
- (7) Prussian Blue, Turnbull's Blue.
- (8) [Co (NH₃)₆] [Co (NO₂)₆]
- (9) cis-[Co(trien) (NO₂)₂] Cl · H₂O
- (10) Hg [Co (SCN)₄]
- (11) [Co (Py)₂Cl₂]
- (12) [Ni (NH₃)₆] Cl₂
- (13) Ni (dmg)₂
- (14) [Cu (NH₃)₄] SO₄ · H₂O

BOOKS SUGGESTED

1. Vogel's Textbook of Quantitative Analysis, rev. Mendham, ELBS.
2. Synthesis and Characterization of Inorganic Compounds, W.L. Jolly, Prentice Hall.

ADSORPTION/SURFACE CHEMISTRY

1. Surface Tension - Concentration relationship for solutions (Gibbs equation).
2. To verify the Freundlich and Langmuir Adsorption isotherms using acetic acid/Oxalic acid and activated charcoal.
3. Determination of CMC of surfactants.

PHASE EQUILIBRIA

1. To Construct the Phase diagram for three component system (e.g., chloroform-acetic acid-water).

CHEMICAL KINETICS

1. Determination of the effect of (a) Change of temperature (b) Change of concentration of reactants and catalyst and (c) Ionic strength of the media on the velocity constant of hydrolysis of an ester/ionic reactions.
2. Determination of the velocity constant of hydrolysis of an ester/ionic reaction in micellar media.
3. Determination of the rate constant for the decomposition of hydrogen peroxide by Fe^{3+} and Cu^{2+} ions.
4. Determination of the primary salt effect on the kinetics of ionic reactions and testing of the Bronsted relationship (iodide ion is oxidized by persulphate ion).

SOLUTIONS/MOLECULAR WEIGHTS

1. Determination of molecular weight of non-volatile substances by Landsberger method.
2. Determination of Molar masses of Naphthelene/acetanilide.
3. Molecular weight of polymers by viscosity measurements.

CONDUCTOMETRY

1. Determination of the velocity constant, order of the reaction and energy of activation for saponification of ethyl acetate by sodium hydroxide conductometrically.
2. Determination of solubility and solubility product of sparingly soluble salts (e.g., PbSO_4 , BaSO_4) conductometrically.
3. Determination of pK_a of Acetic acid and verification of Ostwald dilution law.

POTENTIOMETRY/pH METRY

1. Determination of the strength of strong and weak acids in a given mixture using a potentiometer/pH meter.
2. Determination of the dissociation constant of acetic acid in DMSO, DMF, acetone and dioxane by titrating it with KOH.
3. Determination of the dissociation constant of monobasic/dibasic acid by Albert-Serjeant method.
4. Determination of Redox potential of $\text{Fe}^{++}/\text{Fe}^{+++}$ system.
5. Determination of rate constant for hydrolysis/inversion of sugar using a polarimeter.
6. Enzyme kinetics –inversion of sucrose.
7. Determine the specific and molecular rotation of optically active substances.

BOOKS SUGGESTED

1. Experiments and Techniques in Organic Chemistry, D.Pasto, C. Johnson and M. Miller, Prentice Hall.
2. Macroscale and Microscale Organic Experiments, K.L. Williamson, D.C. Heath.
3. Systematic Qualitative Organic Analysis, H. Middleton, Edward Arnold.
Handbook of Organic Analysis –Qualitative and Quantitative, H. Clark, Edward Arnold.
4. Vogel's Textbook of Practical Organic Chemistry,
5. Practical Physical Chemistry, A.M. James and F.E. Prichard, Longman.
6. Findley's Practical Physical Chemistry, B.P. Levi
Experimental Physical Chemistry, R.C. Das and B. Behera, Tata McGraw Hill.

SECOND SEMESTER

PAPER NO1 . CH - 201

TRANSITION METAL COMPLEXES

Max. Marks 80

UNIT - I

REACTION MECHANISM OF TRANSITION METAL COMPLEXES: Energy profile of a reaction, reactivity of metal complexes, inert and labile complexes, kinetic application of valence bond and crystal field theories, kinetics of octahedral substitution, anation reactions, reactions without metal ligand bond cleavage. Substitution reactions in square planar complexes, the trans effect. Redox reactions, electron transfer reactions, mechanism of one electron transfer reactions, outer sphere type reactions, cross reactions and Marcus-Hush theory, inner sphere type reactions.

UNIT - II

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), Selection rules, mechanism for break down of the selection rules, intensity of absorption, band width, spectra of d-d metal complexes of the type $[M(H_2O)]^{n+}$, spin free and spin paired ML_6 complexes of other geometries, Calculations of Dq , B and parameters, spin forbidden transitions, effect of spin-orbit coupling, Spectrochemical and Nephelauxetic series. Magnetic properties of complexes of various geometries based on crystal field model, spin free-spin paired equilibria in octahedral stereochemistry.

UNIT - III

- A. **TRANSITION METAL COMPLEXES:** Transition metal complexes with unsaturated organic molecules, alkanes, allyl, diene dienyl, arene and trienyl complex, preparations, properties, nature of bonding and structure features. Important reaction relating to nucleophilic and electrophilic attack on ligands and organic synthesis.
- B. **TRANSITION METALS COMPOUND WITH BOND TO HYDROGEN:** Transition Metals Compounds with Bond to Hydrogen.

UNIT-IV

- A. **ALKYLS AND ARYLS OF TRANSITION METALS:** Types, routes of synthesis, stability and decomposition pathways, organocopper in organic synthesis.
- B. **COMPOUNDS OF TRANSITION METAL - CARBON MULTIPLE BONDS :** Alkylidenes, low valent carbenes, nature of bond and Structural characteristics.
- C. **FLUXIONAL ORGANOMETALLIC COMPOUNDS:** Fluxionality and dynamic equilibria in compounds such as olefin, -allyl and dienyl complexes.

BOOKS SUGGESTED :

1. Principles and applications of organotransition metal chemistry, J.P.Collman, L.S.Hegsdus, J. R. Norton and R.G. Finke, University Science Books.
2. The Organometallic chemistry of the Transition metals, R. H. Crabtree, John Wiley.
3. Metallo - organic chemistry, A.J. Pearson, Wiley.
4. Organometallic chemistry, R.C. Mehrotra and A. Singh, New age International.

PAPER NO 2. CH - 202

REACTION MECHANISMS

Max. Marks 80

UNIT - I

- A. ALIPHATIC NUCLEOPHILIC SUBSTITUTION:** The S_N^2 , S_N^1 , mechanisms. The neighbouring group mechanism, neighbouring group participation by π and σ bonds, anchimeric assistance. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, ambident nucleophile and regioselectivity.
- B. AROMATIC NUCLEOPHILIC SUBSTITUTION:** The S_N^1 , S_N^2 mechanisms. Reactivity effect of substrate structure, leaving group and attacking nucleophile. The von Richter, Sommelet-Hauser, and Smiles rearrangements.

UNIT - II

- A. ALIPHATIC ELECTROPHILIC SUBSTITUTION:** Mechanisms of S_E^2 , S_E^1 , electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity.
- B. AROMATIC ELECTROPHILIC SUBSTITUTION:** The arenium ion mechanism, orientation and reactivity. The ortho/para ratio, ipso attack, orientation in other ring systems. Reactivity-Effect of substrates and electrophiles. Vilsmeier reaction and Gattermann-Koch reaction.

UNIT - III

ADDITION TO CARBON-CARBON MULTIPLE BONDS: Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemoselectivity. Addition to cyclopropane ring. Hydrogenation of double and triple bonds, hydroboration 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, acids esters and nitriles. Addition of Grignard Reagents, Organo-Zinc and Organo-lithium to carbonyls and unsaturated carbonyl compounds, Wittig reaction.

Mechanism of condensation reactions involving enolates - Aldol, Knoevenagel and Stobbe reactions. Hydrolysis of esters and amides, ammonolysis of esters.

BOOKS SUGGESTED :

1. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.
2. Modern Organic Reactions, H. O. House, Benjamin.
3. Principles of Organic Synthesis, R. O. C. Norman and J. M. Coxon, Blackie Academic & Professional.
4. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
5. Structures and Mechanism in Organic Chemistry, C. K. Ingold, Cornell University Press.
6. Reaction Mechanism in Organic Chemistry, S. M. Mukherji and S. P. Singh, Macmillan

QUANTUM CHEMISTRY, THERMODYNAMICS AND CHEMICAL DYNAMICS - II

Max. Marks 80

UNIT –I

- A. **APPLICATION OF MATRICES IN QUANTUM CHEMISTRY:** Addition and multiplication, inverse and transpose of matrices. Determinants, in quantum Chemistry.
- B. **ANGULAR MOMENTUM IN QUANTUM CHEMISTRY:** Angular momentum, angular momentum Operators. Eigen functions and Eigen values Angular momentum, ladder operators.
- C. **APPROXIMATE METHODS:** The variation theorem, linear variation principle. Perturbation theory (first order and non-degenerate). Applications of variation method and perturbation theory to the Helium atom.

UNIT –II

STATISTICAL THERMODYNAMICS: Probability, permutations and combinations concepts of probability, Maxwell Boltzmann distribution. Different ensembles and Partition functions translational, rotational, vibrational and Electronic. Thermodynamic function using appropriate Partition function. Fermi-Dirac and Bose-Einstein Statistics and statistical basis of entropy. Heat capacity of solids, Debye and Einstein Models.

UNIT –III

ELECTROCHEMISTRY –II: Structure of electrified interfaces. Gouy-Chapman, Stern, Over potentials and exchange current density, Derivation of Butler –Volmer equation, Tafel plot. Semiconductor interfaces, Theory of double layer at semiconductor, electrolyte solution interfaces, structure of double layer interfaces. Effect of light at semiconductor solution interfaces. Electro catalysis influence of various parameters. Hydrogen electrode.

