SR&BGNR. Govt. Arts & Science College (Autonomous), Khammam.

KAKATIYA UNIVERSRITY

M.SC - CHEMISTRY

(ORGANIC CHEMISTRY)

NEW SYLLABUS – 2021-22 Onwards

Dept. Of Chemistry

SR&BGNR. Govt. Arts & Science College (A), Khammam.

DEPARTMENT OF CHEMISTRY
KAKATIYA UNIVERSITY

M.Sc. Chemistry (2 Year course)

Revised syllabi with effect from the academic year 2021-2022
[Under CBCS system]

Semester –I

Curriculum						Scheme of Examination		
S. No	Paper Code	Paper no.	Title of the paper	Instruction Hrs/ Week	No. of Credits	Marks		Total marks
						External	Internal	
1	ICHT1	Paper-I	Inorganic Chemistry	4	4	80	20	100
2	ICHT2	Paper-II	Organic Chemistry	4	4	80	20	100
3	ICHT3	Paper-III	Physical Chemistry	4	4	80	20	100
4	ICHT4	Paper- IV	Group Theory and Spectroscopy	4	4	80	20	100
5	ICHP1	Paper-V	Inorganic Practicals	6	3	75	----	75
6	ICHP2	Paper-VI	Organic Practicals	6	3	75	----	75
7	ICHP3	Paper-VII	Physical Practicals	6	3	75	----	75
8	----	----	Seminar	----	1	----	----	25
	Total	----	----	34	26	----	----	650

(Prof. G. Hanumanthu)

(Dr. J. MADHUKAR)

[Dr. T. Savitha Jyosthna]

(Prof. G. Brahmeshwari)

(Prof. N. Vasudeva Reddy)

I SEMESTER

PAPER-I: INORGANIC CHEMISTRY (1CHT1)

(Marks-100, Total hrs: 60)

Unit I Bonding Theories of Metal Complexes:

Crystal field theory: Salient features, splitting of d-orbitals in distorted octahedral, square pyramidal, trigonal bipyramidal, trigonal planar, pentagonal bipyramidal and linear geometries. Crystal field stabilization energy, Pairing energy, Calculation of crystal field stabilization energy (CFSE) in octahedral and tetrahedral complexes. Spectrochemical series. Factors affecting the magnitude of crystal field splitting, Jahn-Teller distortion. General applications and limitations of crystal field theory. Special applications of crystal field theory to spinels in site selection.

Metal-ligand bonding: σ and π bonding in octahedral complexes and their effects on the Oxidation states of transition metals.

Molecular orbital theory (MOT): Introduction, Racah Parameters, Nephelauxetic effect. Molecular orbital energy level diagrams of octahedral, tetrahedral and square planar complexes. Molecular orbital treatment of π bonding in complexes.

Unit II Reaction Mechanisms of Metal Complexes:

Energy profile of a reaction-Activated complex and Transition states. Linear free energy relations. Rearrangements-Berry pseudo rotations.

Langford and Grey Classification, types of Substitution reaction mechanisms- SE, SN-SN^1, SN^2, Id (Interchange dissociative Mechanism), Ia (Interchange associative mechanism) and Intimate Mechanism.

Nucleophilic substitution reactions in octahedral complexes: Acid hydrolysis, factors affecting acid hydrolysis, Base hydrolysis, Conjugate base mechanism (SN^1CB), Evidences in favour of conjugate base mechanism; Substitution reaction without breaking Metal-Ligand bond and Anation reactions.

Ligand Substitution reaction in square planar complexes- Mechanism of Substitution, Trans Effect-Trans influence, theories of trans effect - Grienberg's polarization theory and π-bonding theory.

(Prof. G. Hanumanthu) (Dr. T. MADHUKAR) [Dr. T. Savitha Jyostna]

(Prof G. Brahmeshwari) (Prof. N. Vasudeva Reddy)

Electron transfer reactions- Mechanism of one-electron transfer reactions, Atom or group transfer or inner sphere Mechanism. Direct electron Transfer or Outer Sphere mechanism. Factors effecting direct electron transfer reactions. Cross reactions and Marcus-Hush theory.

Unit III Metal-Ligand Equilibria in Solution:

Solvation of metal ions, metal complex formation in solution – Binary metal complexes. Stability constants (Types), stepwise and overall formation constants and their interpretation, trends in stepwise formation constants. Factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand. HSAB rule and its application to stability of complexes and metal-ligand interactions in the biological systems.

Metal Chelates: Characteristics, Chelate effect and its thermodynamic origin, the factors affecting stability of metal chelates. Macrocyclic ligands, crown ethers, cryptands, Ring size effect.

Determination of stoichiometry of complex formation, Determination of binary formation constants of complexes by pH –metry, spectrophotometry and polarographic methods

Unit IV Magnetochemistry:

Origin of Magnetic moment, factors determining paramagnetism, application of magneto chemistry in co-ordination chemistry- spin moment and orbital moment, quenching of orbital angular moment by ligand fields, Magnetic properties of metal complexes with A, E and T ground terms, Spin-orbit coupling contribution to magnetic moment, Spin cross-over in complexes. Magnetic susceptibility (diamagnetic, paramagnetic), magnetic moments from magnetic susceptibilities (Gouy method) temperature dependence of magnetic susceptibility. antiferromagnetism-inter and intra molecular interaction.

Superconductivity: Introduction, magnetic properties of superconductors- Type I and Type II superconductors and Meissner effect. Applications of superconductors.

(Prof. G. Hanumanthu)

(Dr. J. MADHUKAR)

[Dr. T. Savitha Jyosthna]

(Prof. N. Vasudeva Reddy)

Recommended books:

1. Inorganic chemistry, J. E. Huheey, E. A. Keiter and R. L. Keiter, 4th ed., Harper Collins College Publishers.
2. Advanced Inorganic Chemistry, F. A. Cotton and G. Wilkinson, 6th ed., Wiley Interscience.
3. Coordination Chemistry- Experimental Methods – K.Burger
4. Comprehensive Coordination Chemistry – Wilkinson, Gillars and McCleverty.
5. Inorganic Chemistry, D. F. Shriver and P. W. Atkins, 3rd ed., Oxford.
6. Concise Inorganic Chemistry, J. D. Lee, Blackwell Science.
7. Coordination Chemistry, D. Banerjea.
8. Inorganic reaction mechanism- M.L. Tobe and Jhon Burgess Addison Wesley Longmann (1990)
9. Inorganic reaction mechanisms, F. Basolo and R. G. Pearson NewYork 1967.
10. Mechanism of reactions in transition metal sites, R. A. Henderson, Oxford Science Publications.
11. Metal ions in reaction Mechanism K.Veera Reddy Golgotia Publications
12. Coordination Chemistry, F. Basolo and R. Johnson, Benzamin Inc.
13. Concepts and models of Inorganic Chemistry, B. E. Douglas, D. H. McDaniel and J. J. Alexandar, 3rd ed., John-Wiley.
14. Chemistry of complex equilibria, M. T. Beck, Von Nostrand Reinhold.
15. Metal complexes in aqueous solutions, A. E. Martell and R. D. Hancock, Plenum Press.
16. Inorganic Chemistry, K. F. Purcell and J. C. Kotz, Holt-Saunders International editions.
17. Magnetochemistry – R.L.Carlin
18. Introduction to Magnetochemistry – A.Earnshaw, Academic Press.
19. Physical Methods in Inorganic Chemistry - R.S.Drago

