हेमचंद यादव विश्वविद्यालय, दुर्ग (छ.ग.)

एम. एस–सी. रसायन शास्त्र
पाठ्यक्रम
सेमेस्टर परीक्षा– 2022–24

SYLLABUS

M. Sc. CHEMISTRY

SEMESTER EXAMINATION

2022-2024

11.5.22 11.5.22 11.5.22

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	COURSE	CREDIT	DURATION	INTERNAL ASSESSMENT	THEORY MARKS	TOTAL MARKS
CH - 1	GROUP THEORY AND CHEMISTRY OF METAL COMPLEXES	4	3 Hrs	20	80	100
CH - 2	CONCEPTS IN ORGANIC CHEMISTRY	4	3 Hrs	20	80	100
CH - 3	QUANTUM CHEMISTRY, THERMODYNAMICS AND CHEMICAL DYNAMICS - I	4	3 Hrs	20	80	100
CH - 4	THEORY AND APPLICATIONS OF SPECTROS COPY-I	4	3 Hrs	20	80	100

PRACTICAL (4 CREDIT)

PAPER	COURSE	CREDIT	DURATION	MARKS
CH - 5	Lab Course – I	2	8 Hrs	100
CH - 6	Lab Course – II	2	8 Hrs	100

SEMESTER –II (20 CREDIT)

THEORY (16 CREDIT)

PAPER	COURSE	CREDIT	DURATION	INTERNAL ASSESSMENT	THEORY MARKS	TOTAL MARKS
CH - 7	TRANSITION METAL COMPLEXES	4	3 Hrs	20	80	100
CH - 8	REACTION MECHANISM	4	3 Hrs	20	80	100
CH - 9	QUANTUM CHEMISTRY, THERMODYNAMICS AND CHEMICAL DYNAMICS - II	4	3 Hrs	20	80	100
CH - 10	THEORY AND APPLICATIONS OFSPECTROSCOPY-II	4	3 Hrs	20	80	100

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PRACTICAL (4 CREDIT)

PAPER	COURSE	CREDIT	DURATION	MARKS
CH - 11	Lab Course – III	2	8 Hrs.	100
CH - 12	Lab Course – IV	2	8 Hrs.	100

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

PAPER	COURSE	CREDIT	DURATION	INTERNAL ASSESSMEN	THEORY MARKS	TOTAL MARKS
CH – 13	RESONANCE SPECTROSCOPY, PHOTOCHEMISTRY AND ORGANOCATALYSIS	4	3 Hrs	20	80	100
CH – 14	CHEMISTRY OF BIOMOLECULES	4	3 Hrs	20	80	100
CH – 15	CATALYSIS, SOLID STATE AND SURFACE CHEMISTRY	4	3 Hrs	20	80	100
CH – 16	ANALYTICAL TECHNIQUES AND DATA ANALYSIS	4	3 Hrs	20	80	100

PRACTICAL (4 CREDIT)

PAPER	COURSE	CREDIT	DURATION	MARKS
CH – 17	Lab Course - V	2	8 Hrs.	100
CH – 18	Lab Course - VI	2	8 Hrs.	100

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SEMESTER –IV (20 CREDIT)

THEORY (16 CREDIT)

PAPER	COURSE	CREDIT	DURATION	INTERNAL ASSESSMENT	THEORY MARKS	TOTAL MARKS
CH – 19	INSTRUMENTAL METHODS OF ANALYSIS	4	3 Hrs	20	80	100
CH – 20	NATURAL PRODUCTS AND MEDICINAL CHEMISTRY	4	3 Hrs	20	80	100
CH – 21	MATERIAL AND NUCLEAR CHEMISTRY	4	3 Hrs	20	80	100
CH - 22	ENVIRONMENTAL & APPLIED CHEMICAL ANALYSIS	4	3 Hrs	20	80	100
	OPTIONAL PAPERS					
	In place of CH 22 students can opt any optional papers CH 22a to CH 22c					
CH – 22 a	CHEMISTRY OF SURFACTANTS	4	3 HRS	20	80	100
22 b	NANOCHEMISTRY	4				
22 c	POLYMERS	4				

PRACTICAL (4 CREDIT)

PAPER	COURSE	CREDIT	DURATION	MARKS
CH - 23	Lab Course - VII	2	8 Hrs.	100
CH - 24	Lab Course - VIII	2	8 Hrs.	100

SCHEME FOR PRACTICAL EXAMINATION

EXPERIMENT	MARKS
Experiments	60
Viva-voce	20
Sessional Marks	20
TOTAL MARKS	**100**

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FIRST SEMESTER

PAPER NO. CH –1

GROUP THEORY AND CHEMISTRY OF METAL COMPLEXES

Max. Marks 80

UNIT - I

SYMMETRY AND GROUP THEORY IN CHEMISTRY: Symmetry elements and symmetry operation- Centre of Symmetry- Plane and its types of Symmetry-Proper and Improper axis of Symmetry- Principal axis and subsidiary axes- The concept of groups- Assigning Point groups with illustrative examples- Symmetry operations and order of a group - Group theoretical rules (Group postulates) - Reducible and Irreducible representations- Matrix representations of symmetry operations. Definitions of group, subgroup, relation between orders of a finite group and its subgroup. Conjugacy relation and classes. Point symmetry group. Schoen flies 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 of C_2v, C_2h, C_3v 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. π-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.