UNIT –IV

CHEMICAL DYNAMICS –II: General features of fast reactions by flow method, relaxation method, flash photolysis and the nuclear magnetic resonance method. Molecular reaction dynamics, Dynamics of molecular motions, probing the transition state, dynamics of barrierless chemical reactions in solutions, dynamics of unimolecular reaction. [Lindemann –Hinshelwood , RRK and Rice-Ramsperger-Kassel-Marcus {RRKM}] theories of unimolecular reactions.

BOOKS SUGGESTED :

1. The Chemistry Mathematics Book, E. Steiner, Oxford University Press.
2. Mathematics for Chemistry, Doggett and Sutcliffe, Longman.
3. Mathematical Preparation for Physical Chemistry, F. Daniels, McGraw Hill.
4. Chemical Mathematics, D.M, Hirst, Longman.
5. Applied Mathematics for Physical Chemistry, J.R. Barrante, Prentice Hall.
6. Basic Mathematics for Chemists, Tebbutt, Wiley.
7. Physical Chemistry, P.W. Atkins, ELBS.
8. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill.
9. Quantum Chemistry, Ira N. Levine, Prentice Hall.
10. Coulson's Valence, R. McWeeny, ELBS.
11. Chemical Kinetics, K. J. Laidler, Pearson.
12. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman and J. Kuriacose, McMillan.
13. Modern Electrochemistry Vol. I and Vol. II, J.O.M. Bockris and A.K.N. Reddy, Plenum.
14. Thermodynamics for Chemists, S. Glasstone EWP.
15. An Introduction to Electrochemistry S. Glasstone EWP.
16. Physical Chemistry, Ira N. Levine McGraw Hill.
17. Physical Chemistry, Silbey, Alberty, Bawendi, John-Wiley.

THEORY AND APPLICATIONS OF SPECTROSCOPY –II

Max. Marks 80

UNIT - I

ULTRAVIOLET AND VISIBLE SPECTROSCOPY:

Introduction, intensity of vibrational-electronic spectra and Frank-Condon principle for dissociation energy, rotational fine structure of electronic-vibrational spectra, Shape of some molecular orbitals

viz., H₂, He₂, N₂, O₂. Electronic spectra of organic molecules, chromophores, application of electronic spectroscopy: spectrophotometric studies of complex ions, determination of ligand/metal ratio in a complex, identification of compounds, determination of stability constants.

UNIT -II

SCATTERING SPECTROSCOPY:

Principle, instrumentations and application of Auger spectroscopy, Scanning Electron Microscopy, Electron diffraction of gases and vapours, The Wierl equation and co-related method.

Theory, instrumentation and application of turbidimetry, nephelometry, fluorometry. Fluorescence and phosphorescence and factors affecting them.

UNIT - III

MASS SPECTROMETRY:

Introduction, basic principles, separation of the ions in the analyzer, resolution, molecular ion peak, mass spectral fragmentation of organic compounds, factors affecting fragmentation, McLafferty rearrangement. Instrumentation, Characteristics of mass spectra of Alkanes, Alkenes, Aromatic hydrocarbons, Alcohols, Amines. Nitrogen rule, ring rule, Molecular weight and formula determination, Gas chromatography-Mass spectrometry.

UNIT - IV

NUCLEAR RESONANCE SPECTROPHOTOMETRY:

Theory of NMR spectroscopy, interaction of nuclear spin and magnetic moment, chemical shift, precessional motion of nuclear particles in magnetic field, spin-spin splitting, coupling constants, factor affecting the chemical shift, shielding effect, effect of chemical exchange, hydrogen bonding, instrumentation of Fourier transform NMR spectrophotometer, structure determination of organic compounds, Carbon-13 NMR spectroscopy, Multiplicity-proton (¹H) decoupling-noise decoupling, off resonance decoupling, selective proton decoupling, chemical shift.

BOOKS SUGGESTED

1. Modern Spectroscopy, J.M. Hollas, John Wiley.
2. Fundamentals of Molecular Spectroscopy, C.N. Banwell.
3. Spectroscopy, B.K. Sharma, Goel Publication.
4. Organic Spectroscopy : Principles and Application, Jag Mohan, Narosa Publication.
5. Spectroscopic Methods in Organic Chemistry, D.H. Williams & I. Fleming, Tata Mcgraw-Hill Publication.
6. Spectrophotometric Identification of Organic Compounds, R.M. Silverstein & F.X. Webster, John Wiley Publications.

PAPER NO 5. CH - 205

LABORATORY COURSE –III

Max. Marks 100

1. **GENERAL METHODS OF SEPARATION AND PURIFICATION OF ORGANIC COMPOUNDS WITH SPECIAL REFERENCE TO:**
 - 1) Solvent Extraction
 - 2) Fractional Crystallization
2. **DISTILLATION TECHNIQUES:**

Simple distillation, steam distillation, Fractional distillation and distillation under reduced pressure.
3. **ANALYSIS OF ORGANIC BINARY MIXTURE:**

Separation and Identification of organic binary mixtures containing at least one component with two substituents.
(A student is expected to analyse at least 10 different binary mixtures.)
4. **PREPARATION OF ORGANIC COMPOUNDS: SINGLE STAGE PREPARATIONS.**
 - 1) **Acetylation:** Synthesis of β -Naphthyl acetate from β -Naphthol / Hydroquinone diacetate from Hydroquinone.
 - 2) **Aldol condensation:** Dibenzal acetone from benzaldehyde.
 - 3) **Bromination:** p-Bromoacetanilide from acetanilide.
 - 4) **Cannizzaro Reaction:** Benzoic acid and Benzyl alcohol from benzaldehyde.
 - 5) **Friedel Crafts Reaction:** o-Benzoyl Benzoic acid from phthalic anhydride.
 - 6) **Grignard Reaction:** Synthesis of triphenylmethanol from benzoic acid,
 - 7) **Oxidation:** Adipic acid by chromic acid oxidation of cyclohexanol.
 - 8) **Perkin's Reaction:** Cinnamic acid from benzaldehyde.
 - 9) **Sandmeyer Reaction:** p-Chlorotoluene from p-toluidine/o-Chlorobenzoic acid from anthranilic acid.
 - 10) **Schotten Baumann Reaction:** β -Naphthyl benzoate from: β -Naphthol / Phenyl benzoate from phenol.
 - 11) **Sulphonation Reaction:** Sulphanilic acid from aniline.

BOOK SUGGESTED :

1. Practical Organic chemistry by A. I. Vogel.
2. Practical Organic chemistry by Mann and Saunders.
3. Practical Organic chemistry by Garg and Salija.
4. The Systematic Identification of Organic compounds, R. L. Shriner and D. Y. Curtin.
5. Semimicro Qualitative Organic Analysis, N.D. Cheronis, J. B. Entrikin and E. M. Hodnett.
6. Practical Physical chemistry by Alexander Findlay.
7. Experimental Physical chemistry, D. P. Shoemaker, G. W. Garland and J. W. Niber, Mc Graw Hill Interscience.
8. Findlay's Practical Physical chemistry, revised B

PAPER NO 6. CH –206

LABORATORY COURSE –IV

Max. Marks 100

I. ERROR ANALYSIS AND STATISTICAL DATA ANALYSIS

1. Linear Regression Analysis
2. Curve Fitting
3. Student “t” Test
4. Data Analysis Using Basic Statistical Parameters
5. Calibration of volumetric Apparatus, Burette, Pipette Weight Box etc.

II. USE OF COMPUTER PROGRAMMES

The students will learn how to operate a PC and how to run standard programmes and packages. Execution of linear regression, X-Y plot, numerical integration and differentiation as well as differential equation solution programmes. Monte Carlo and Molecular dynamics. Programmes with data preferably from physical chemistry laboratory. Further, the student will operate one or two or the packages such as MICROSOFT ECCEL, WORLD, POWERPOINT, SPSS, ORIGIN, MATLAB, EASYPLOT.

III. A. FLAME PHOTOMETRIC DETERMINATIONS

1. Sodium and potassium when present together.
2. Sodium/potassium in solid samples.
3. Solid Sodium and Potassium in Liquid Samples.
4. Lithium/calcium/barium/strontium.
5. Cadmium and magnesium in tap water.

B. NEPHELOMETRIC DETERMINATIONS

1. Sulphate
2. Phosphate
3. Silver

IV. ELECTROPHORESIS

1. To separate cations of inorganic salts by paper electrophoresis.
2. Capillary Electrophoresis of water –soluble Vitamines

V. SPECTROSCOPY

1. Verification of Beer’s Lambert Law.
2. Determination of stoichiometry and stability constant of inorganic (e.g. ferric –salicylic acid) and organic (e.g. amine-iodine) complexes, thiocyanate.
3. Characterization of the complexes by electronic and IR, UV spectral data.
4. Determination of Indicator constant (pK_a) of methyl red.

BOOK SUGGESTED :

1. Computer and Common Sense, R. Hunt and J. Shelley, Prentice Hall.
2. Computational Chemistry, A.C. Norris.
3. Microcomputer Quantum Mechanics, J.P. Killingbeck, Adam Hilger.
4. Computer Programming in FORTRAN IV, V. Rajaraman, Prentice Hall.
5. An Introduction to Digital Computer Design, V. Rajaraman and T. Radhakrishnan, Prentice Hall.
6. Experiments in Chemistry, D.V. Jahagirgar.