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Paper – V INORGANIC CHEMISTRY - PRACTICALS (1CHP1)

(6 Hours per week)

1. a) Determination of total, permanent and temporary hardness of water
   b) Determination of COD of water
   c) Back titration of Ni^{+2} by EDTA
   d) Back titration of Al^{+3} by EDTA
   e) Substitution titration of Ca^{+2} by EDTA
2. One component gravimetric estimations
   i) Estimation of Zn^{2+}
   ii) Estimation of Ba^{2+} (as $BaSO_4$)
3. Preparation of the following complexes and their characterization by metal estimation and conductance measurement
   i) $[Cu(NH_3)_4]SO_4$ ii) $Hg[Co(SCN)_4]$ iii) $K_3[Fe(C_2O_4)_3]$
   iv) $[Ni(en)_3]S_2O_3$ v) $[Co(NH_3)_5Cl]Cl_2$ vi) $[Mn(acac)_3]$

Scheme of valuation

Marks: 75 Time: 4Hrs

Standardization	– 18
Estimation of sample	– 30
Preparation of sample	– 12
Viva, Record and samples	–15

Recommended Books:

1. Vogel's Text Book of quantitative chemical analysis (6^{th} edition)
2. Analytical chemistry- Gary D. Christian (6^{th} edition)

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I SEMESTER
PAPER-II: ORGANIC CHEMISTRY (1CHT2)
(Marks-100, Total hrs: 60)

Unit I Stereochemistry-I: **(15h)**

Introduction, Chirality and Symmetry elements, classifications of chiral molecules based on symmetry (dissymmetric and asymmetric molecules). Configuration: R,S and E,Z, nomenclature, threo, erythro nomenclature. Stereochemistry of the compounds containing –C=N and –N=N–, Dynamic enantiomerism.

Axial, planar and helical chiral molecules and their configurational nomenclature: Axially chiral allenes. spiranes, alkylidene cycloalkanes. chiral biaryls (atropisomerism), planar chiral ansa compounds, helically chiral compounds.

Relative and absolute configuration: Determination of configuration by chemical correlation methods. Racemization, Racemic modifications and methods of Racemic resolution.

Conformational analysis (acyclic systems): Conformational isomerism, Conformational diastereomers and conformational enantiomers. Study of conformations in 1,2-disubstituted ethane derivatives like butane, dihalobutanes, halohydrin, ethylene glycol, butane-2, 3-diol amino alcohols and 1,1,2,2-tetrahalobutanes.

Conformational effects on the stability and reactivity of acyclic diastereoisomers: Steric and stereoelectronic factors-examples. Conformation and reactivity: The Winstein-Holness equation and the Curtin – Hammett principle.

Unit II Reaction Mechanism-I: **(15h)**

Introduction, Thermodynamic and Kinetic requirements of a reaction. Thermodynamically and Kinetically controlled reactions. Methods of determination of reaction mechanisms: i) Product analysis ii) Intermediate analysis (isolation, trapping) iii) Crossover experiments iv) Isotopic effects (primary and secondary) and Isotopic labelling. Aliphatic nucleophilic substitution reactions - Mechanism and Stereochemistry of S_N^1, S_N^2, S_N^i reactions. Reactivity: The effect of substrate structure, attacking nucleophile, leaving group and reaction medium. Competition between S_N^1 and S_N^2 reactions. Ambient nucleophiles- Regioselectivity. Mechanism of $S_N^{1'}$, $S_N^{2'}$ reactions. Aromatic nucleophilic substitution reactions- S_N^1Ar, S_N^2Ar, and Benzyne mechanisms with evidences. Neighbouring group participation of O, S, N, halogens, aryl groups, alkyl and cycloalkyl groups in nucleophilic substitution reactions. Sigma, Pi bond participation in acyclic and bicyclic systems (non-classical carbocations).

Elimination reactions: Mechanistic pathways of eliminations - E^2, E^1, E^1CB, Orientation of the double bond- Hofmann versus Saytzeff eliminations. Stereochemistry of eliminations (syn & anti). Competition between substitution and elimination reactions.

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Unit III Reagents in Organic Synthesis: **(15h)**

Introduction, Preparation and applications of the following reagents in organic synthesis and functional group transformations: 1,3-Dithianes (Reactivity and umpolung effect), Organolithium reagents (Alkyl lithium and phenyl lithium, LDA, LiHMDS), Borane and Organoboranes (9BBN, Thexyl borane andDisiamyl borane).

Organo Zinc Compounds: Simmons-Smith reagent, Organozinc halides (R -Zn – X), Diorganozincs (R-Zn-R). Coupling reagents (DCC, EDC, HOBt, CDI, PyBOP). Trimethylsilyl iodide, Tri-n-butyl tin hydride, Phase transfer catalysts: Tetra alkyl ammonium halides and Crown ethers.

Unit IV Heterocyclic compounds-I:

Classification and nomenclature of the heterocycles based on number of heteroatoms and size of the ring. π-excessive and π-deficient heterocycles with suitable examples – comparative reactivity of furan, pyrrole, and thiophene (preparation not necessary). Synthesis, reactivity, and reactions of pyridine, coumarin, benzofuran, indole, benzothiophene, quinoline, isoquinoline, oxazole, isoxazoles, imidazoles, and thiazoles.

Recommended books:

1. Stereochemistry of carbon compounds – E.L. Eliel
2. Stereochemistry of organic compounds – D. Nasipuri
3. Stereochemistry: conformation and mechanism – P.S. Kalsi
4. Advanced Organic Chemistry, Part A: Structure and Mechanisms – Francis A. Carey and Richard J. Sundberg
5. March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure– Michael B. Smith
6. Modern Synthetic Reactions (Monograph Series)- Herbert O. House
7. Modern textbook of organic chemistry – Furguson
8. A guide book to reaction mechanisms in organic chemistry – Peter Sykes
9. Mechanism and structure in organic chemistry - S.M.Mukherji & S.P.Singh
10. Organic Chemistry –Clayden, Greeves, Warren and Wothers
11. Organic Chemistry – Paula Y. Bruice
12. Modern Organic Chemistry- M. K. Jain and S. C. Sharma
13. Modern textbook of organic chemistry – Furguson
14. Modern methods of organic synthesis – William Carruthers and Iain Coldham
15. Reagents for organic synthesis – Louis Fieser and Mary Fieser
16. Advanced Organic Chemistry: Part B: Reaction and Synthesis – Francis A. Carey and Richard J. Sundberg
17. Essential reagents for organic synthesis – Philip L. Fuchs, Andre B. Charette, Tomislav Rovis and Jeffrey W. Bode
18. Principles of organic synthesis – Richard O.C. Norman and James M. Coxon
19. Organic Chemistry – Volume-I & II – I.L. Finar
20. Reactions Rearrangements And Reagents – S.N. Sanyal
21. Heterocyclic chemistry – John A. Joule and Keith Mills
22. Heterocyclic chemistry – Raj K Bansal
23. An introduction to chemistry of heterocyclic compounds – R. Moorin Acheson
24. Heterocyclic Chemistry - Thomas. L. Gilchrist

(Prof. G. Hanumanthu) N. Reddy [Dr. T. Savitha Jyosthna]

PAPER- VI: ORGANIC CHEMISTRY - PRACTICALS (1CHP2)

(6 Hours per week)

I. **Some important techniques in practical organic chemistry**: Recrystallization, mixed melting point, drying of solvents and steam distillation.