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UNIT – IV

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

BOOKS 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. Earnshow, Pergamon.
4. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
5. Comprehensive Coordination Chemistry, Eds.G. Wilkinson, R.D. Gillars and J.A. McCleverty, Pergamon.

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PAPER NO. CH –2
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 benzonoid and non-benzenoid compounds, Huckel's rule 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 E_2, E_1 and E_1c B 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 cheleotropic reactions. Sigmatropic rearrangements - suprafacial and antarafacial shifts of H, sigmatrophic shifts involving carbon moieties, 3, 3- and 5, 5- sigmatropic rearrangements. Claisen, Cope and Aza-Cope rearrangements. Ene reaction.

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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, Blackle, Academic and Professional.
7. Pericyclic Reactions, S. M. Mukherji, Macmillan, India.
8. Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh, Macmillian.
9. Stereo chemistry of Organic Compounds, D. Nasipuri, New AgeInternational.
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.

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PAPER NO. CH – 3

QUANTUM CHEMISTRY, THERMODYNAMICS AND CHEMICAL DYNAMICS – I

Max. Marks 80

UNIT - I

A. MATHEMATICAL CONCEPT 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 isotherm, 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 solutions. Debye-Huckel Onsager treatment and its extension, ion solvent interactions. Debey-Huckel-Limiting Law. Debye-Huckel theory for activity coefficient of electrolytic solutions. Determination of activity and activity coefficient, Ionic strength, Thermodynamics of electrified interface. 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)

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BOOKS SUGGESTED:

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

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PAPER NO. CH - 4

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.

UNIT- II

MICROWAVE SPECTROSCOPY:

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

UNIT- III

SCATTERING SPECTROSCOPY:

A. **Electron Diffraction Spectroscopy** :Principle, instrumentations and application of Auger spectroscopy and Scanning Electron Microscopy for chemical characterization, electron diffraction of gases and vapours, The Wierl equation and co-related method, application of electron diffraction.

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

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 CO_2, N_2O, SO_2, NO_2, ClF_3.

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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. Spectrophometric Identification of Organic Compounds, R.M. Silversteion & F. X. Webster, John Wiley Publication

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PAPER NO. CH - 5
LABORATORY COURSE–I

Max. Marks 100

One Experiment from each section is compulsory

Sec-A (24 Marks)

01. Qualitative analysis of mixture containing 8 radicals including 2 less common metals from among the following by semimicro method.

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.

Acid Radicals:

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

Sec-B (20 Marks)

02. QUANTITATIVE ANALYSIS:

Separation and determination of two metal ions in ores, alloys, or mixtures in solution, one by volumetric and the other by gravimetric methods.

Sec-C (16 Marks)

03. ESTIMATION OF:

01. Phosphoric acid in commercial orthophosphoric acid.
02. Boric acid in borax.
03. Ammonia in ammonium salt.
04. Manganese dioxide in pyrolusite.
05. Available chlorine in bleaching powder.
06. Hydrogen peroxide in a commercial sample.

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04. 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) $TiO(C_9H_8NO)_2 . 2H_2O$

(3) cis-K $[Cr(C_2O_4)_2(H_2O)_2]$

(4) Na $[Cr (NH_3)_2(SCN)_4]$

(5) Mn $(acac)_3$

(6) $K_2[Fe(C_2O_4)_3]$

(7) Prussian Blue, Turnbull's Blue.

(8) $[Co (NH_3)_6] [Co(NO_2)_6]$

(9) cis-[Co(trien) (NO2)2]Cl.H2O

(10) Hg [Co(SCN)4]

(11) $[Co(Py)_2Cl_2]$

(12) $[Ni (NH_3)_6]Cl_2$

(13) $Ni(DMG)_2$

(14) $[Cu (NH_3)_4] SO_4.H_2O$

Mark Scheme:-

Ex. 1	**24**
Ex 2	**20**
Ex 3/Ex 4	**16**
Sessional	**20**
Viva	**20**
Total	**100**

BOOKS SUGGESTED:

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

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PAPER NO. CH –6
LABORATORYCOURSE–II

Max. Marks 100

One Experiment from each section is compulsory

Sec- A (30 marks)

ADSORPTION/SURFACE CHEMISTRY

1. To Study 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 $Fe^{+++}$and Cu^{++}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 Lands berger method.
2. Determination of Molar masses of Naphthalene/acetanilide
3. Molecular weight of polymers by viscosity measurements.

Sec- B (30 Marks)

CONDUCTOMETRY

1. Determination of the velocity constant, order of the reaction and energy of activation for hydrolysis 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 Fe^{++}/Fe^{+++} system.

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POLARIMETRY

1. Determination of rate constant for hydrolysis/inversion of sugar using a polarimeter.
2. Enzyme kinetics –inversion of sucrose.
3. Determination of the specific and molecular rotation of optically active substances.