THIRD SEMESTER

PAPER NO 1. CH - 301

RESONANCE SPECTROSCOPY, PHOTOCHEMISTRY AND ORGANOCATALYSIS

Max. Marks 80

UNIT –I

- A. **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).
- B. **NUCLEAR QUADRUPOLE RESONANCE SPECTROSCOPY:** Quadrupole nuclei, quadrupole moments, electric field gradient, coupling constant, splitting, applications.

UNIT –II

- A. **PHOTOELECTRON SPECTROSCOPY:** Basic principle both for atoms and molecules; Photo-electric effect, ionization process, Koopman's theorem, Spectra of simple molecules, Auger electron spectroscopy, Determination of Dipole moment.
- B. **PHOTOACOUSTIC SPECTROSCOPY:** Basic principle of Photo acoustic Spectroscopy (PAS), PAS – gases and condensed system Chemical and Surface application.

UNIT –III

- A. **PHOTOCHEMICAL REACTIONS :** Interaction of electromagnetic radiation with matter, Photophysical processes , Stern Volmer equation, types of excitations, fate of excited molecule, quantum yield, transfer of excitation energy, Actinometry.
- B. **DETERMINATION OF REACTION MECHANISM:** Classification, rate constants and life times of reactive energy states –determination of rate constants of reactions. Effect of light intensity on the rate of photochemical reactions.
- C. **MISCELLANEOUS PHOTOCHEMICAL REACTIONS:** Photo-Fries reactions of anilides, Photo-Fries rearrangement. Barton reaction. Singlet molecular oxygen reactions. Photochemical formation of smog. Photodegradation of polymers, Photochemistry of vision.

UNIT –IV

A. ORGANOCATALYSIS

General Principles: Energetic, Catalytic cycles, catalytic efficiency and life time, selectivity. Type of organometallic reaction: Ligand substitution, Oxidative addition, reductive elimination and insertion and deinsertion. Homogeneous catalysis: Hydrogenation of alkenes, Hydroformylation, Monsanto acetic acid synthesis, Wacker oxidation of alkenes, Alkenes metathesis, Palladium-Catalysed C-C bond forming reactions, asymmetric oxidation. Heterogeneous catalysis: The nature of heterogeneous catalysts, Fischer-Tropsch synthesis, alkene polymerization.

BOOK SUGGESTED:

1. Infrared and Raman Spectra: Inorganic and Coordination Compounds, K. Nakamoto, Wiley.
2. Fundamentals of Photochemistry, K.K. Rohtagi-Mukherji, Wiley-Eastern.
3. Essentials of Molecular Photochemistry, A. Gilbert and J. Baggott, Blackwell Scientific Publications.
4. Molecular Photochemistry, N.J. Turro, W.A. Benjamin.
5. Introductory Photochemistry, A. Cox and T. Camp, McGraw-Hill.
6. Photochemistry, R.P. Kundall and A. Gilbert, Thomson Nelson.
7. Application of Spectroscopy of Organic Compounds, J.R. Dyer, Prentice Hall.
8. Photochemistry, R.P. Kundall and A. Gilbert, Thomson Nelson.
9. Organic Photochemistry, J. Coxon and B. Halton, Cambridge University Press.
10. Shriver & Atkins Inorganic Chemistry: P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong, Oxford University Press
11. Inorganic Chemistry: C.E. Housecroft, A.G. Sharpe, Pearson Education Limited.
12. Inorganic Chemistry: Principles of Structure and Reactivity: J.E. Huheey, E.A. Keiter, R.L. Keiter, O.K. Medhi, Pearson Education
13. Organometallic Chemistry: A Unified Approach: R.C. Mehrotra, A. Singh, New Age International Publishers.

CHEMISTRY OF BIOMOLECULES

Max. Marks 80

UNIT –I

- A. **BIOENERGETICS:** Standard free energy change in biochemical reactions, exergonic, endergonic. Hydrolysis of ATP, synthesis of ATP from ADP.
- B. **ELECTRON TRANSFER IN BIOLOGY:** Structure and function of metalloproteins in electron transport processes –cytochromes and iron-sulphur proteins, synthetic models.
- C. **TRANSPORT AND STORAGE OF DIOXYGEN:** Heme proteins and oxygen uptake, structure and function of haemoglobin, myoglobin, haemocyanins and haemerythrin, model synthetic complexes of iron, cobalt and copper.

UNIT –II

- A. **METALLOENZYMES:** Zinc enzymes –carboxypeptidase and carbonic anhydrase. Iron enzymes – catalase, peroxidase and cytochrome P-450. copper enzymes- superoxide dismutase. Molybdenum oxotransferase enzymes –xanthine oxidase.
- B. **ENZYME MODELS:** Host-guest chemistry, chiral recognition and catalysis, molecular recognition, molecular asymmetry and prochirality. Biomimetic chemistry, Cyclodextrin-based enzyme models, calixarenes, ionophores, synthetic enzymes or synzymes.

UNIT –III

- A. **ENZYMES :** Nomenclature and classification of Enzyme. Induced fit hypothesis, concept and identification of active site by the use of inhibitors.
- B. **CO-ENZYME CHEMISTRY:** Structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD⁺, NADP⁺, FMN, FAD, lipoic acid, vitamin B₁₂.
- C. **BIOTECHNOLOGICAL APPLICATIONS OF ENZYMES:** Techniques and methods of immobilization of enzymes, effect of immobilization on enzyme activity, application of immobilization enzymes in medicine and industry. Enzymes and Recombinant DNA Technology.

UNIT –IV

- A. **BIOPOLYMER INTERACTIONS:** forces involved in biopolymer interaction. Electrostatic charges and molecular expansion, hydrophobic forces, dispersion force interactions. Multiple equilibria and various types of binding processes in biological systems. Hydrogen ion titration curves.
- B. **THERMODYNAMICS OF BIOPOLYMER SOLUTIONS:** Thermodynamics of biopolymer solution, osmotic pressure, membrane equilibrium, muscular contraction and energy generation in mechanochemical system.
- C. **CELL MEMBRANE AND TRANSPORT OF IONS:** Structure and functions of cell membrane, ion transport through cell membrane, irreversible thermodynamic treatment of membrane transport and Nerve conduction.

BOOK SUGGESTED:

1. Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.
2. Bioinorganic Chemistry, I. Bertini, H.B. Gray, S.L. Lippard and J.S. Valentine, University Science Books.
3. Inorganic Biochemistry vols II and I. Ed G.L. Eichhorn, Elsevier.
4. Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.
5. Bioinorganic Chemistry, I. Bertini, H.B. Gary, S.J. Lippard and J.S. Valentine, University Science.
6. Inorganic Biochemistry vols I and II ed. G.L. Eichhorn, Elsevier.
7. Bioorganic Chemistry: A Chemical Approach to Enzyme Action, Hermann Dugas and C. Penny, Springer-verlag.
8. Understanding Enzymes, Trevor palmer, Prentice Hall.
9. Enzyme Chemistry : Impact and Applications, Ed. Collin J Suckling, Chapman and Hall.
10. Enzyme Mechanisms Ed, M.I. Page and A. Williams, Royal Society of Chemistry.
11. Fundamentals of Enzymology, N.C. Price and L. Stevens, Oxford University Press.
12. Immobilized Enzymes: An Introduction and Applications in Biotechnology, Michael D. Trevan, and John Wiley.

13. Enzymatic Reaction Mechanisms, C. Walsh, W.H. Freeman.
14. Enzyme Structure and Mechanisms, A Fersht, W.H. Freeman.
15. Biochemistry: The Chemical Reactions of Living Cells, D.E. Metzler, Academic Press.
16. Principles of Biochemistry, A.L. Lehninger, Wroth Publishers.
17. Biochemistry, L. Stryer, W.H. Freeman.
18. Biochemistry, J. David Rawn, Neil Patterson.
19. Biochemistry, Voet and Voet, John Wiley.
20. Outlines of Biochemistry, E.E. Conn and P.K. Stumpf, John Wiley.
21. Bioorganic Chemistry : A Chemistry Approach to Enzyme Action, H. Dugas and C. Penny, Springer-Verlag.
22. Biochemistry and Molecular Biology of Plants, Buchanan, Griseham and Jones, I.K. International Pvt. Ltd.

CATALYSIS, SOLID STATE AND SURFACE CHEMISTRY

Max. Marks 80

UNIT –I

ACIDS, BASES, ELECTROPHILES, NUCLEOPHILES AND CATALYSIS:

Acid-base dissociation, Electronic and structural effects, acidity and basicity. Acidity function and their applications. Hard and soft acids and bases. Nucleophilicity scales. Nucleofugacity. The alpha effect. Ambivalent Nucleophilies. Acid base catalysis-specific and general catalysis. Bronsted catalysis, Enzyme Catalysis.

UNIT –II

MICELLES AND ADSORPTION :

Micelles : Classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of Surfactants. Thermodynamics of micellization - phase separation and mass action models. Reverse micelles, micro-emulsion. Micellar Catalysis, Surface tension capillary action, pressure difference across curved surface (Laplace equation), vapor pressure of droplets (Kelvin equation), Gibbs adsorption isotherm.

UNIT –III

SOLID STATE CHEMISTRY - I :

Crystal defects and Non-stoichiometry - Perfect and imperfect crystals, intrinsic and extrinsic defects - point defect, line and plane defects, vacancies - Schottky defects and Frankel defects. Thermodynamics of Schottky and Frenkel defect, formation of color centres, non-stoichiometry and defects. Electronic properties and Band theory of semiconductors.

UNIT –IV

MACROMOLECULES :

Polymer - Definition types of polymers, electrically conducting, fire resistant, liquid crystal polymers, kinetics of polymerization, mechanism of polymerization.

Molecular mass and average molecular mass. Molecular mass determination (Osmometry, Viscometry, diffusion and light scattering methods), Sedimentation, chain configuration of macromolecules, calculation of average dimensions of various chain structures.