II. Preparation of

i) Methyl orange ii) Coumarin

iii) Pyrazolone iv)Azalactone

III. Preparation of

i) Benzanilide by Beckmann's rearrangement:

(a) Preparation of benzophenone oxime

(b) Beckmann's rearrangement to benzanilide

ii) Benzilic acid from benzoin:

(a) Benzil from benzoin

(b) Benzilic acid from benzil

iii) Anthranilic acid from phthalic anhydride:

(a) Phthalimide from Phthalic anhydride

(b) Hoffmann's rearrangement to anthranilic acid

iv) m-Nitroaniline from Nitrobenzene:

(a) m-Dinitrobenzene from Nitrobenzene

(b) m-Nitroaniline from m-Dinitrobenzene

Scheme of valuation

Marks: 75 Time: 4Hrs

Single step preparation and Recrystallization	–	20
Two step preparation and Recrystallization	–	40
Viva, Record and Samples	–	15

Recommended books:

1) Vogel's textbook of practical organic chemistry – Arthur Israel Vogel, B. S. Furniss
2) Practical Organic Chemistry – Frederick George Mann and Bernard Charles Saunders
3) Advanced Practical Organic Chemistry N K Vishnoi
4) Laboratory Manual of Organic Chemistry - R. K. Bansal

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I SEMESTER
PAPER-III: PHYSICAL CHEMISTRY (1CHT3)

(Marks-100, Total hrs: 60)

Unit I Chemical Thermodynamics:

Concept of Entropy: Standard entropies and entropy changes in chemical reactions, entropy of mixing. Third law of thermodynamics, calculation of absolute entropies of solids, liquids, and gases, tests and exceptions.

Free energy changes: Gibb's and Helmholtz free energy, Standard free energy of formation, Variation of free energy with temperature and pressure. Free energy change in phase transformations, Clausius-Clapeyron equation, Maxwell's relationships and applications.

Thermodynamics of Non-ideal gases and solutions: Fugacity of a gas, determination of fugacity using graphical and general method. Activity and activity coefficients of electrolyte solutions – determination using Debye-Huckel and EMF method. Vant Hoff's reaction isotherm. Concept of partial molar properties – partial molar free energy–chemical potential-determination of partial molar properties and variation of chemical potential with temperature and pressure. Gibbs–Duhem equation.

Unit II Electro Chemistry-I:

Conductance of Ions: Conductance of strong electrolytes – interionic attraction theory – Thickness of ionic atmosphere (no derivation).

Debye-Huckel-Onsager treatment and derivation of conductance equation – tests and deviations – ion association (Debey-Huckel-Bjerrum equation) – ion pair formation-association constant – conductance minima and triple ions.

Electrochemical cells: Reversible and irreversible cells – Nernst equation of cell emf (thermodynamic formulation) – relation to equilibrium constant of cell reaction and other thermodynamic parameters. Chemical cells and Concentration cells with and without transference. Liquid junction potential and its determination. Applications of emf measurements –determination of pH, pKa and K_{sp} –Potentiometric titrations (acid-base, redox and precipitation).

Polarization: Electrode polarization and concentration polarization – Decomposition potential and overvoltage – theories of overvoltage – factors influencing overvoltage.

Unit III Chemical Kinetics-I:

Theories of Reaction Rates: Simultaneous reactions, derivation of first order rate expression for parallel, opposing and consecutive reactions. Theory of absolute reaction rates – application to reactions between atoms and molecules. Thermodynamical formulations of reaction rates–calculations of activation parameters.

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Theories of Unimolecular Reactions: Lindemann's theory of unimolecular reactions and Hinshelwood modification. Effect of Solvent, Ionic strength and Isotopic effect on reaction rates. Solvent -solute interaction solvation parameters-effect of solvent on reactivity-solvolysis and nucleophilic substitution reactions. Grunwald-Winstein equation, Swain-Scott equation, Edward equation.

Unit IV Basic principles of Quantum Mechanics-I:

Planck's quantum theory and derivation of Planck's temperature radiation law–Derivation of time independent Schrödinger wave equation-wave function and significance of Ψ and Ψ^2 – Normalization and orthogonality of wave function – well behaved functions – Operators like linear momentum (p), angular momentum (L), Energy (E), Hamiltonian (H), operator ∇ and ∇^2. Properties of Hermitian operator. Eigenfunction,eigenvalue, commutation and eigen properties of angular momentum properties. Operator algebra – Postulates of quantum mechanics.

Applications: Application of Schrodinger wave equation to particle in a one-dimensional box and three-dimensionalbox, derivation of energy expressions – plots of Ψ and Ψ^2 – degenerate states – quantum mechanical tunnelling (qualitative treatment).

Polynomials: Hermite, Legendre, Associated Legendre, Laguerre and Associated Laguerre Polynomials (no derivation). Derivation of energy expression and wave function for a linear harmonic oscillator, plots of Ψ and Ψ^2

Recommended books:

1. Physical Chemistry by Donal D; Mcquarrie & John D Simon.
2. Physical Chemistry by Peter Atkins and Julio de Paula
3. Principles of Physical Chemistry by Samuel H.Maron and Carl F. Prutton
4. Advanced Physical Chemistry by Gurdeep Raj
5. Quantum Chemistry by R.K.Prasad
6. Thermodynamics by Samuel Glasstone, D.Van
7. Chemical Kinetics by K.J. Laidler
8. Chemical Kinetic Methods–Principles of Relaxation techniques & Applications by C. Kalidas.
9. An Introduction to Electrochemistry- Samuel Glasstone (10^{th}Ed)
10. Electrochemistry by M.S. Yadav
11. An introduction to Chemical Thermodynamics by R.P. Rastogi and R.R. Misra.
12. Principles of Chemistry by Paul Ander Anthony J. Sonnessa.

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Paper – VII PHYSICAL CHEMISTRY PRACTICALS (1CHP3)

(6 Hours per week)

1. Kinetics:

(i) Acid catalyzed Acetone – Iodine reaction.
(Comparison of rate constants at different acid concentrations)

(ii) Acid catalyzed hydrolysis of methyl acetate.
(Comparison of rate constants at different acid concentrations)

(iii) Persulphate – Iodide reaction.
(Comparison of rate constants at different iodide concentrations)

2. Polarimetry:

(i) Specific rotation of sucrose and glucose.

(ii) Acid catalysed inversion of sucrose-Pseudo first order rate constants.
(Comparison of rate constants at different acid concentrations)

3. Conductometry: Titrations of

(i)Mixture of strong and weak acids with Strong base

(ii) Salt with Strong base

(iii) Dibasic acids Vs NaOH

(iv) Determination of pKaof chloroacetic acid

b. Verification of Ostwald's dilution law and determination of Ka.

c. Solubility product of AgCl.