Mark Scheme:-

Ex-1	**30**
Ex -2	**30**
Sessional	**20**
Viva	**20**
Total	**100**

BOOKS SUGGESTED:

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

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SECOND SEMESTER
PAPER NO. CH - 7
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 and 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, Selection rules, mechanism for breakdown of the selection rules, intensity of absorption, band width correlation, Orgel and Tanabe-Sugano diagram for transition metal complexes (d^1-d^9 states), spectra of d-d metal complexes of the type $[M\ (H_2O)_6]^{n+}$, spin free and spin paired ML6 complexes of other geometries, Calculations of Dq, B and β parameters, spin forbidden transitions, effect of spin-orbit coupling, Spectrochemical and Nephelouxetic series. Magnetic properties of complexes of various geometries based on crystal field model, spin free-spin paired equillibria in octahedral stereochemistry.

UNIT - III

A. **TRANSITION METAL COMPLEXES:** Tranisition 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 Metal Complexes 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.

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BOOKS SUGGESTED :

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

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PAPER NO. CH - 8
REACTION MECHANISM

Max. Marks 80

UNIT-I

A. **ALIPHATIC NUCLEOPHILIC SUBSTITUTION**: The SN2 and SN1 mechanisms. The neighboring group mechanism, neighboring group participation by π and σ bonds, anchimeric assistance. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis, ambident nucleophile and regioselectivity.

B. **AROMATIC NUCLEOPHILIC SUBSTITUTION**: The SNAr, SN1 and benzyne 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 – SE1, SE2 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. Theortho/para ratio, ipso attack, orienation in other ring systems. Reactivity-Effect of substrates and electrophiles. Vilsmeir 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, hydrogenation of aromatic rings, Hydroboration, Micheal 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–Perkins, Aldol, Claisen, benzoin, Mannich, Knoevengel, Stobbereactions. Hydrolysis of esters and amides, ammonolysis of esters.

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BOOKS SUGGESTED:

1. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, Johan Wiley.
2. Modern Organic Reactions, H. O. House, Benjamin.
3. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackle Academic & Professional.
4. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
5. Structures and Mechanismin Organic Chemistry, C.K. Ingold, Cornell University Press.
6. Reaction Mechanismin Organic Chemistry, S.M. Mukherji and S.P. Singh, Macmillian
7. Organic Chemistry Concepts and Application, Jagdamba Singh, Pragati Prakashan
8. Organic reactions and mechanisms, P.S. Kalsi, New Age International.

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PAPER NO. CH –9
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 for 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 partition functions. Thermodynamic function using appropriate Partition functions. 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 and Stern models. Over potentials and exchange current density, Derivation of Butler – Volmer equation, Tafelplot. 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.

UNIT –IV

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

11.5.22 11.5.22 11.5.22

BOOKS SUGGESTED:

1. The Chemistry Mathematics Book, E. Steiner, Oxford University Press.
2. Mathematics for Chemistry, Doggett and Sutclilffe, Longman.
3. Mathematical Preparation for Physical Chemistry, F. Daniels, McGraw Hall.
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 Electro chemistry 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.

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PAPER NO. CH - 10

THEORY AND APPLICATIONS OF SPECTROSCOPY –II

Max. Marks 80

UNIT - I

ULTRAVIOLET AND VISIBLE SPECTROSCOPY:

Introduction, Intensity of vibrational – electronic spectra, Frank-Condon principle, dissociation energy, Rotational fine structure of electronic – vibrational transitions, shape of molecular orbitals of some molecules viz., H_2, He_2, N_2, O_2. Electronic spectra of organic molecules, chromophores, Applications of electronic spectroscopy and identification of organic molecules. Spectrophotometric studies of complex ions, determination of ligand/metal ratio in a complex, determination of stability constants.

UNIT - II

INFRA RED SPECTROSCOPY:

Introduction, simple and enharmonic oscillators in vibrational spectroscopy, diatomic-vibrating rotor, 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 and phenols aldehydes and ketones, ethers, esters, carboxylic acids, amines and amides.

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 spectrophotometry: Introduction.

UNIT - IV

NUCLEAR RESONANCE SPECTROPHOTOMETRY:

Theory of NMR spectroscopy, interaction of nuclear spin and magnetic moment, chemical shift, processional 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 (aliphatic, olephinic, alkyne, aromatic and carbonyl carbon)

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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. Spectrophometric Identification of Organic Compounds, R.M. Silverstein & F.X. Webster, John Wiley Publications.

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PAPER NO. CH - 11
LABORATORY COURSE –III

Max. Marks 100

One Experiment from each section is compulsory

Sec- A (10 Marks)

01. GENERAL METHODS OF SEPARATION AND PURIFICATION OF ORGANIC COMPOUNDS WITH SPECIAL REFERENCE TO:

Solvent Extraction

Fractional Crystallisation

02. DISTILLATION TECHNIQUIES:

Simple distillation, steam distillation, Fractional distillation and distillation under reduced pressure.

Sec- B (30 Marks)

01. 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 analyses at least 10 different binary mixtures.)