BOOK SUGGESTED :

1. G.W. Castellan, "Physical Chemistry", Addison- Lesley Publishing Co.
2. E.A. Moelwyn Hughes, "Physical Chemistry", Pergamon Press.
3. Denbigh, "Chemical Equilibria", D. Van Nostrand.
4. J. Rose, "Dynamic Physical Chemistry" Sir Issac Pitman and Sons.
5. Solid state "Chemistry and its Applications, A.R. West, Plenum.
6. Principle of Solid State H.V. Kar, Wiley Eastern.
7. Solid State Chemists, D.K. Chakrabarty, New Age International (P) Ltd.
8. Micelles, Theoretical and Applied Aspects, V. Moral Plenum.
9. The Chemistry Mathematics Book, E. Steiner, Oxford University Press.
10. Mathematics for Chemistry, Doggett and Sutcliffe, Longman.
11. Mathematical Preparation for Physical Chemistry, F. Daniels, McGraw Hill.
12. Chemical Mathematics, D.M. Hirst, Longman.
13. Applied Mathematics for Physical Chemistry, J.R. Barrante, Prentice Hall.
14. Basic Mathematics for Chemists, Tebbutt, Wiley.
15. Quantum Chemistry, Ira N. Levine, Prentice Hall.
16. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill.

ANALYTICAL TECHNIQUES AND DATA ANALYSIS

Max. Marks 80

UNIT –I

SAMPLE PREPARATION, DEGESTION AND STATISTICAL ANALYSIS

- A. Sampling - Collection, Preservation and preparation of sample, Techniques of sampling of solid, liquid and gaseous samples, Operation of drying and preparing a solution of the analyte.
Principle, methodology and application of different types of digestions such as acid digestion, base digestion, enzymatic and microwave digestion for liquid and solid materials.
- B. Evolution and procession of Analytical Data, Precision and Accuracy, Types of Errors, Propagation of errors, Normal Distribution Curve, Standard deviation, Confidence limit, Graphical presentation of result-method of average, Method of Linear least square, Significant figures, Statistical aid to hypothesis of testing- t-test, F-test, Correlation coefficient, Rejection of data.

UNIT –II

SEPARATION TECHNIQUES

- A. Principle of Solvent Extraction, Methods of Extraction, Efficiency of extraction, Selectivity of extraction, applications.
- B. Principle, classification of chromatographic techniques, Technique and applications of paper chromatography, Thin-layer chromatography, HPTLC, Column chromatography.

UNIT –III

THERMAL AND AUTOMATED METHODS

- A. Principle, Instrumentation, Applications of TGA, DTA and DSC methods.
- B. Automated methods, Principle, instrumentation and application of flow injection analysis.

UNIT –IV

ELECTROCHEMISTRY

- A. Principles and instrumentation of pH potentiometry, coulometry and conductometry.
- B. Basic principles, Diffusion current, polarized electrode, Micro electrode, Dropping Mercury Electrode Ilkovic equation, Polarographic wave, Qualitative analysis Stripping methods, Cyclic Voltammetry, Amperometric titration :-curves, Differential pulse polarography and Square wave polarography.

BOOK SUGGESTED :

1. Fundamental of Analytical Chemistry- Skoog D.A. and West D.M. Saunders, College Publication.
2. Textbook of Quantitative Inorganic Analysis-Vogel A.I.
3. Principles and Practice of Analytical Chemistry-Fifield F.W and Kealey D. Black well Science
4. Instrumental Analysis R. Braun, McGraw Hill, International Edition.
5. Analytical Chemistry, Christian, G.D., WSE/Wiley.
6. Instrumental Analysis, Willard Meritt Dean, CBS.
7. Chemical Analysis, Brawn, McGraw Hill.
8. Fundamental of Analytical Chemistry-Skoog D.A. and West D.M.
9. Principles of instrumental analysis, Skoog Holler - Niemann.
10. Instrumental analysis, Wizard Dean and Merit.
11. Principle and PRACTICAL analytical chemistry, Fifield and Kealey.

PAPER NO 5. CH - 305

LABORATORY COURSE –V

Max. Marks 100

1. To calculate the activity with given radioactive source.
2. Determination of the half-life of Radionuclide.
3. Determination of absorption coefficient & half
4. Determination of absorption coefficient & half thickness of lead for gamma radiation.
5. Determination of range and energy of β particle
6. Prove the inverse square law for gamma rays.
7. Measurement of gamma ray energy by gamma ray spectrometry.
8. Determination of the partition coefficient for iodine between carbon tetrachloride & (a) Water, (b) aqueous potassium iodide.
9. Study of kinetics of exchange between ethyl iodide & the iodide ion.
10. Determination of the solubility product of lead iodide.
11. Determination of the dissociation constant of Barium Nitrate.
12. Determination of the concentration of iodine in a given sample (KI), by isotope dilution technique.
13. To study the effect of temperature, concentration of the reactant and catalyst on the rate of a chemical reaction (Hydrolysis/Nucleophilic Substitution).
14. Reaction between Sodium Formate and Iodine by
 - (i) Volumetric Method.
 - (ii) Conductometric Method.
16. Saponification of ethyl acetate
 - (i) Volumetric Method.
 - (ii) Conductometric Method.
17. Reaction between Acetone and Iodine.
18. To study the autocatalytic reaction between KMnO_4 and Oxalic acid.
19. Reaction between $\text{K}_2\text{S}_2\text{O}_8$ and Iodine.
20. Determination of pK_a by Kinetic Measurement.
21. Evaluation of Equilibrium constants from kinetic data.
22. Determination of rate constant of the decomposition of benzene diazonium chloride at different temperature.
23. To study the photolysis of uranyl oxalate.
24. To study the effect of substrate catalyst etc (i) HCl , $\text{K}_2\text{S}_2\text{O}_8$ (ii) KOH , NaOH .
25. To study the Activation parameters.
26. To study the solvent effect using some Aprotic & Protic Solvents.
27. To examine the substituent effect (Hammett equation).
28. To study the effect of Electrolyte on the rate hydrolysis (KCl , NaCl .)
29. To study some simple enzyme catalyzed reaction.
30. To study the Micellar Catalyzed Reaction.

Some advanced level sophisticated instrument based (FTIR, NMR, GC-MS, AAS, FLUORESCENCE SPECTROPHOTOMETER, TENSIO METER etc) experiments may be given to the students.

BOOK SUGGESTED:

1. Basic Experiment with radioisotopes by John, N. Andrews & David J. Hornsey, Pitam Publishing New York.
2. Practical radiochemistry by M.F.C. Ladd & W.H. Lee, Cleaver Hune press Ltd.
3. Practical Physical Chemistry by Alexander Findlay.
4. Experimental Physical Chemistry, D.P. Shoemaker, C.W. Garland and J.W. Niber, Mc Graw Hill Interscience.
5. Findlay's Physical Practical Chemistry, revised B.Phys.Levitt, Longman.

PAPER NO 6. CH –306

LABORATORY COURSE –VI

Max. Marks 100

A. SPECTROPHOTOMETRIC DETERMINATIONS

- I. Manganese / Chromium, Vanadium in steel sample.
- II. Nickel / Molybdenum / Tungsten / Vanadium / Uranium by extractive spectrophotometric method.
- III. Fluoride / Nitrate / Phosphate.
- V. Zirconium –Alizarin Red –S complex: Mole-ratio method.
- VI. Copper –Ethylene diamine complex: Slope-ratio method.

B. pH METRY

Stepwise proton-ligand and metal-ligand stability constant of complexes by Leving –Rossoti methods.

C. POLAROGRAPHY

Composition and stability constant of complexes.

D. FLAME PHOTOMETRIC DETERMINATIONS.

- (i) Sodium and potassium when present together
- (ii) Lithium / calcium / barium / strontium.
- (iii) Cadmium and magnesium in tap water.

E. REFRACTOMETRY

1. Determination the specific and molar refraction of a given liquid by abbe Refractometer.
2. Determine the variation of refractive index.
3. To verify law of refraction of mixture (glycerol + water).

F. SEPARATION AND QUANTITATIVE ESTIMATION OF BINARY AND TERNARY MIXTURES BY THE USE OF FOLLOWING SEPARATION TECHNIQUES:

1. Paper chromatography –Cadmium and Zinc, Zinc and Magnesium.
2. Thin –layer chromatography –separation of nickel, manganese, cobalt and zinc.
3. Ion-exchange.
4. Solvent extraction.
5. Electrophoretic separation.

Some advanced level sophisticated instrument based (FTIR, NMR, GC-MS, AAS, FLUORESCENCE SPECTROPHOTOMETER, TENSIO METER etc) experiments may be given to the students

BOOK SUGGESTED :

1. Quantitative Inorganic Analysis, A.I. Vogel.
2. Test book of quantitative chemical analysis, A.I. Vogel.
3. Practical Physical chemistry, A.M. James and F.E. Prichard, Longman.
4. Findley's Practical Physical Chemistry, B.P. Levi
5. Experimental Physical Chemistry, R.C. Das and B. Behera, Tata McGraw Hill.

FOURTH SEMESTER

PAPER NO 1. CH - 401

INSTRUMENTAL METHODS OF ANALYSIS

Max. Marks 80

UNIT –I

ADVANCED CHROMATOGRAPHY:

- A. Ion chromatography: Ion exchange equilibrium, Ion-exchange packing and Inorganic Applications.
- B. Size exclusion chromatography: Column packing, Theory of size of exclusion chromatography and applications.
- C. Supercritical fluid chromatography: Properties of supercritical fluid SFC-Instrumentation and operating variables, comparison with other types of chromatography, applications.
- D. Capillary Electrophoresis and capillary electro chromatography : overviews and applications

UNIT –II

X-RAY AND PROTON INDUCED SPECTROSCOPY:

- A. X-Ray fluorescent method: Principles-Characteristics x-ray emission. Instrumentation x-ray tube, Radioactive sources. Wavelength dispersive instruments. Energy dispersive instruments. Analytical Applications-Qualitative Analysis.
- B. Proton Induced X-Ray Spectroscopy : Theory, instrumentation and application.