4. a. Density and viscosity of liquids.

b.Determination of molecular weights of polyethylene glycol or polyvinyl alcohol.

5. Determination of heat of solution of benzoic acid by solubility method.

Scheme of valuation

Marks:75 Time: 4Hrs

Two Experiments	30 + 30 =	60
Experiments includes - Tables, graphs, calculations		
Principle record and viva	–	15

Recommended books:

1. Practical Physical Chemistry by A. Findlay, Longman-London.
2. Practical Physical Chemistry by B. Vishwanathan and P.S. Raghavan,
3. Practical Physical Chemistry by B.D.Khosla and V.C. Garg.
4. Systematic Experimental Physical Chemistry -S.W. Raj Bhoj and Dr.T.K. Chondhekar.

(Prof. G. Hanumanthu) (Dr. T. Savitha Jyosthna)

I SEMESTER

Paper-IV: Group Theory and Spectroscopy (1CHT4)

(Marks-100, Total hrs 60)

Unit I Symmetry & Group Theory **15h**

Concept of Symmetry in Chemistry-Symmetry Operations and Elements of Symmetry: Rotational Axis of Symmetry, Plane of Symmetry, Improper Rotational Axis of Symmetry (Alternate Axis of Symmetry), Centre of Symmetry and Identity Element. Mathematical concepts of group theory for symmetry. Point group and classification of molecules into C_1, Cs, Ci, Cn,Cnv, Cnh, C∞v, Dn, Dnh, Dnd, D∞h, Sn(n=even), Td and Oh groups with examples Abelian and non-abelian groups. Descent in Symmetry of molecules with substitution. Symmetry Criteria for Optical Activity. Symmetry Restrictions on Dipole Moment. Matrix representation of symmetry operations and point groups.

UNIT II - Rotational, Vibrational and Raman Spectroscopy: **15h**

Rotational (Microwave) spectroscopy: Types of molecular energies and molecular spectroscopy. Classification of molecules based on moment of inertia. Rotational energy levels and selection rules of rotational spectra – Calculation of bond lengths of diatomic molecules. Isotope effect on rotational spectra.

Infrared Spectroscopy: Vibrational energy of a diatomic molecule-anharmonic oscillator–Selection rules-Overtones-hot bands. Zero-point energy-Calculation of force constant of diatomic molecules. Rotational –Vibrational spectra of diatomic molecules. Normal modes of vibrations for linear and non-linear molecules. Types of stretching and bending vibrations.Factors influencing vibrational frequencies-Isotopic effect, Coupled vibrations and Fermi resonance-combinational bands. Characteristic absorptions in common classes of compounds. Applications of infrared spectroscopy: Structure elucidation of organic molecules-Functional groups, the nature of substituents, benzene and substituted benzene, cis-trans isomers, keto-enol tautomers and hydrogen bonding (inter and intra molecular)–Analysis of metal nitrates and carbonates by IR spectroscopy.

Raman spectroscopy: Raman effect-Quantum theory-selection rules-Rotational and Vibrational Raman effect. Instrumentation, Mutual exclusion principle and Raman spectra of Hg_2^{2+}, NO_3^-, ClO_3^-, N_2O, CO_2 and CH_4.

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UNIT III - UV & Visible (Electronic) Spectroscopy and ESR Spectroscopy:

Origin of electronic spectra, Lambert-Beer's absorption law. Types of electronic transitions. Chromophores and auxochromes. Bathochromic, hypsochromic, hyperchromic and hypochromic shifts. Effect of solvent onabsorption maxima. Effect of substituent and conjugation on electronic transitions. Electronic spectra of benzene and its derivatives. Woodward-Fieser rules for calculating absorption maximum of dienes and α, β-unsaturated carbonyl compounds. Applications of UV-visible spectroscopy: In qualitative analysis of polyenes/aromatic (hetero & homo) systems geometrical isomers and keto-enol tautomers. In quantitative analysis of mixture analysis, ionization constants of acids and bases. Determination of composition of complexes by Job's slope ratio method. Charge transfer spectra of complexes. UV spectra of Mesityl Oxide, Phenol and Benzoic acid.

Electron spin resonance spectroscopy (ESR): Introduction-Principles involved in ESR spectroscopy. Instrumentation, presentation of ESR spectra, hyperfine coupling constant. ESR spectrum of hydrogen atom. Lande's splitting factor, calculation of g from resonance equation. Significance of g. ESR spectra of methyl, ethyl, isopropyl, benzene (anion and cation radicals), 1,4-benzosemiquinone, naphthalene anion and bis salicylaldimine copper(II) complex.

Unit IV NMR Spectroscopy (1H-NMR):

Nuclear Magnetic Resonance Spectroscopy (NMR): Theory of NMR-Quantum approach and Classical Approach-Relaxation phenomenon. Equivalent and non-equivalent protons. Chemical shift, Factors affecting the chemical shift-Shielding and Deshielding, Anisotropic effects in alkanes, olefins, acetylenes, carbonyl compounds and aromatic systems.

Spin-Spin coupling, theory of Spin-Spin coupling, coupling constant, Types of coupling constants, Factors affecting the coupling constants. Signal integration. First order and non-first order spectra, e.g., AX, AX_2, AX_3, A_2X_3, AMX, AB, ABC, ABX type. Simplification of non-first order spectra: Increased field strength, Lanthanide shift reagents and Double resonance techniques. Nuclear Over Hauser enhancement (NOE).

Applications of NMR spectroscopy: Proton exchange reactions (alcohols, amines and carboxylic acids), deuterium exchange reactions, hydrogen bonding, keto-enol tautomers, cis-trans isomers, conformational analysis, C-N restricted rotation and Reaction mechanism (cyclic bromonium ion).

NMR spectra of pure and impure ethanol,vinyl chloride, acrolein, crotonaldehyde, styrene oxide, monosubstituted benzenes -ethyl benzenes, anisole, acetophenone and nitrobenzene. Disubstituted benzenes - paracetamol, p-Toluidine, p-Chloroaniline, 4-Methoxy-benzaldehyde.

(Prof. G. Hanmanthu) NV Reddy [Dr. T. Savitha Jyosthna]

Recommended Books:

1. Chemical Applications of Group Theory – F. A. Cotton
2. Atomic structure and chemical bonding – Manas Chanda
3. Fundamentals of Molecular spectroscopy-Banwell &McCash
4. Molecular spectroscopy-Patel and Patel
5. Spectroscopy organic compounds-P. S. Kalsi
6. Organic Spectroscopy-Jag Mohan
7. Elementary Organic Spectroscopy-Y.R. Sharma
8. Organic spectroscopy-W. Kemp.
9. Nuclear Magnetic Resonance: Basic Principles - Atta ur Rahman.
10. Introduction to Spectroscopy - Donald L. Pavia, Gary M. Lampman, George S. Kriz, James A. Vyvyan.
11. Instrumental methods of chemical analysis-G. R. Chatwal & S. K. Anand.
12. Group Theory and Molecular spectroscopy-K. Veera Reddy.
13. Spectrometric Identification of Organic compounds, 6th Ed. Rober M. Silverstein & Francis Webster.
14. Applications of spectroscopy-J. Dyer.