Sec- C (20 Marks)

01. PREPARATION OF ORGANIC COMPOUNDS: SINGLE STEP REPARATIONS.

a. **Acetylation:** Synthesis of β-Naphthyl acetate from β-Naphthol/Hydroquinone diacetate from Hydroquinone.
b. **Aldol condensation:** Dibenzal acetone from benzaldehyde.
c. **Bromination:** p-Bromoacetanilide from acetanilide.
d. **Cannizzaro Reaction:** Benzoic acid and Benzyl alcohol from benzaldehyde.
e. **Friedel Crafts Reaction:** O-Benzoyl Benzoic acid from phthalic anhydride.
f. **Grignard Reaction:** Synthesis of triphenyl methanol from benzoic acid.
g. **Oxidation:** Adipic acid by chromic acid oxidation of cyclohexanol.
h. **Perkin's Reaction:** Cinnamic acid from benzaldehyde.
i. **Sandmeyer Reaction:** p-Chlorotoluene from p-toluidine/o-Chlorobenzoic acid from anthranilic acid.
j. **Schotten Baumann Reaction:** β-Naphthyl benzoate from: β-Naphthol / Phenyl benzoate from phenol.
k. **Sulphonation Reaction:** Sulphanilic acid from aniline.

Mark Scheme:-

Ex. 1	10
Ex. 2	30
Ex .3	20
Sessional	20
Viva	20
Total	100

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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 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. Practical Physical chemistry by Alexander Findlay.
7. Experimental Physical chemistry, D. P. Shoemaker, G. W. Garland and J. W. Niber, McGraw Hill Inter science.
8. Findlay's Practical Physical chemistry.

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PAPER NO. CH –12
LABORATORY COURSE –IV

Max. Marks 100

One Experiment from section A and two exercises from section B are compulsory.

Sec- A (10 Marks)

01. 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.

02. 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 EXCEL, WORD, POWERPOINT, SPSS, ORIGIN, MATLAB, EASYPLOT.

Sec- B (2×25 Marks)

1 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

2. ELECTROPHORESIS

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

3. SPECTROSCOPY

01. Verification of Beer's Lambert Law.
02. Determination of stoichiometry and stability constant of inorganic (e.g. ferric –salicylclic acid) and organic (e.g. amine-iodine) complexes, thiocynam.
03. Characterization of the complexes by electronic and IR, UV spectral data.
04. Determination of Indicator constant (pKa)of methyl red.

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Mark Scheme:-

Ex. 1	**10**
Ex 2	**25**
Ex 3	**25**
Sessional	**20**
Viva	**20**
Total	**100**

BOOKS 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. Killngbeck, Adam Hilger.
4. Computer Programmingin FORTRANIV, V.Rajaraman, PrenticeHall.
5. An Introduction to Digital Computer Design, V. Rajaraman and T. Radhakrishnan, PrenticeHall.
6. Experiments in Chemistry, D.V. Jahagirdar.

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THIRD SEMESTER

PAPER NO. CH - 13

RESONANCE SPECTROSCOPY, PHOTOCHEMISTRY AND ORGANOCATALYSIS

Max. Marks 80

UNIT –I

A. **ELECTRON SPIN RESONANCE SPECTROSCOPY:** Introduction, principle, 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, splittings, applications.

UNIT –II

A. **PHOTOELECTRON SPECTROSCOPY:** Basic principle for atoms and molecules;

Photo-electric effect, ionization process, Koopman's theorem, Auger electron spectroscopy,

Determination of Dipolemoment. Photoelectron spectra of simple molecules-ESCA.

B. **PHOTOACOUSTIC SPECTROSCOPY:** Basic principle of Photo acoustic Spectroscopy (PAS), PAS –gases and condensed system. Chemical and Surface applications.

UNIT –III

A. **PHOTOCHEMICAL REACTIONS:** Interaction of electromagnetic radiation with matter, 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 photo chemical reactions.

C. **MISCELLANEOUS PHOTOCHEMICAL REACTIONS:** Photo-Fries reactions of anilides, Photo-Fries rearrangement. Barton reaction. Singlet molecular oxygen reactions. Photochemical formation of smog. Photo degradation of polymers, Photochemistry of vision.

UNIT –IV

A. **ORGANOCATALYSIS**

General Principles: Energetics, Catalytic cycles, catalytic efficiency and life time, selectivity. Type of organometallic reactions: Ligand substitution, Oxidative addition, reductive elimination and insertion and de-insertion. Homogeneous catalysis: Hydrogenetion of alkenes, Hydroformylation, Monosubstituted acetic acid synthesis, Wacker oxidation of alkenes. Alkenes metathesis, Palladium-Catalysed C-C bond forming reactions, asymmetric oxidation. Heterogenous catalysis: The nature of heterogenous catalysts, Fischer- Tropsch synthesis, alkene polymerization.