UNIT –III

ATOMIC EMISSION SPECTROSCOPY

- A. Selectivity, sensitivity and interferences of atomic spectroscopy.
- B. Theory, instrumentation and application of flame photometer, AES, ICP-AES and AFS.

UNIT –IV

ATOMIC ABSORPTION SPECTROSCOPY AND HYPHENATED TECHNIQUES

- A. Theory instrumentation and application of flame and graphite furnace AAS, cold-vapor and hydride generation AAS.
- B. Theory, instrumentation and application of hyphenated techniques i.e. GC/HPLC/-MS, GC/IC/HPLC-ICP-MS.

BOOK SUGGESTED:

1. Instrumental methods of analysis, Willard, Meritt and Dean.
2. Basic concepts of analytical chemistry, S.M. Khopkar, John Wiley & Sons.
3. Metallurgical analysis, S.C. Jain.
4. Material Science and Engineering. An Introduction, W.D. Callister, Wiley.
5. Material Science, J.C. Anderson, K.D. Leaver, J.M. Alexander and R.D. Rawlings, ELBS.
6. Fundamentals of Analytical Chemistry, Skoog, Welt, Holler and Crouch Thomson Learning Inc.

PAPER NO 2. CH - 402
NATURAL PRODUCT AND MEDICINAL CHEMISTRY

Max. Marks 80

UNIT-I

- A. **Terpenoids and Carotenoids:** Classification, nomenclature, occurrence, isolation, general methods of structure determination of Citral, Geraniol, α -Terpeneol, Menthol, Farnesol, Zingiberene, Santonin, Phytol, Abietic acid and β – Carotene.
- B. **Alkaloids:** Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on Nitrogen heterocyclic ring, role of alkaloids in plant. Synthesis and biosynthesis of the following: Ephedrine, (+)- Coline, Nicotine, Atropine, Quinine and Morphine.

UNIT-II

- A. **Steroids:** Isolation, structure determination and synthesis of Cholesterol, Bile acids, Androsterone, Testosterone, Esterone, Progesterone, Aldosterone and Biosynthesis of cholesterol.
- B. **Plant Pigments:** Occurrence, nomenclature and general method of structure determination. Isolation and synthesis of Apigenin, Luteolin, Quercetin, Myrcetin, Quercetin-3-glucoside, Vitexin, Diadzin, Butein, Aureusin, Cyanidin-7-arebinoside, Cyanidin, Hirsutidin.

UNIT- III

Drug Design

- A. Development of new drugs procedures followed in drug design, concepts of lead compound and lead modification, concepts of prodrugs and soft drugs, Structure-Activity Relationship (SAR), Factors affecting bioactivity, resonance, inductive effect. Theories of drug activity: occupancy theory, rate theory, induced fit theory. Quantitative Structure Activity Relationship (QSAR).
- B. Concepts of drug receptors, lipophilicity, pharmacophore, pharmacological activity and typical range of parameters related to drug likeness.
- C. General introduction of pharmacokinetics and pharmacodynamics.

UNIT – IV

- A. **Anteoplastic Agents:** Introduction, Alkylating agents, antimetabolites, carcinolytic antibiotics, mitotic inhibitors.
- B. **Antibiotics:** Constitution and synthesis of penicillins, chloramphenicol, tetracycline and streptomycin.
- C. **Antimalarials:** Synthesis and properties of the following Antimalarial: 8-amino quinolone derivatives-Pamaquine, Primaquine, Pentaquine, Isopentaquine, 4- amino quinolone derivatives-Santoquine, Camaquine, Acridine derivatives-Mepacrine, Azacrine, Pyrimidine and Biguanid derivatives- Paludrine Pyrimethamine.

Book Suggested:

1. Natural Products: Chemistry and Biological Significance, J. Mann, R. S. Davidson, J. B. Hobbs.
2. D. V. Banthorpe and J. B. Harborne, Longman, Essex., Organic Chemistry, Vol. 2, I. L. Finar, ELBS.
3. Chemistry, Biological and Pharmacological properties of Medicinal Plants from the Americas, Ed. Kurt Hostettmann, M. P. Gupta and A. Marston, Harwood Academic Publishers.
4. Introduction to Flavonoids, B. A. Bhom, Harwood Academic Publishers.
5. New Trends in Natural Product Chemistry, Att-ur-Rahman and M. I. Choudhary, Harwood, Academic Publishers.

6. Insecticides of Natural Origin, Sukh Dev, Harwood Academic Publishers.
7. Introduction to medicinal Chemistry, A Gringuage, Wiley-VCH.
8. Burger's Medicinal Chemistry-1 (Chapter-9 and Ch- 14), Drug Ed. M. E. Discovery, Wolff, John Wiley.

MATERIAL AND NUCLEAR CHEMISTRY

Max.Marks 80

UNIT- I

NON EQUILIBRIUM THERMODYNAMICS: Fundamental concepts, Forces and Fluxes, Entropy production, Phenomenological Laws and Onsager's r for biological systems, coupled reactions.

UNIT- II**MATERIAL CHEMISTRY:**

Preparation and Properties of Nanoparticles, Materials-Metals, Ceramics (Oxide, carbides, sulphides, nitrides). Physical and chemical Methods, Size and Shape controlled Synthesis, Sol-gel methods, Optical Properties, Electrical and Magnetic Properties, Application of Nanoparticles. Characterization of Nanoparticles (SEM, TEM etc.)

UNIT-III**SUPRAMOLECULAR CHEMISTRY:**

Properties of covalent bonds, bond length, inter bond angles, Force constant, bond and molecular dipole moment, molecular and bond polarizability.

Intermolecular Forces, hydrophobic effects, Electro static, induction, dispersion and resonance energy, Hydrogen bond, Magnetic interactions. Principles of molecular association and organization Biological macromolecules, Molecular receptors and design principal, cryptands, Cyclophanes, calixarenes and cyclodextrins. Supramolecular reactivity and catalysis.

UNIT-IV**NUCLEAR AND RADIOCHEMISTRY****NUCLEAR THEORY :**

Nuclear cross section and nuclear radii, nuclear shells and magic numbers, theory of nuclear shell model, nuclear potentials, square well and simple harmonic oscillator potentials, application, liquid drop model, semi-empirical mass equation, application and limitations.

NUCLEAR FISSION :

Mass, energy and charge distribution of fission products, decay chains, prompt and neutrons, liquid drop model of nuclear fission.

NUCLEAR ENERGY :

Nuclear fission, chain reaction, multiplication factor, nuclear reactors

APPLIED RADIOCHEMISTRY :

Radioactive isotopes, purity and strength of radioisotopes. Radiochemical principle in the use of tracers, Application of Tracers in Chemical investigations, Physico-chemical methods, Analytical applications, Age determinations, Medical applications, Agricultural application.

BOOKS SUGGESTED:

1. Nuclear and Radiochemistry by G. Friedlander, J.W. Kennedy & J.M. Miller, John Wiley and Sons, New York.
2. Source Book on Atomic Energy – S. Glasstone, Affiliated East –West Press Pvt. Ltd. New Delhi.
3. Nuclear Physics by I. Kaplan, Addison –Wiley Publishing company, London.
4. Nuclear Chemistry and its applications, M. Haissinsky, Addison –Welsley, Publishing Company, London.
5. Essentials of Nuclear chemistry, H.J. Arnikar, Wiley Eastern Ltd, New Delhi.
6. Molecular Mechanics, U. Burkert and N.L. Allinger, ACS Monograph 177, 1982.
7. Mechanism and Theory in Organic Chemistry, T.H. Lowry and K.C. Richardson, Harper and Row.
8. Introduction to Theoretical Organic Chemistry and Molecular Modelling, W.B. Smith, VCH, Weinheim.
9. Physical Organic Chemistry, N.S. Isaacs, ELBS./ Longman.
10. Supramolecular Chemistry: concept and Perspectives, J.M. Lehn, VCH.
11. The Chemistry Mathematics Book, E. Steiner, Oxford University Press.
12. Chemical Mathematics, D.M. Hirst, Longman.
13. Applied Mathematics for Physical Chemistry, J.R. Barrante, Prentice Hall.
14. Quantum Chemistry, Ira N. Levine, Prentice Hall.
15. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill.

ENVIRONMENTAL & APPLIED CHEMICAL ANALYSIS

Max. Marks 80

UNIT –I

AIR POLLUTION MONITORING AND ANALYSIS

Classification of air pollution monitoring levels, air quality, standards and index, monitoring and analysis of selected air borne pollutants: SO₂, NO_x, SPM, VOC's, Pb, CO₂, POP's, Hg, carbon and ozone. Air pollution control devices Viz ESP, scrubber technique, baghouse filters etc. Atmospheric chemistry of acid rains, photochemical smog, green house effect, global warming, ozone hole.

UNIT –II

SOIL AND WATER POLLUTION

Soil and water quality standards, monitoring and analysis of selected soil water contaminants: COD, pesticides, heavy metals, POPs, fluoride, cyanide, nitrate, phosphate, oil & grease, Geobiochemical impact of municipal solid waste, steel plants effluent, domestic sewage. Control devices of water pollutants.