(Prof. G. Hanmanthu) (Dr. V. Veera Reddy) [Dr. T. Savitha Jyosthna]

M.Sc - CHEMISTRY

(Effective from the academic year 2021-22)

SEMESTER-II

Curriculam						Scheme of Examination		
S.No	Paper Code	Paper No	Title of the Paper	Instruction Hrs/Week	No. of Credits	Marks		Total Marks
						External	Internal	
1.	2CHT5	Paper-I	Inorganic Chemistry	4	4	80	20	100
2.	2CHT6	Paper-II	Organic Chemistry	4	4	80	20	100
3.	2CHT7	Paper-III	Physical Chemistry	4	4	80	20	100
4.	2CHT8	Paper-IV	Spectroscopy	4	4	80	20	100
5.	2CHP4	Paper-V	Inorganic Chemistry Practicals	6	3	75	-	75
6.	2CHP5	Paper-VI	Organic Chemistry Practicals	6	3	75	-	75
7.	2CHP6	Paper-VII	Physical Chemistry Practicals	6	3	75	-	75
8.	-	-	Seminar	-	1	-	25	25
Total				**34**	**26**	**545**	**105**	**650**

II SEMESTER

PAPER-I: INORGANIC CHEMISTRY (2CHT5)

(Marks-100, Total hrs: 60)

Unit I Electronic spectra of metal complexes:

Free ion terms and energy levels - Electron configuration, Microstates and Terms. Calculation of microstates for **p** and **d** configurations, Russel-Saunders (L-S) coupling. Derivation of terms for $\mathbf{p^2}$ and $\mathbf{d^2}$ configurations, Ground state term symbols for **d** configurations, Hole formalism, Hund's rules to determine ordering of energy levels, Effect of weak fields on free ion terms, Selection rules governing electron transitions and breakdown of selection rules, Orgel diagrams for $\mathbf{d^1}$ to $\mathbf{d^9}$ systems, Electronic spectra of $[Ti(H_2O)_6]^{3+}$, $[Cu(H_2O)_6]^{2+}$, $[V(H_2O)_6]^{3+}$, $[Ni(H_2O)_6]^{2+}$, $[CoF_6]^{3-}$, $[CoCl_4]^{2-}$ and $[NiCl_4]^{2-}$ complexes, Charge transfer Spectra, Calculation of ligand field parameters - Racah parameter (**B),** Crystal field splitting (**10DQ)** and Nephelauxetic ratio (**β).**

Unit II Organometallic Compounds:

Principles of synthesis of organometallic compounds. Types of organometallic reactions. Classification of carbon-based ligands by donor atoms and number of electrons donated by the ligand. Transition metal organometallics with σ-donor and π- acceptor ligands. 16/18 valence electron rule and its applications to the stability of organotransition metal compounds. Synthesis, structure and properties of organometallic compounds of **Al** and **Sn.** Synthesis, structure and bonding of olefin, allyl and cyclopentadienyl organometallic compounds of **Fe, Pt,** and **Pd**. Applications of organometallic compounds of **B** and **Si** in organic synthesis. Organometallic compounds in homogeneous catalysis – Hydrogenation, Hydroformylation and Isomerization processes.

Unit III Bioinorganic Chemistry:

Metal ions in biological systems - Brief survey of metal ions in biological systems, Basic principles underlying biological selection of elements, Physiological effects of metal ion concentration.

Oxygen transport and storage - Haemoglobin and Myoglobin, Geometric, electronic and magnetic aspects of dioxygen binding, oxygen adsorption isotherms and cooperativity and its mechanism, Physiological significance of haemoglobin, Role of globin chain in haemoglobin. Comparison of Hemerythrin and Hemocyanin with Haemoglobin

Photosynthesis Structural aspects of chlorophyll. Photosystem I and Photosystem II. Biological and chemical nitrogen fixation

Metalloenzymes containing zinc, iron, cobalt, and copper

Metal compounds in medicine - Metals used for diagnosis and radiodiagnosis; Lithium, Gold, and Platinum compounds used in therapy. Metal deficiency and diseases of Iron, Zinc and Copper

Unit IV Ligational aspects of diatomic molecules:

Metal Carbonyls: Classification of metal carbonyls, General methods of preparing metal carbonyls, Ligational properties of Carbon monoxide (CO), Donor and acceptor molecular orbitals of CO, Bonding modes of CO, Evidence for multiple bonding, Eighteen electron rule and its applications

Metal carbonyl clusters- Factors favouring metal-metal bond, Classification of metal carbonyl clusters.

Low nuclearity clusters- M_3 and M_4 clusters Structures of $Mn_2(CO)_{10}$, $Co_2(CO)_8$, $Fe_3(CO)_{12}$, $Ru_3(CO)_{12}$, and $Co_4(CO)_{12}$, Metal carbonyl scrambling.

High nuclearity clusters-M_5, M_6, M_7 and M_8 clusters. Polyhedral skeletal electron pair theory and total electron count theory. Structures of $Rh_6(CO)_{16}$ and $[Os_6(CO)_{18}]^{2-}$

Metal nitrosyls: NO as a ligand- donor and acceptor molecular orbitals of nitric oxide (NO), Bonding modes of NO, structural and bonding aspects of $[IrCl(PPh_3)_2(CO)(NO)]^+$ and $[RuCl(PPh_3)_2(NO)_2]^+$. Stereochemical control of valence in $[Co(diars)_2(NO)]^{2+}$ and $[Co(diars)_2(NO)(SCN)]^+$

Metal dinitrogen complexes - Dinitrogen molecule (N_2) as a ligand, Molecular orbitals of N_2, Bonding modes - Terminal and Bridging, Structures of Ru (II) and Os (II) dinitrogen complexes. Chemical fixation of dinitrogen.

Recommended books:

1. Inorganic chemistry, J. E. Huheey, E. A. Keiter and R. L. Keiter, 4th ed., Harper Collins College Publishers.
2. Inorganic Chemistry, Keith F. Purell and John C. Koltz. Holt-Saunders International editions, London
3. The Chemistry of metal cluster complexes D. F. Shriver, H. D. Kaesz and R. D Adams
4. Inorganic biochemistry edited by G. L Eichhorn volume I Elsevier
5. Basic organometallic chemistry, B. D Gupta, A. J Elias
6. Inorganic Chemistry, G. L Miessler, D. A Tarr , 3rd Edition Pearson education
7. Inorganic Chemistry, G. Wulfsberg
8. Introduction to ligand fields, B. N. Figgis, Wiley.
9. Concise Inorganic Chemistry, J. D. Lee, Blackwell Science.
10. Organometallic Chemistry, R. C. Mehrotra and A. Singh, New age international.
11. Metalorganic Chemistry, A. J. Pearson, Wiley.
12. Physical methods in chemistry, R. S Drago
13. Bioinorganic Chemistry, L. Bertini, H.B. Gray, S. J. Lippard and S. J. Valentine
14. Principles of Bioinorganic Chemistry, S. J. Lippard and Berg.
15. Bioinorganic Chemistry, K. Hussain Reddy, New Age international Publishers.