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BOOK SUGGESTED:

1. Infrared and Raman Spectra: Inorganic and Coordination Compounds, K. Nakamoto, Wiley.
2. Fundamentals of Photo chemsitry, K.K. Rohtagi- Mukherji, Wiley-Eastern.
3. Essentials of Molecular Photo chemistry, A. Gilbert and Baggott, Blackwell Scientific Publications.
4. Molecular Photo chemsitry, N.J. Turro, W.A. Benjamin.
5. Introductory Phto chemistry, 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, PrenticeHall.
8. Organic Photo chemistry, J. coxon and B. Halton, Cambridge University Press.
9. Shriver & Atkins Inorganic Chemistry: P. Atkins, T. Overtone, J. Rourke, M. Weller, F. Armstrong Oxford University Press
10. Inorganic Chemistry: C.E. Housecraft, A.G. Sharpe, Pearson Education Limited.
11. InorganicChemistry:PrinciplesofStructureandReactivity:J.E.Huheey, Keiter, Keiter, OMedhi, Pearson Education

13 . Organo metallic Chemistry: AUnified Approach: R.C. Mehrotra, A.Singh, New Age Publishers.

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PAPER NO. CH - 14
CHEMISTRY OF BIOMOLECULES

UNIT-I **Max. Marks 80**

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 Ion-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 – carboxypeptibase and carbonic anhydrase. Iron enzymes – catalase, peroxidase and cytochrome P-450. Copper enzymes-superoxide dismutase. Molybdenum oxatransferase enzymes –xanthineoxidase.

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 orsynzymes.

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 mechnochemical 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.

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BOOKS 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, Elservier.
4. Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.
5. Bioinorganic Chemistry, I. Bertinin, 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, PrenticeHall.
9. Enzyme Chemistry: Impact and Applications, Ed. Collin J Suckling, Chapman and Hall.
10. Enzyme Mechanisms Ed, M.I. PageandA. Williams, Royal Society of Chemistry.
11. Fundamentals of Enzymology, N.C.PriceandL. Stevens, Oxford University Press.
12. Immobilizaed 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 Reacitons fligingcells, 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, Gruissem and Jones, I.K. International Pvt. Ltd.

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PAPER NO. CH –15
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 micells, micro-emulsion. Micellar Catalysis, Surface tension capillary action, pressure difference across curved surface (Laplace equation), vapour 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 - Schotty defects and Frankel defects. Thermodynamics of Schotty 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, 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.

11.5.22 11.5.22 11.5.22

BOOKS 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, McGrawHill.
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 McGrawHill.

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PAPER NO. CH –16
ANALYTICAL TECHNIQUES AND DATA ANALYSIS

Max. Marks 80

UNIT –I

SAMPLE PREPARATION, DIGESTION AND STATISTICAL ANALYSIS

A. Sampling - Collection, Preservation and preparation of sample, Techniques of sampling solids, liquids and gases, 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 testing-t-test,

F-test, Correlation coefficient, Rejection of data.

UNIT –II

SEPARATION TECHNIQUES

A. Efficiency of extraction, Selectivity of extraction, Extraction system, Method of Extraction, applications.

B. Principle, classification of chromatographic techniques, Technique and applications of paper chromatography, Thin-layer chromatography, HPLC, Column chromatography. Gas Chromatography

UNIT –III

THERMAL AND AUTOMATED METHODS

A. Principle, Instrumentation, Application of TGA, DTA and DSC methods.

B. Automated methods, Principle, instrumentation and application of flow injection analysis.

UNIT –IV

A. **ELECTROCHEMISTRY**

Principles and instrumentation of pH potentiometry, coulometry and conductometry.

B. **POLAROGRAPHY**

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 Squarewave polarography.

11.5.22 11-5-22 11-5-22

BOOK SUGGESTED :

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

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PAPER NO. CH - 17
LABORATORY COURSE–V

Max. Marks 100

Any Two experiments from the following are compulsory

1. Determination of the partition coefficient for iodine between carbon tetrachloride & (a) Water,
   (b) Aqueous potassium iodide.
2. Study of kinetics of exchange between ethyl iodide & the iodide ion.
3. Determination of the solubility product of lead iodide.
4. Determination of the dissociation constant of Barium Nitrate.
5. Determination of the concentration of iodine in a given sample (KI)by isotope dilution technique.
6. To study the effect of temperature, concentration of the reactant and catalyst on the rate of a chemical reaction (Hydrolysis/Nucleophilic Substituttion).
7. To study Reaction between Sodium Formate and Iodine by
   01. Volumetric Method.
   02. Conductometric Method.
8. Saponification of ethylacetate
   01. Volumetric Method.
   02. Conductometric Method.
9. To study the reaction between Acetone and Iodine.
10. To study the autocatalylic reaction between $KMnO_4$ and Oxalic acid.
11. To study the reaction between $K_2S_2O_8$ and Iodine.
12. Determination of pKa by Kinetic Measurement.
13. Evaluation of Equilibrium constants from kinetic data.
14. Determination of rate constant of the decomposition of benzene diazonium chloride at different temperature.
15. To study the photolysis of uranyl oxalate.
16. To study the effect of substate catalyst etc (i) HCl, $K_2S_2O_8$ (ii) KOH, NaOH.
17. To study the Activation parameters.
18. To study the solvent effect using some Aprotic & Protic Solvents.
19. To examine the substituent effect (Hammette quation).
20. To study the effect of Electrolyte on the rate hydrolysis (KCl, NaCl,)
21. To study some simple enzyme catalyzed reaction.
22. To study the Micellar Catalyzed Reaction.