UNIT –III

FOOD ANALYSIS

- A. Introduction to general Constituents of food, Proximate Constituents and their analysis, Additives-Introduction -Types - Study of preservatives colors and Antioxidants and method of estimation, adulteration - Introduction, Types, Test for adulterants.
- B. Introduction standards composition and analysis of following foods : Wheat, Bread, Biscuits, Jam, Jelly, Honey, Milk, Ice Cream, Butter, Cheese, Milk Powder, Oils and Fats, Tea, Coffee, Soft drinks, Alcoholic beverages, Cereal and pulses, Confectionery, Fruits, Vegetables, Egg, Fish, Meat.

UNIT –IV

COSMETICS, CLINICAL AND DRUG ANALYSIS

- A. Introduction of Cosmetics, evaluation of cosmetics materials, raw material and additives, Cosmetics colors, Perfumes in cosmetics, Cosmetics formulating, introduction, standards and methods of analysis, Creams, face powders, Make-up, Shaving preparations, Bath preparations.
- B. Concepts and principles of analytic methods commonly used in the clinical species: i.e. ammonia, blood urea Nitrogen, Ca, Cl, CO₂, Fe, K, Li, Mg, Na, P, urea, glucose.
Method for analysis of proteins (i.e. albumin, bilirubin, creatinine, cholesterol, HDL-cholesterol, triglycerides, creatinine) and Enzymes (i.e. Alanine Aminotransferase, acid phosphatase, alkaline phosphatase, amylase, aspartate, aminotransferase, cholinesterase, lactate, and lipase).

BOOK SUGGESTED :

1. Environmental Chemistry, S.E. Manahan, Lewis Publishers.
2. Environmental chemistry, Sharma and Kaur, Krishna Publishers.
3. Environmental Chemistry, A.K. De, Wiley Eastern.
4. Environmental Chemistry, Analysis, S.M. Khopkar, Wiley Eastern.
5. Standard Method of Chemical Analysis, F.J. Welcher Vol. III, Van Nostrand Reinhold Co.
6. Environmental Toxicology, Ed. J. Rose, Gordon and Breach Science Publication.
7. Environmental Chemistry, C. Baird, W.H. Freeman.
8. Analytical chemistry, G.D. Christian, J. Wiley.
9. Fundamentals of Analytical Chemistry, D.A. Skoog, D.m. West and F.J. Holler, W.B. Saunders.
10. Analytical Chemistry - Principles, J.H. Kennedy, W. Saunders.
11. Analytical Chemistry-Principles, and Techniques, L.G. Hargis, Prentice Hall.
12. Principles of Instrumental Analysis, D.A. Skoog and J.L. Loary, W.B. Saunders.
13. Principles of Instrumental Analysis, D.A. Skoog, W.B. Saunders.
14. Quantitative Analysis, R.A. Day, Jr. and A.L. Underwood, Prentice Hall.
15. Environmental Solution Analysis, S.M. Khopkar, Wiley Eastern.

16. Basic Concepts of Analytical Chemistry, S.M. Khopkar, Wiley Eastern.
17. Handbook of Instrumental Techniques for Analytical Chemistry, F. Settle, Prentice Hall.
18. Environmental Biotechnology, Indushekar Thakur, I.K. International Pvt. Ltd.
19. Fundamental of Analytical Chemistry, D.A. Skoog, D.M. West, F.J. Holler and S.R. Crouch, Thompson Learning Inc.
20. APHA, 1977, "Methods of Analysis of air, water and soil" Washington US.

OPTIONAL PAPERS

CH-404 a

MEDICINAL CHEMISTRY

UNIT I

(a) **DRUG DESIGN:** Development of new drugs, procedures followed in drug design, concepts of lead compound and lead modification, concepts of prodrugs and soft drugs, structure – activity relationship (SAR). Theories of drug activity: Occupancy theory, rate theory, induced fit theory. Quantitative structure activity relationship. History and development of QSAR. Concepts of drug receptors. Lipophilicity and Lipinski Rule of 5.

(b) **PHARMACOKINETICS:** Introduction to drug absorption, disposition, elimination using pharmacokinetics, important pharmacokinetics parameters in defining drug disposition and in therapeutics.

(c) **PHARMACODYNAMICS:** Introduction, elementary treatment of enzyme stimulation, enzyme inhibition, membrane active drugs, drug metabolism, biotransformation significance of drug metabolism in medicinal chemistry.

UNIT II

(a) **ANTINEOPLASTIC AGENTS:** Introduction, role of alkylating agents and antimetabolites in treatment of cancer. Mention of carcinolytic antibiotics and Mitotic inhibitors. Mechlorethamine, cyclophosphamide, melphalan, uracil, mustards, and 6-mercaptopurine.

(b) **CARDIOVASCULAR DRUGS:** Introduction, cardiovascular diseases, drug inhibitors of peripheral sympathetic function. Direct acting arteriolar dilators. Synthesis of amyl nitrate, sorbitrate, diltiazem, quinidine, verapamil, methyldopa, atenolo, oxypropeno.

UNIT III

(a) **LOCAL ANTIINFECTIVE DRUGS:** Introduction and general mode of action. Synthesis of sulphonamides, furazolidine, nalidixic acid, ciprofloxacin, norfloxacin, dapson, amino salicylic acid, isoniazid, ethionamide, ethambutal, fluconazole, econazole, griseofulvin, chloroquin and primaquin.

(b) **ANTIBIOTICS:** Cell wall biosynthesis, inhibitors, β -lactam rings, antibiotic inhibiting protein synthesis.

Synthesis of penicillin G, penicillin V, ampicillin, amoxicillin, chloramphenicol, cephalosporin, tetracycline and streptomycin.

UNIT IV

PSYCHOACTIVE DRUGS- THE CHEMOTHERAPY OF MIND : Introduction, neurotransmitters, CNS

depressants, mode of action of hypnotics, sedatives, anti-anxiety drugs, benzodiazepines, busipirone. Antipsychotic drugs – the neuroleptics, antidepressants, butyrophenones, serendipity and drug development, stereochemical aspects of psychotropic drugs. Synthesis of diazepam, oxazepam, chlorazepam, alprazolam, phenytoin, ethosuximide, trimethadione, barbiturates, thiopental sodium, glutethimide.

Books Suggested

1. Introduction to Medicinal Chemistry, A Gringuage, Wiley-VCH
2. Wilson and Gisvold's Text Book of Organic Medicinal and Pharmaceutical Chemistry, Ed Robert F. Dorge
3. An Introduction to Drug Design, S. S. Pandeya and J.R.Dimmock, New Age International.
4. Burgers's Medicinal Chemistry and Drug Discovery, Vol-1(Chapter-9 and Chapter-14), Ed. M.E. Wolff, John Wiley.
5. Goodman and Gilman's Pharmacological Basis of Therapeutics, Mc-Graw Hill.
6. The Organic Chemistry of Drug Design and Drug Action, R. B. Silverman, Academic Press.
7. Strategies for Organic Drug Synthesis and Design, D.Lednicer, John Willey

CHEMISTRY OF SURFACTANTS

CH-404 b

UNIT- I

OVERVIEW OF SURFACTANTS: Classification of Surfactants, Physicochemical Properties of Surfactants, Critical Micelle Concentration , Determination, Effect of Additives, Aggregate Shapes , Structure and Morphology, Novel and New Generation Surfactants, Aggregation Behavior.

UNIT-II

PRINCIPLES OF SELF-ASSEMBLY: Closed and Continuous Association , Surfactant Micellization Pseudo-Phase Model , Mass Action Model, Estimation of Micelle Size , Size Dispersion of Micelles, Concentration Dependence of Micelle Size , Phase Behavior, Aggregation Behavior.

UNIT-III

SURFACTANT MIXTURES: Ideal and Non-Ideal Mixed Micelles , Regular Solution Model Size and Composition Distribution of Aggregates , Nonionic –ionic Surfactant Mixtures , Ionic -Ionic Surfactant Mixtures, Origin of Ideal and Non-Ideal Mixing Behavior, Polymer Surfactant Interaction.

UNIT-IV

APPLICATIONS OF SURFACTANTS: Micellar Catalysis, Quantitative Models , Micellar Enzymology, Phenomenon of Solubilization , Solubilization in Mixed Micelles, Drug Surfactant Interaction, Protein Surfactant Interactions, Microemulsions and its applications, Industrial Application of Surfactants.

Books:

1. Surfactants Edited by Th. F. Tadros, Academic Press
2. Micelles : Theoretical and Applied Aspects by Y. Moroi
3. Chemistry and Technology of Surfactants by R. J. Farn Wiley

CHEMISTRY AND APPLICATION OF PESTICIDES

CH-404c

UNIT-1

INTRODUCTION: What is pesticides, classification of pesticides, utility of pesticides, categories of toxicity, Threshold limit value, LD 50 value, Effect of pesticides in food, House hold and Human health.

UNIT-2

CHEMICAL TOXICOLOGY: Biochemical effects of pesticides, pesticides persistence, bioaccumulation and biomagnifications of pesticides, Toxicology of pesticides, Toxicology of organophosphates, carbamates, organochlorine and Dermal Toxicology of pesticides.

UNIT-3

INSTUMENTAL TECHNIQUES IN PESTICIDES DETECTION: Spectrophotometry, paper chromatography, Thin layer chromatography (TLC), GC-MS, indicator tube, High performance (pressure) Liquid chromatography (HPLC).

UNIT-4

PESTICIDES AND ITS RESIDUE ANALYSIS: Steps in pesticides residue analysis, clean-up, concentration (evaporation), Analysis, Extent of residue of pesticides in different commodities.