16. Structure and bonding Vol. 55 H. J. Clark.
17. Modern Inorganic Chemistry, W. L. Jolly, McGraw-Hill.
18. Concise coordination Chemistry, R. Gopalan and V. Ramalingam, Vikas Publishing Home Pvt. Ltd.

Paper – V INORGANIC CHEMISTRY PRACTICALS (2CHP4)

I. Estimations:

1. Glucose by using Fehling's solution
2. Vitamin – C
3. Calcium in Milk
4. Iodine value of Oil
5. Chlorine in Bleaching Powder

II. Analysis of Binary Mixtures:

1. Determination of Cu^{2+} and Ni^{2+}
2. Determination of Fe^{3+} and Al^{3+}
3. Determination of Cu^{2+} and Zn^{2+}
4. Determination of Ca^{2+} and Mg^{2+}
5. Determination of Ferrocyanide & Ferricyanide

Scheme of valuation

Marks: 75 Time: 4Hrs

Standardization	–	24
Estimation of sample	–	36
Viva and Record	–	15

Recommended Books:

1. A Text Book of quantitative inorganic analysis (3^{rd} and 6^{th} editions)
2. Analytical chemistry 6^{th} edition Gary D. Christian
3. Practical Inorganic chemistry G. Marr and B. W. Rockett

II SEMESTER

PAPER-II: ORGANIC CHEMISTRY (2CHT6)

(Marks-100, Total hrs: 60)

Unit I Modern methods in organic synthesis:

a) Metal mediated C-C and C-X coupling reactions: Heck, Stille, Suzuki, Nozaki-Hiyama, Sonogashira, Buchwald-Hartwig and Ullmann coupling reactions. b) Construction of Ring Systems: (i) Pauson-Khand reaction and Nazarov cyclization (ii) Ring closing metathesis- Grubb's 1st and 2nd generation catalysts. c) Multicomponent reactions: Ugi reaction and Multicomponent Mannich reaction. d) Carbene insertions: Rh based carbene complexes, cyclopropanations.

e) C-H Activation: Introduction, Rh catalysed C-H activation. f) Other important synthetic reactions: Baylis-Hillman reaction, Mitsunobu reaction, Robison annulation, Corey-Fuchs reaction, Sakurai reaction and Shapiro reaction.

Unit II Stereochemistry-II:

Conformational analysis of Cycloalkanes: Conformations of small and medium sized rings. Study of conformations of mono and disubstituted cyclohexanes-optical activity, stability-factors affecting the stability of conformations (steric, electronic and stereoelectronic effects). Conformations of cyclohexanone (2-alkyl and 3-alkyl ketone effect) and 2-halo cyclohexanones. Stereochemistry of bicyclic systems involving five and six numbered rings. Conformation and reactivity in cyclohexane systems: Steric and stereoelectronic effects in S_N1, S_N2 and S_Ni reactions, E_2 eliminations, neighboring group participation, epoxide formation and opening of epoxide in cyclohexyl systems (Furst Plattner rule). Reactions at exocyclic centers present on cyclohexane-esterification and ester hydrolysis. Stereochemistry of addition to the carbonyl group in rigid cyclohexanone system.

ORD studies: Optical rotation and optical rotatory dispersion, octant rule, axial haloketone rule, applications of ORD studies in the determination of configuration and conformation of organic molecules.

Unit III Protection of functional groups and Nonbenzenoid aromatic compounds:

(a) **Protection of functional groups:** (1) Protection of alcohols – Ether formation: methyl, benzyl, alkoxymethyl groups (MEM, MOM, BOM and THP), silyl, and TBDMS ethers; Ester formation- methyl, benzoyl, tosyl, and p-nitro benzoyl ester (2) Protection of diols–acetal, ketal and carbamate formation (3) Protection of carboxylic acids – Ester formation: methyl, benzyl, t-butyl, p-nitrobenzyl, p-bromophenacyl, and silyl esters. (4) Protection of amines by CBZ,

BOC, FMOC, phthaloyl, and triphenyl methyl groups. (5) Protection of carbonyls by acetal, ketal and thiol acetal (Umpolung) groups.

(b) **Nonbenzenoid aromatic compounds:** Concept of aromaticity, Robinson's sextet theory, Huckel's rule, limitations of the Huckel's rule, Alternant and Non-alternant hydrocarbons Craig's rule. Antiaromatic compounds. Aromaticity in various non-benzenoid aromatic molecules –3,4,5,6,7 and 8-membered rings, metallocenes, annulenes, heteroannulenes, azulenes, fullerenes(C_{60}), and Sydnones. Synthesis and properties of azulene, tropylium cation and ferrocene.

Unit IV Biomolecules:

Polypeptides and Proteins: Determination of structures of polypeptides – N-terminal and C-terminal amino acid determination – Sequence determination in polypeptides – polypeptide synthesis – Merrifield resins – Solid phase polypeptide synthesis. Classification, structures, and functions of primary, secondary and tertiary proteins.

Carbohydrates: Determination of the relative and absolute configuration in D-glucose and D-fructose. Structural features of Maltose, Lactose, Sucrose, Cellobiose, Starch, and Cellulose. Synthesis of Sucrose and Maltose.

Nucleic acids: Isolation, structure, and properties of RNA & DNA – chemical synthesis of nucleosides and nucleotides.

Recommended Books:

1. Stereochemistry of carbon compounds – E.L. Eliel
2. Stereochemistry of organic compounds – D. Nasipuri
3. Stereochemistry: conformation and mechanism – P.S. Kalsi
4. Reaction mechanisms – Jerry March
5. Organic Chemistry – Volume-I & II – I.L. Finar
6. Textbook of organic chemistry – Morrison and Boyd
7. Organic reagents – Fieser and Fieser
8. Modern textbook of organic chemistry – Furguson
9. Reaction mechanisms – Jerry March
10. Modern methods of organic synthesis – William Carruthers and Iain Coldham
11. Organic Chemistry – Greeves, Warren, and Wothers Clayden
12. Advanced Organic Chemistry: Part B: Reaction and Synthesis – Francis A. Carey and Richard J. Sundberg
13. Organic Chemistry – Volume-I & II – I.L. Finar
14. Carbohydrate chemistry – Davidson

15. Reagents for organic synthesis – Louis Fieser and Mary Fieser
16. Reactions Rearrangements and Reagents – S.N. Sanyal
17. Essential reagents for organic synthesis – Philip L. Fuchs, Andre B. Charette, Tomislav Rovis and Jeffrey W. Bode.
18. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken.
19. Transition metals in the synthesis of Complex Organic Molecules- Louis S. Hegedus

Paper - VI ORGANIC CHEMISTRY PRACTICALS (2CHP5)

Identification of Organic compounds – Systematic qualitative analysis:

Physical data – Boiling points/ Melting points; Ignition test, Solubility classification, Detection of extra elements N,S and Halogens (Lassaigne sodium fusion test, Beilstein test). Functional group tests and preparation of two rational derivatives - determine the melting points of solid derivatives and reference to literature to identify the compounds.