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

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Marks Distribution

Ex. 1	-	**30**
Ex. 2	–	**30**
Viva	–	**20**
Sessional	–	**20**
Total	-	**100**

BOOK SUGGESTED:

1. Practical Physical Chemistry by Alexander Findlay.
2. Experimental Physical Chemistry, D.P. Shoemaker, C.W. Garland and J.W. Niber, McGraw Hill Inter science.
3. Findlay'sical Practial Chemistry, revised B.Phys. Levitt, Longman.

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PAPER NO. CH –18
LABORATORY COURSE –VI

Max. Marks 100

Any Two experiments from the following are compulsory

Sec A (25 Marks)

01. SPECTROPHOTOMETRIC DETERMINATIONS

A. Manganese / Chromium, Vanadium in steel sample.

B. Nickel / Molybdenum / Tungsten / Vanadium / Uranium by extractive spectrophotometric method.

C. Fluoride / Nitrate /Phosphate.

D. Iron –phenanthroline complex; Job'sMethod for determination of stability constant of complex.

E. Zirconium –Alizarin Red –S complex: Mole-ratio method.

F. Copper –Ethylenediamine complex: Slope-ratio method.

02. POLAROGRAPHY

Composition and stability constant of complexes.

Sec B (25 Marks)

01. pHMETRY

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

02. FLAME PHOTOMETRIC DETERMINATIONS.

(i) Sodium and potassium when present together

(ii) Lithium / Calcium / Barium /Strontium.

(iii) Calcium and Magnesium in tap water.

03. REFRACTOMETRY

1. Determination of 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).

Sec C (10 Marks)

01. 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, TENSIOMETER etc.) experiments may be given to the students**

Marks Distribution

Ex. 1	–	**25**
Ex. 2	–	**25**
Ex. 3	–	**10**
Viva	–	**20**
Sessional	–	**20**
Total	–	**100**

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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.Leviu7
5. Experimental Physical Chemistry, R.C. Das and B. Behera, Tata McGrawHill.

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FOURTH SEMESTER
PAPER NO. CH - 19
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 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 electrochromategraphy: 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. Wave length dispersive instruments. Energy dispersive instruments. Analytical Applications-Qualitative Analysis.

B. Proton Induced X-Ray Spectroscopy: Theory, instrumentation and applications.

UNIT –III

ATOMIC EMISSION SPECTROSCOPY

A. Selectivity, sensitivity and interferences of atomic spectroscopy.

B. Theory, instrumentation and application of flame photometry, AES, ICP-AES and AFS.

UNIT –IV

ATOMIC ABSORPTION SPECTROSCOPY AND HYPHENATED TECHNIQUES

A. Theory, instrumentation and applications of flame and graphite furnace AAS, cold-vapour and hydride generation AAS.

B. Theory, instrumentation and application of hyphenated techniques i.e. GC/HPLC/MS-GC/IC/HPLC- ICP-MS.

BOOKS SUGGESTED:

1. Instrumental methods of analysis, Willard, Meritt and Dean.
2. Basic concepts of analytical chemistry, S.M. Khopkar, JohnWiley & 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. Alex ander and R.D. Rawlings, ELBS.
6. Fundamentals of Analytical Chemistry, Skoog, Welt, Holler and Crouch Thomson Learning Inc.

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PAPER NO. CH - 20
NATURAL PRODUCTS 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,
(+) - Conine, Nicotine, Atropine, Quinine and Morphine.

UNIT-II

A. **Steroids:** Isolation, structure determination and synthesis of Cholesterol, Bile acids, Androsterone, Testosterone, Esterone, Progestrone, Aldostrone and Biosythesis 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, Diadzine, Butein, Aureusin, Cyanidin, Hirsutidin.

UNIT- III

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), Factors affecting bioactivity, resonance, inductive effect. Theories of drug activity: occupancy theory, rate theory, induced fit theory. Quantitative Structure Activity Relationship (QSAR)-Hansch approach-free Wilson model, relationship between free Wilson and Hans analysis

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. **Antineoplastic 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 drug: 8-amino quinoline derivatives- Pamaquine, Primaquine, Pentaquine, Isopentaquine.

D. **aminoquinoline derivatives**- Santoquine, Camaquine, Acridine derivatives-Mepacrine, Azacrin, Pyrimidine and Biguanidine derivatives-Paludrine, Pyremethamine.