References

- Environmental chemistry. A.K De. New Age International Pvt. Ltd. 6th edition.
- Soil Testing and Analysis, plant, water and pesticide residues- Patiram, Bajendra N.S. Azad, Thakur and T.Ramesh. Agricultural, Horticultural, Food and Veterinary Science Book. 2nd edition.
- Toxicology of pesticides: Experimental, clinical and regulatory perspectives. Edited by: Lucio G. Costa, Corrado L. Galli Sheldon D. Murphy. Springer, 1st edition.
- Persistent Pesticide in the Environment- C.A Edward, CRC Press Inc., Florida 2nd edition.
- Agricultural chemicals and chemical mutagens- C.L. Canoria.
- Progress in pesticide Biochemistry and Toxicology- D.H Hutson and T.R Roberts. Willey, 7th edition.
- Air pollution from Pesticides and Agricultural process. Lee, R.F., Jr. CRC Press Inc., Florida, 1976, 174.

MOLECULAR SYMMETRY, COORDINATION AND ORGANOMETALLIC CHEMISTRY CH-404 d

UNIT – I

SYMMETRY AND GROUP THEORY IN CHEMISTRY: Symmetry elements and symmetry operation, definitions of group, subgroup, relation between orders of a finite group and its subgroup. Conjugacy relation and classes. Point symmetry group. Schonflies symbols, representations of groups by matrices (representation for the C_n , C_{nv} , C_{nh} , D_{nh} etc. groups to be worked out explicitly). Character of a representation. The great orthogonality theorem (without proof) and its importance. Character tables and their use; spectroscopy.

UNIT – II

A. METAL-LIGAND BONDING: Limitation of crystal field theory, molecular orbital theory, octahedral, tetrahedral and square planar complexes, bonding and molecular orbital theory.

B. 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), Selection rules, mechanism for break down of the selection rules, intensity of absorption, band width, spectra of d-d metal complexes of the type $[M(H_2O)]^{n+}$, spin free and spin paired ML_6 complexes of other geometries, Calculations of Dq , B and parameters, spin forbidden transitions, effect of spin-orbit coupling, Spectrochemical and Nephelouxetic series.

UNIT – III

A. REACTION MECHANISM OF TRANSITION METAL COMPLEXES: Energy profile of a reaction, reactivity of metal complexes, inert and labile complexes, kinetic application of valence bond and crystal field theories, kinetics of octahedral substitution, anation reactions, reactions without metal ligand bond cleavage. Substitution reactions in square planar complexes, the trans effect. Redox reactions, electron transfer reactions, mechanism of one electron transfer reactions, outer sphere type reactions, cross reactions and Marcus-Hush theory, inner sphere type reactions.

B. METAL-LIGAND EQUILIBRA IN SOLUTION: Stepwise and overall formation constants and their interaction, trends in stepwise constants, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, chelate effect and its thermodynamic origin, determination of binary formation constants by pH-metry and spectrophotometry.

UNIT – IV

METAL π -COMPLEXES: Metal carbonyls, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls; preparation, bonding, structure and important reactions of transition metal nitrosyl, dinitrogen and dioxygen complexes; tertiary phosphine as ligand. B. Transition metal complexes with unsaturated organic molecules, alkanes, allyl, dienedienyl, arene and trienyl complex, preparations, properties, nature of bonding and structure features. Important reaction relating to nucleophilic, electrophilic attack on ligands and organic synthesis. Alkylidenes, low valent carbenes nature of bond and Structural characteristics.

NANOCHEMISTRY

CH-404 e

UNIT I

GENERIC METHODOLOGIES FOR NANOCHEMISTRY AND NANOTECHNOLOGY

Introduction and classification, What is nanotechnology?, Classification of nanostructures, Nanoscale architecture, Summary of the electronic properties of atoms and solids, The isolated atom, Bonding between atoms, Giant molecular solids, The free electron model and energy bands, Crystalline solids, Periodicity of crystal lattices, Electronic conduction, Effects of the nanometre length scale, Changes to the system total energy, Changes to the system structure, How nanoscale dimensions affect properties

UNIT -II

MATERIAL CHEMISTRY

Preparation and Properties of Nanoparticles, Materials-Metals, Ceramics (Oxide, carbides, sulphides, nitrides).physical and chemical Methods, Size and Shape controlled Synthesis, Sol-gel methods, Optical Properties, Electrical and Magnetic Properties, Application of Nanoparticles.

UNIT-III

CHARACTERIZATION METHODS

X-ray diffraction, Debye-Scherrer formula, dislocation density, micro strain, Synchrotron Radiation, Principle and Applications, Raman Spectroscopy and its Applications, Dynamic Light Scattering (DLS). Electron microscopes: scanning electron microscope (SEM), transmission electron microscope (TEM), atomic force microscope (AFM), scanning tunneling microscope (STM), XPS, Working Principle, Instrumentation and Applications. Differential scanning calorimeter (DSC), Thermogravimetric/Differential Thermal Analyzer (TG/DTA), UV – Visible Spectrophotometer, FTIR, Principle and Applications, Photoluminescence (PL) Spectroscopy.

UNIT-IV

APPLICATIONS ON NANOCHEMISTRY

Nanobiology, Introduction, Bio-inspired nanomaterials, Interaction Between Biomolecules and Nanoparticle Surfaces, Different Types of Inorganic Materials Used for the Synthesis of Hybrid Nano-bio Assemblies, Applications of Nano in Biology, Nanoprobes for Analytical Applications, Current Status of Nanobiotechnology, Future Perspectives of Nanobiology; Nanosensors, Electrochemical, Nanobiosensors, Smart Dust; Nanomedicines, Nanodrug Administration Diagnostic and Therapeutic Applications.

References:

1. Nanoparticles: From Theory to Application Edited by Gu"nter Schmid, @ 2004 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim
2. Nanoparticles and Catalysis Edited by Didier Astruc @ 2008 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim
3. Peter Atkins, Tina Overton, Jonathan Rourke, Mark Weller, Fraser Armstrong, Mike HagermanShriver and Atkin's Inorganic Chemistry, Fifth Edition, Oxford, 2010.
4. Nanoscale Science and Technology, Robert W. Kelsall, Ian W. Hamley and Mark Geoghegan, John Wiley & Sons, Ltd., UK, 2005.
5. Introduction to Nanotechnology, Charles P. Poole Jr and Frank J. Owens, Wiley Interscience, 2003.
6. Nano:The Essentials: Understanding Nanoscience and Nanotechnology, T.Pradeep, Tata McGraw-Hill Publishing Company Limited, New Delhi, 2008.

CHEMISTRY OF NATURAL PRODUCTS

CH-404 f

UNIT-I	Terpenoids and Carotenoids	15 Hrs
	Classification; nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Structure determination, stereochemistry, biosynthesis and synthesis of the following representative molecules; Citral, Geraniol, α -Terpeneol, Menthol, Farnesol, Zingiberene, Santonin, Phytol, Abietic acid and β -Carotene.	
UNIT-II	Alkaloids	15 Hrs
	Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation classification based on nitrogen heterocyclic ring, role of alkaloids in plants. Structure, stereochemistry, biosynthesis and synthesis of the following: Ephedrine, (+)- Coniine, Nicotine, Atropine, Quinine and Morphine.	
UNIT-III	Gteroids	
	Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of Cholesterol, Bile acids, Androsterone, Testosterone, Estrone, Progesterone, Aldosterone.	
UNIT -IV	Plant Pigments	7 Hrs
	Occurrence, nomenclature, general methods of structure determination, isolation and synthesis of Apigenin, Luteolin, Quercetin, myrcetin, Quercetin-3-glucoside, Vitexin, Diadzein, Butein, Aureusin, Cyanidin-7-arabinoside, Cyanidin, Hirsutidin. Biosynthesis of flavonoids: Acetate pathway and Shikimic acid pathway.	
	Porphyryns	
UNIT -V	Structure and synthesis of Haemoglobin and Chlorophyll.	
	Prostaglandins	
UNIT -VI	Occurrence, nomenclature, classification, biogenesis and physiological effects. Synthesis of PGE ₂ and PGF _{2α} .	
	Pyrethroids and Rotenones	
	Synthesis and Reaction of Pyrethroids and Rotenones	
UNIT-VII .	Books Suggested :	
	1. Natural Products : Chemistry and Biological Significance, J. Mann, R.S. Davidson,	
	2. J B Hobbs, D.V. Banthrope and J B Harborne, Longman Organic Chemistry, Vol 2 , IL Finar ELBS	
	3. New Trends in Natural Products Chemistry , A R Rahman and M I Choudhury, Harwood Academic Publishers	
	4. Roods Chemistry of Carbon Compounds, Ed S. Coffey, Elsevier	

POLYMERS

CH-404 g

8 Hrs

UNIT- I Basics

Importance of polymers. Basic concepts: Monomers, repeat units, degree of polymerization. Linear, branched and network polymers. Classification of polymers. Polymerization: condensation, addition, radical chain-ionic and co-ordination and co-polymerization. Polymerization conditions and polymer reactions. Polymerization in homogeneous and heterogeneous system.

UNIT- II Polymer Characterization

14 Hrs

Polydispersion-average molecular weight concept. Number, weight and viscosity average molecular weights. Polydispersity and molecular weight distribution. The practical significance of molecular weight. Measurement of molecular weights. End-group, viscosity, light scattering, osmotic and ultracentrifugation methods. Analysis and testing of polymers-chemical analysis of polymers, spectroscopic methods, X-ray diffraction study. Microscopy. Thermal analysis and physical testing-tensile strength. Fatigue, impact. Tear resistance. Hardness and abrasion resistance.

UNIT-III Structure and Properties

14 Hrs

Morphology and order in crystalline polymers-configurations of polymer chains. Crystal structure of polymers. Morphology of crystalline polymers, strain-induced morphology, crystallization and melting. Polymer structure and physical properties-crystalline melting point T_m - melting point of homogeneous series, effect of chain flexibility and other steric factors, entropy and heat of fusion. The glass transition temperature, T_g -Relationship between T_m and T_g , effects of molecular weight, diluents, chemical structure, chain topology, branching and cross linking. Property requirements and polymer utilization.