A minimum of eight following compounds to be studied as unknown covering at least one from each of the solubility classes.

List of suggested compounds:

Glucose, Fructose, Benzaldehyde, p-Anisaldehyde, p-Chlorobenzaldehyde, Acetophenone, p-Nitroacetophenone, Benzophenone, Benzoic acid, p-Nitrobenzoic acid, p-Chlorobenzoic acid, Anisic acid, Phenol, p-Cresol, β–Naphthol, p-Chlorophenol, Aniline, p-Toluidine, p-Anisidine, o-Chloroaniline, m-Chloroaniline p-Chloroaniline,

Diphenylamine, N-methyl aniline N, N-dimethyl aniline, Benzamide, Ethyl benzoate, methyl benzoate, Nitrobenzene, Chlorobenzene, Bromobenzene, Naphthalene and Anthracene, Biphenylanthracene.

Scheme of valuation

Marks: 75	Time: 4Hrs
Determination of M.P/ B.P, Extra element test, Solubility test	– 18
Functional group test	– 24
Preparation of derivatives	– 18
Viva, Record and samples	– 15

Recommended books:

1. Vogel's textbook of practical organic chemistry – Arthur Israel Vogel, B. S. Furniss
2. Practical Organic Chemistry – Frederick George Mann and Bernard Charles Saunders

II SEMESTER
PAPER-III: PHYSICAL CHEMISTRY (2CHT7)

(Marks-100, Total hrs: 60)

Unit I Thermodynamics – II:

Statistical Thermodynamics: Thermodynamic probability of distinguishable and indistinguishable particles-most probable distribution–entropy and probability (Boltzmann–Planck equation), Derivation of Maxwell–Boltzmann distribution law.

Partition Function: Translational, rotational, vibrational and electronic functions–Relation between thermodynamic functions (E, H, S and G) and partition functions-factorization into translational, rotational, vibrational and electronic contributions of monoatomic and diatomic molecules. Sackur-tetrode equation of entropy. Equilibrium constant, Calculations of Partition Functions and Thermodynamical Functions.

Quantum Statistics: Basic concepts of quantum statistics–Bose–Einstein and Fermi- Dirac statistics–comparison with Maxwell–Boltzmann statistics.

Unit II Electrochemistry – II

Ion selective electrodes: Membrane electrodes, theory of glass membrane potential.

Reference electrodes: Polarizable and non-polarizable systems, Types of reference and working electrodes.

Batteries: Battery parameters, Energy density and power density, measure of battery performance, primary and secondary batteries, Zn/Mno_2, Lead-acid, Ni-Cd batteries, Zn-air and lithium batteries.

Fuel cells: Types of fuel cells, H_2/O_2 and methanol/O_2, Phosphoric acid, High temperature fuel cells, use of porous electrode in fuel cells, Advantages and limitations of fuel cells, Voltaic cells, Semi-conductor based photochemical energy from solar energy.

Corrosion: Different types of corrosion: influence of environment corrosion rate measurements, Stern Geary equation: mixed potential theory and prevention of corrosion.

Unit III Chemical Kinetics - II:

Effect of substituent on the rate of reaction – Hammett's and Taft's equations– use of σ and ρ constants and extended Hammett equation. Yukawa–Tsuno equation–Nonlinear Hammett's Plots–Isokinetic temperature and its determination.

Acid-Base Catalysis: Homogeneous acid–base catalysis–mechanism of acid-base catalysis-protolytic and prototropic mechanism.

Enzyme Catalysis: Specific action and classification of enzymes–Kinetics and mechanism of single substrate reaction–Michaelis–Menten Kinetics. Production detection and estimation of free radicals.

Chain Reactions: General Characteristics–Kinetics of Chain reactions–Mechanisms of thermal reaction of hydrogen with chlorine and bromine and their rate expressions–thermal decomposition of N_2O_5 and C_2H_6-general kinetic schemes-Inhibition of chain reactions by NO.

Unit IV Quantum Chemistry - II:

Rigid rotator: Application of Schrodinger equation to rigid rotator– derivation of energy expression and wave function of a rigid rotator–solution of (ϕ) and (ɵ) parts of wave functions–total wave function of rigid rotator.

Hydrogen atom: Separation of (r), (ϕ) and (ɵ) equations–Solution of radial equation–Total wave function for hydrogen atom–radial and angular plots–probability functions and radial probability density plots for 1s and 2s orbitals.

Approximation methods: Variation method–principle and its application to hydrogen atom–perturbation method–First order correction terms of energy and wave function–application to particle in a one-dimensional box under an electric field.

Bonding in molecules: Born-Oppenheimer approximation - construction of molecular orbitals by LCAO. MO theory of H_2^+ ion. Energy and wave function expressions (no derivation). Basic postulates of Huckel's π electron theory and its applications to ethylene system.

Recommended books:

1. Physical Chemistry by Donald A McQuarrie & John D. Simon.
2. Physical Chemistry - Peter Atkins and de Pulpa Oxford University Press.
3. Principles of Physical Chemistry - Samuel H. Maron and Carl F. Prutton.
4. Advanced Physical Chemistry -Gurdeep Raj Goel Publishers House, Meerut.
5. Quantum Chemistry - R. K. Prasad
6. Electrochemistry - Samuel Glasstone
7. Chemical Kinetics by K.J. Laidler
8. Quantum Chemistry - Levine
9. Chemical Kinetic Methods–Principles of Relaxation techniques & Applications - C. Kalidas.
10. Text book of physical chemistry -Puri & Sharma

11. Engineering Chemistry by PC Jain and M Jain, Dhanapathi Rai publishing Co.
12. Text Book of Engineering Chemistry by Shashi Chawla, Dhanapathi Rai publishing Co.

Paper – VII PHYSICAL CHEMISTRY - PRACTICALS (2CHP6)

1. Potentiometry:
   a. Acid –Base titrations:
      (i) Strong acid with strong base.
      (ii) Weak acid with strong base and determination of P^{ka} of weak acid.
      (iii) Mixture of acids with strong base.
   b. Redox titrations:
      (i) Ferrous ion with $KMnO_4$ or $K_2Cr_2O_7$
      (ii) Ferrous ion with Ce^{+4}
   c. Precipitation titrations:
      (i) KCl or KI with $AgNO_3$
      (ii) Mixture of (KCl + KI) with $AgNO_3$
2. Colorimetry**:**
   Verification of Lambert-Beer's law and determination of concentration of unknown solutions -$KMnO_4$, $CuSO_4$, $K_2Cr_2O_7$, $[Cu(NH_4)_6]SO_4$
3. Verification of Freundlich adsorption isotherm-Acetic acid–activated charcoal system.
4. Distribution of Iodine between CCl_4 and aqueous KI. (Determination of unknown concentration of KI)
3. Determination of partial molar volume of methanol in aqueous methanol.