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Book Suggested:

1. Natural Products: Chemistry and Biological Significance, J. Mann, R.S. Davidson, J.B. Hobbs.
2. D.V. Banthrope and J.B. Harbrone, Longman, Essex., Organic Chemistry, Vol.2, I.L. Finar, ELBS.
3. Chemistry, Biologcal and Pharmacological properties of Medicinal Plants from the Americans, Ed. Kurt Hostettmann, M. P. Gupta and A. Marston, Harwood Academic Publishers.
4. Introductionto Flavonoids, B.A. Bhom, Harwood Academic Publishers.
5. New Trendsin 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'sMedicinalChemistry-1(Chapter-9andCh-14), DrugEd. M.E. Discovery, Wolff, John Wiley.
9. The Science of Flavanoids, Erich Groteworld, Springer

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PAPER NO. CH – 21

MATERIAL AND NUCLEAR CHEMISTRY

Max. Marks 80

UNIT- I

NON EQUILIBRIUM THERMODYNAMICS:

Fundamental concepts, Forces and Fluxes, Entropy production, Phenomenological Laws and Onsager's theory 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, TEMetc.)

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, Electrostatic, induction, dispersion and resonance energy, Hydrogen bond, Magnetic interactions. Principles of molecular association and organization. Biological marcomolecules, Molecular receptors and design principle, cryptands, Cyclophanes, calixarenes and cyclodextrins.

Supramoleular 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 delayed 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.

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BOOKS SUGGESTED:

1. Nuclear and Radio chemistry by G. Friedlander, J.W. Kennedy & J.M. Miller, John Wittey and Sons, Ine New York.
2. Source Book Atomic Energy–S. Glasstone, Affiliated East–West Press Pvt. Ltd. New Delhi.
3. Nuclear Physics by I. Kaplan, Addision –Welsly. Publishing company London.
4. Nuclear Chemistry and its applications, M. Haissinsky, Addision– Welsley, Publishing Company, London.
5. Essentials of Nuclear chemistry, H.J. Arnikar, Wiley Eatern Ltd, New Delhi.
6. Molecular Mechanics, U. Burkert and N.L. Allinger, ACS Monograph 177, 1982.
7. Mechanism and Theoryin Organic Chemistry, T.H. Lowry and K.C. Richrdson, 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. Quantum Chemistry, Ira N. Levine, PrenticeHall.
12. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGrawHill.

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PAPER NO. CH – 22
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: SO_2, NO_x, SPM, Volatile organic compounds, Pb, CO_2, Persistent organic compounds, Hg, carbon and ozone. Air pollution control devices Viz ESP, scrubber technique, baghouse filters etc. Atmospheric chemistry of acid rains, photochemical smog, greenhouse effect, global warming, ozone hole.

UNIT –II

SOIL AND WATER POLLUTION

Soil and water quality standards, monitoring and analysis of selected soil and water contaminants: COD, pesticides, heavy metals, POP's, 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

1. Introduction to general constituents of food- Proximate Constituents and their analysis, Additives- Introduction, types, study of preservatives colors and antioxidants and methods of estimation, adulteration - Introduction, types, test for adulterants.
2. Introduction of 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 analytical methods commonly used in the clinical species: i.e. ammonia, Nitrogen, Ca, Cl, CO_2, Fe, K, Li, Mg, Na, P, urea, glucose.

Method for analysis of proteins (i.e. albumin, bilirubin, creatinine, cholesterol, HDL-cholesterol, triglycerides) and Enzymes (i.e. Alanine Aminotransferase, acid phosphatase, alkaline phosphatase, amylase, aspartate, aminotransferase, cholinesterase, lactate, and lipase).

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

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OPTIONAL PAPERS

CH-22a

CHEMISTRY OF SURFACTANTS

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 SUGGESTED:

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

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CH-22b

NANO CHEMISTRY

Max Marks 80

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-Scherer 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/Diffferential 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,

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Nanoprobes for Analytical Applications, Current Status of Nanobiotechnology, Future Perspectives of Nanobiology; Nanosensors, Electrochemical, Nanobiosensors, Smart Dust; Nanomedicines, Nanodrug Administration Diagnostic and Thenrapeutic Applications.

BOOKS SUGGESTED :

01. Nanoparticles: From Theory to Application Edited by Gu¨nter Schmid, @ 2004 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim
02. Nanoparticles and Catalysis Edited by Didier Astruc @ 2008 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim
03. Peter Atkins, Tina Overton, Jonathan Rourke, Mark Weller, Fraser Armstrong, Mike Hagerman Shriver and Atkin's Inorganic Chemistry, Fifth Edition, Oxford, 2010.
04. Nanoscale Science and Technology, Robert W. Kelsall, Ian W. Hamley and Mark Geoghegan, John Wiley & Sons, Ltd., UK, 2005.
05. Introduction to Nanotechnology, Charles P. Poole Jr and Frank J. Owens, Wiley Interscience, 2003.
06. Nano:The Essentials: Understanding Nanoscience and Nanotecnology, T.Pradeep, Tata McGraw-Hill Publishing Company Limited, New Delhi, 2008.
07. Handbook of Nanotechnology, Bharat bhushan, Springer
08. Textbook of Nanoscience and Nanotechnology, B.S.Murty, Baldev Raj, James Murday. Springer

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CH-22c

POLYMERS

Max Marks 80

UNIT-I

I Basics **8Hrs**

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.