UNIT-IV Polymer Processing

12 Hrs

Plastics, elastomers and fibres. Compounding. Processing techniques: Calendering, die casting, rotational casting, film casting, injection moulding, extrusion moulding, thermoforming, foaming, reinforcing and fibre spinning.

UNIT-V Properties of Commercial Polyme

12 Hrs

Polyethylene, polyvinyl chloride, polyamides, polyesters, phenolic resins, epoxy resins and silicone polymers. Functional polymers- Fire retarding polymers and electrically conducting polymers. Biomedical polymers- contact lens, dental polymers, artificial heart, kidney, skin and blood cells.

Books Suggested :

1. Textbook of Polymer Science, F W . Billmeyer Jr. Wiley
2. Polymer Science, V R Gowarikar, N V Viswanathan and J Sreedhar, Wiley Eastern
3. Contemporary Polymer Chemistry, H R Alcock and F W Lambe, Prentice Hall
4. Physics and Chemistry of Polymers, J M G Cowie, Blackie Academic and Professional

FORENSIC CHEMISTRY

Course -404h

Unit-I

Introduction to Forensic Science

Forensic science : methodologies and applications used in the forensic context. Organic and inorganic chemical analyses of physical evidence, principles of serology and DNA analysis, ballistics, arson, fingerprint analysis, drug analysis,

Unit-II

Forensic Chemistry

Chemical aspects of forensic science as it applies to criminal investigation and laboratory preparation. Instrumentation and chemistry associated with crimes. properties of the chemical evidence.. Details of the methods employed for analysis, such as color test, Chromatography (GC, GLC, HPLC), mass spectrometry (MS), GC-MS. Laboratory course. Instrumental Aspects of Liquid Chromatography Solvent delivery systems, sample inlets, temperature control, coupled column systems, detectors, and indirect detection other Separation Techniques

Unit-III

Toxicology

General principles and fundamentals of forensic toxicology, poisons, action, toxicity, postmortem characteristics, samples required for toxicological analysis and methods of collection, methods of preservation and analysis. Chemical, toxicological and pathological characteristics of commonly abused drugs, including the following: ethanol, barbiturates, narcotics, stimulants, and hallucinogens

Unit-IV

Applications of Forensic Chemistry

Investigation of crime against society, food adulteration, environmental pollution, use and distribution of unsafe chemicals, career in criminal investigation, in the laboratory analysis of forensic evidence,. Drug Enforcement Administration, Food and Drug Administration, Environmental Protection Agency, and Occupational Safety and Health Administration. environmental sciences, industrial hygiene,.

**(Combination should be- Lab course VII + Lab course VIII OR
Seminar + Project work)**

LABORATORY COURSE-VII

Max. Marks 100

A. MULTI-STEP SYNTHESIS OF ORGANIC COMPOUNDS

- (i) Beckmann Rearrangement: Benzanilide from benzene (Benzene Benzophenone Benzophenone oxime Benzanilide).
- (ii) Benzilic Acid Rearrangement: Benzilic acid from Benzoin (Benzoin Benzil Benzilic acid)
- (iii) Skraup's synthesis (Synthesis of heterocyclic Quinoline from o - Amino phenol
- (iv) p-Bromoaniline from Aniline (Aniline Acetanilide p - Bromoacetanilide p -Bromoaniline)
- (v) p-Nitroacetanilide from Acetanilide (Aniline Acetanilide p - Nitroacetanilide p - Nitroaniline)
- (vi) m Nitroaniline from Benzene (Benzene Nitrobenzene m - dinitrobenzene m- nitroaniline)
- (vii) Acridone from Anthranilic acid (Anthranilic acid o - Chlorobenzoic acid N -Phenylanthranilic acid Acridone)
- (viii) Enzymatic Synthesis Enzymatic reduction : Reduction of ethylace enantiomeric excess of S(+) ethyl - 3 - hydroxybutanone and determine its optical purity.

B. QUANTITATIVE ORGANIC ANALYSIS

- (i) Estimation of Sulphur by Messenger's Method.
- (ii) Estimation of Nitrogen by Kjeldahl Method.

C. ESTIMATION OF FUNCTIONAL GROUP

- (i) Estimation of Aniline.
- (ii) Estimation of Amino Group By Acetylation Method.
- (iii) Estimation of Hydroxyl Group By Acetylation Method.
- (iv) Estimation of Carbonyl Group By Hydrazone Formation Method.
- (v) Estimation of Carboxyl Group By Titration Method.
- (vi) Determination of Equivalent Weight of Carboxylic Acid By Silver Salt Method.
- (vii) Estimation of Glucose By Fehling Solution Method.
- (viii) Estimation of Glycine By Titration Method.

D. EXTRACTION OF ORGANIC COMPOUNDS FROM NATURAL SOURCES

- (i) Isolation of caffeine from leaves.
- (ii) Isolation of Casein from milk.
- (iii) Isolation of lactose from milk.
- (iv) Isolation of nicotine dipicrate from tobacco.
- (v) Isolation of Cinchonine from cinchona bark.
- (vi) Isolation of Piperine from black pepper.
- (vii) Isolation Lycopene from tomatoes.
- (viii) Isolation of β -Carotene from carrots.
- (ix) Isolation of Limonene from citrus rinds.

- (x) Isolation of protein and carbohydrates from seeds –colour test
- (xi) Extraction of Fatty oil from seeds and determination of refractive index of the oil.
- (xii) Isolation of protein and carbohydrate (as reducing sugars) from seed-colour test.

E. Some advanced level sophisticated instrument based (FTIR, NMR, GC-MS, AAS, FLUORESCENCE SPECTROPHOTOMETER, TENSIO METER etc) experiments may be given to the students. SUGGESTED BOOKS:

1. Practical Organic chemistry by A. I. Vogel.
2. Practical Organic chemistry by Mann and Saunders.
3. Practical Organic chemistry by Garg and Saluja.
4. The Systematic Identification of Organic compounds, R. L. Shriner and D. Y. Curtin.
5. Semimicro Qualitative Organic Analysis, N.D. Cheronis, J. B. Entrikin and E. M. Hodnett.
6. Experimental Organic chemistry, M. P. Doyle and W. S. Mungall.
7. Small Scale Organic preparation, P. J. Hill.
8. Experimental Biochemistry, by B.S.Roa and V.Deshpande. I.K. International Pvt.Ltd.
9. Comprehensive Practical Organic Chemistry, Preparation and Qualitative Analysis, V.K.Ahluwalia and Renu Aggarwal, University Press.

OR

Seminars

Seminar topics should be related to M. Sc. Syllabus or research oriented topics on recent trends in chemical sciences

**(Combination should be- Lab course VII + Lab course VIII OR
Seminar + Project work)**

LABORATORY COURSE –VIII

Max. Marks 100

A. TITRIMETRIC/GRAVIMETRIC DETERMINATIONS

- (i) Manganese in iron / Steel by Bismuthate / Lingane –Karplus/Periodate methods.
- (ii) Manganese in pyrolusite ores.
- (iii) Nickel in steel by dimethylglyoxime method.
- (iv) Lead by dithizone precipitation.

B. SPECTROPHOTOMETRIC DETERMINATIONS

- (i) Manganese/Chromium / Vanadium / Copper / Lead in Steel and Environmental / Industrial effluent samples.
- (ii) Nickel / Molybdenum / Tungsten / Vanadium / Uranium by extractive spectrophotometric method.
- (iii) Fluoride / Nitrite / Phosphate in tap / pond / river industrial waste water.
- (iv) Iron in water samples by thiocyanate and phenanthroline methods.

C. CHROMATOGRAPHIC SEPARATION

- (i) Separation and identification of the sugars present in the given mixture of glucose, fructose and sucrose by paper chromatography and determination of R_f values.
- (ii) Thin layer chromatography – separation of nickel, manganese, cobalt and zinc, Determination of R_f values.

D. FLOW INJECTION ANALYSIS.

Determination of the following anions/cations in synthetic/real/ environmental samples.

- (i) Ca^{2+} , Mg^{2+} , Al^{3+} , Mn^{2+} , Cr^{6+} , Fe^{3+}
- (j) (ii) F^- , Cl^- , PO_4^{3-} , NO_2^- , NO_3^- , SO_4^{2-} , BO_3^{3-} .

E. ATOMIC ABSORPTION SPECTROPHOTOMETER

Determination of metal contents (Fe/Pb/As/Zn/Co/Ni etc.) in real and environmental samples.

F. MISCELLANEOUS

- (i) Nutrient and micronutrient analysis in plant/soil/sediment.
- (ii) Speciation of toxic metals i.e. As, Hg, Se, etc.
- (iii) Analysis of clinical samples i.e. blood, urine, hair, etc.

Some advanced level sophisticated instrument based (FTIR, NMR, GC-MS, AAS, FLUORESCENCE SPECTROPHOTOMETER, TENSIMETER etc) experiments may be given to the students.

SUGGESTED BOOK:

1. Quantitative Inorganic Analysis, A.I. Vogel.
2. Standard Methods of Water Analysis.
3. Colorimetric Determination of Traces of Metals, E.B. Sandell.
4. GBC, Manuals on AAS analysis, Austria.

OR
Projects

- ☐ Recent trends in chemical sciences
- ☐ Based on synthesis of organic compounds, characterization
- ☐ Kinetic, thermodynamic studies
- ☐ Analysis of chemical substances from environmental, biological, food and pharmaceutical samples with analytical techniques
- ☐ Ore, rocks, coal, cement analysis

Note: The Project work will be based on research facilities available in colleges, institutions or university