II PolymerCharacterization14Hrs

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 ultra-centrifugation 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-II

III Structure and Properties **14Hrs**

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 Tm- melting point of homogeneous series, effect of chain flexibility and other steric factors, entropy and heat of fusion. The glass transition temperature, Tg-Relationship between Tm and Tg, effects of molecular weight, diluents, chemical structure, chain topology, branching and cross linking. Property requirements and polymer utilization.

IV Polymer Processing **12Hrs**

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

UNIT-IV

V Properties of Commercial Polymers **12Hrs**

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.

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BOOKS SUGGESTED

1. Textbook of Polymer Science, F W. BillmeyerJr. 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, JMGCowie, Blackie Academic and Professional.
5. Polymer Chemistry introduction , Malcom T Stevens, Addison-Wesley Educational Publishers Inc.

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PAPER NO. CH –23

LABORATORY COURSE –VII

MAX MARKS 100

One Experiment from each section is compulsory

Sec-A (25 marks)

A. MULTI - STEP SYNTHESIS OF ORGANIC COMPOUNDS

(i) Beckmann Rearrangement: Benzanilide from benzene
(Benzene Benzophenone Benzo phenoneoxime Benzanilide).

(ii) Benzilic Acid Rearrangement: Benzilic acid from Benzoin
(Benzoin Benzil Benzilic acid)

(iii) Skraup's synthesis
(Synthesis of heterocyclic Quinoline from o – Aminophenol)

(iv) p –Bromoaniline from Aniline
(Aniline Acetanilide p - Bromoacetanilide p - Bromoaniline)

(v) p –Nitroacetanilide from Acetanilide
(Aniline Acetanilide p - Nitroactanilide 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 ethylaceenantiomeric
Excess of S (+) ethyl - 3 - hydroxybutanone and determine its optical purity.

Sec-B (20 marks)

A. QUANTITATIVE ORGANIC ANALYSIS

(i) Estimation of Sulphur by Messenger's Method.

(ii) Estimation of Nitrogen by Kjeldahl Method.

B. 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.

Sec-C (15 marks)

A. EXTRACTION OF ORGANIC COMPOUNDS FROM NATURALSOURCES

(i) Isolation of caffeine from leaves.

(ii) Isolation of Casein from milk.

(iii) Isolation of lactose from milk.

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(iv) Isolation of nicotine dipicrate from tobacco.
(v) Isolation of Cinchonine from cinchona bark.
(vi) Isolation of Piperine from blackpepper.
(vii) Isolation Lycopene from tomatoes.
(viii) Isolation of β–Carotene from carrots.
(ix) Isolation of Limonene from citrusrinds.
(x) Isolation of protein and carbohydrates from seeds –colourtest
(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-colourtest.

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

Marks Distribution

Ex. 1	–	**25**
Ex. 2	–	**20**
Ex. 3	–	**15**
Viva	–	**20**
Sessional	–	**20**
Total	–	**100**

BOOKS SUGGESTED:

1. Practical Organic chemistry by A. I.Vogel.
2. Practical Organic chemistry by Mann and Saunders.
3. Practical Organic chemistry by Gargand 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, byB.S. Roa and V. Deshp and e.I.K. International Pvt. Ltd.
9. Comprehensive Practical Organic Chemistry, Preparation and Qualitative Analysis, V.K. Ahluwalia and Renu Aggarwal, University Press.

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LABORATORY COURSE–VIII

Max. Marks 100

One Experiment From each section is compulsory

Sec –A (25 Marks)

A. SPECTROPHOTOMETRIC DETERMINATION

(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.

B. FLOW INJECTION ANALYSIS.

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

(xiii) Ca^{2+}, Mg^{2+}, Al^{3+}, Mn^{2+}, Cr^{6+}, Fe^{3+}

(xiv) F^-, Cl^-, NO^-_2 , NO^-_3, PO_4^{3-}, SO^{2-}_4 BO^{3-}_3

C. ATOMIC ABSORPTION SPECTROPHOTOMETER

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

Sec –B (25 Marks)

A. TITRIMETIC/GRAVIMETRIC DETERMINATIONS

a. Manganese in iron/Steelby Bismuthate/Linganane – Karplus/Periodate Methods.

b. Manganese in pyrolusiteores.

c. Nickel in steel by dimethylglyoxine method.

d. Lead by dithizone precipitation.

Sec –C (10 Marks)

A. CHROMATOGRAPHIC SEPARATION

1. Sepraration and identification of the sugars present in the given mixture of glucose, fructose and sucrose by paper chromategraphy and determination of Rf values.

2. Thin layer chromatography – separation of nickel, manganese, cobalt and zinc, Determination of Rf values.

B. MISCELLANEOUS

a. Nutrient and micronutrient analysis in plant/soil/sediment.

b. Speciation of toxic metals i.e. As, Hg, Se, etc.

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c. Analysis of clinical samples i.e. blood, urine, hair, etc.

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

Marks Distribution

Ex. 1	–	**25**
Ex. 2	–	**25**
Ex. 3	–	**10**
Viva	–	**20**
Sessional	–	**20**
Total	–	**100**

BOOK SUGGESTED:

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.

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