Scheme of valuation

Marks: 75 Time: 4 Hrs

Two Experiments		30+30 = 60
Experiments includes- Tables, Graphs, Calculation Principle, Record and Viva	-	15

Recommended Books:

1. Practical Physical Chemistry -A. Findlay, Longman-London.
2. Practical Physical Chemistry -B. Vishwanathan and P.S. Raghavan,
3. Practical Physical Chemistry - B.D. Khosla and V.C. Garg. R. Chand & Co. Delhi.
4. Systematic Experimental Physical Chemistry by S.W. Raj Bhoj and Dr. T.K. Chondhekar

II Semester

Paper-IV SPECTROSCOPY (2CHT8)

(Marks 100, Total Hours 60)

Unit-I ^{13}C NMR and 2D NMR Spectroscopy:

Recording of ^{13}C NMR spectra (PFT technique), Types of ^{13}C NMR spectra: Undecoupled, proton decoupled, selective proton decoupled and off-resonance decoupled spectra – Spin decoupling method-Double resonance. ^{13}C chemical shifts and factors affecting the chemical shifts. Calculation of chemical shifts of alkanes, alkenes, alkynes and mono substituted benzenes. Heteronuclear coupling of **^{13}C** to ^{19}F and ^{31}P. Applications of ^{13}C NMR spectra in structure determination of organic molecules. ^{13}C-NMR spectral editing techniques: principle and applications of INEPT and DEPT methods.

2D NMR Spectroscopy: Principles of 2D NMR, Different types of 2D-experiments with suitable examples. Correlation spectroscopy (COSY): HOMOCOSY (^{1}H-^{1}H COSY) and HETERO- COSY (^{1}H-^{13}C COSY), HMBC, HMQC, Homonuclear and Heteronuclear 2D-J-resolved spectroscopy, NOESY and 2D– INADEQUATE experiments and their applications.

Study of ^{13}C-NMR, DEPT, HOMOCOSY and HETEROCOSY spectra of isopentyl acetate, ethyl crotonate, natural products viz., citronellol, menthol, ipsenol and geraniol.

Unit-II Mass Spectrometry:

Origin of mass spectrum, principles of EI mass spectrometer- Instrumentation. Types of fragments: odd electron and even electron containing neutral and charged species (even electron rule), Nitrogen rule, Isotopic peaks, Metastable ion peaks, determination of molecular formula and High-resolution mass spectrometry. Calculation of ratio of Isotopic peaks in halo substituted organic compounds (mono, di, tri chloro/bromo; with both chloro and bromo) Salient features of fragmentation pattern of organic compounds– α-cleavage, β-cleavage, McLafferty rearrangement, Retro-Diels-Alder fragmentation and ortho effect. Mass spectra of aliphatic and aromatic hydrocarbons, halogen compounds, alcohols, ethers, phenols, carbonyl compounds, carboxylic acids and their derivatives, nitrogen compounds, heterocyclic systems (furan, pyrrole, thiophene and pyridine) with fragmentation mechanisms. Preliminary account of chemical ionization.

Unit-III Electron Spectroscopy and Mössbauer Spectroscopy

(i) Electron Spectroscopy:

a) Photoelectron spectroscopy – Principles, Koopman's theorem, Ultraviolet photoelectron spectroscopy (UPS), and X-ray photoelectron spectroscopy (XPES) photoelectron spectrometer Applications of UPS to O_2 and N_2 molecules.

Chemical shift with reference to N_2O, $S_2O_3^{-2}$, S^{-2}, S^0, SO_3^{-2}, SO_4^{-2} and $CH_3CH_2COOCF_3$ Applications of XPES in qualitative analysis, Structural analysis and surface studies.

b) AUGER Electron Spectroscopy – Principles, Instrumentation and Applications of the technique in qualitative analysis of solid surfaces and line scanning.

c) Mössbauer Spectroscopy–Principles, experimental considerations, Mössbauer spectrometer, presentation of Mössbauer spectrum, Factors that influence the absorption of γ-rays by a sample- Isomer shift, Quadrupole splitting and magnetic splitting, Applications of Mössbauer Spectroscopy in the study of iron compounds- high spin and low spin Fe (II) and Fe (III) complexes, high spin -low spin cross over, structure with reference to FeO_4^{-2}, Fe^{4+}, Fe^{+3} and Fe^{+2}, bonding in $Na_2[Fe(CN)_5NO]$ and structural aspects of $Fe(CO)_5$, $Fe_2(CO)_9$, $Fe_3(CO)_{12}$ and tin compounds-tin halides and organo tin compounds, Biological applications of the technique.

<u>Unit-IV</u> Structure Elucidation from Spectral Data in Organic Chemistry:

Introduction, structure elucidation of following organic molecules by combined application of UV, IR, ^{1}H-NMR, ^{13}C-NMR and Mass spectral data.

2-Bromopropane, Isobutyl alcohol, Diethyl ether, Diisopropylether, 2-Butanone, Ethyl acetate, Methyl pentanoate, Methyl-3,3-dimethylbutanoate, Ethylbenzene, Benzyl alcohol, Anisole, Acetophenone, Benzoic acid, Acetanilide, Benzyl acetate, Ethyl benzoate, Dibenzyl ketone, 3-phenylpropanoicacid, Acraldehyde, Crotanaldehyde (E and Z), Cinnamaldehyde (E and Z), Prop-1-en-2-ylbenzene, o-Cresol, o-Toluic acid, p-Toluidine, p-Anisaldehyde, Furfural. and Pyridine.

Recommended Books:

1. Spectroscopic identification of organic compounds –Robert M. Silverstein, Francis X. Webster.
2. Application of absorption spectroscopy – John R. Dyer
3. Organic Spectroscopy – William Kemp
4. Spectroscopic methods in Organic chemistry – DH Williams and I Fleming
5. Modern Nuclear Magnetic Resonance Techniques for Chemistry Research (Tetrahedron Organic Chemistry) by Andrew E. Derome.
6. Introduction to spectroscopy – Donald L. Pavia, Gary M. Lampman, George S. Kriz and James Vyvyan.
7. Carbon-13 NMR for organic chemists – GC Levy and O L Nelson
8. Nuclear Magnetic Resonance Basic principles – Atta-Ur-Rahman
9. Spectroscopy of Organic compounds- P. S. Kalsi.

10. Mass Spectrometry -Basics, Herbert, Christopher G. Johnstone, Robert A.W., CRC Press.
11. Physical methods for chemists– R.S. Drago, 2nd ed. (Saunders College Publishers).
12. Mössbauer spectroscopy-N.N. Greenwood and T.C. Gibb
13. Instrumental methods of Analysis- Willard, Dean & Settle.
14. Principles of Instrumental Analysis - Skoog, Holler and Nieman
15. Introduction to photoelectron spectroscopy - P. K. Ghosh
16. Structural Inorganic chemistry-Mössbauer spectroscopy – Bhide
17. Organic Structures from Spectra- L D Field, S Sternhell, J R Kalman.

III Semester- Inorganic Chemistry

Curriculum						Scheme of Examination		
S. No	Paper Code	Paper no.	Title of the paper	Instruction Hrs/ Week	No. of Credits	Marks		Total marks
						External	Internal	
1	3CHT9	Paper-I	Analytical Chemistry	4	4	80	20	100
2	3CHT10	Paper-II	Synthetic Organic Chemistry-I	4	4	80	20	100
3	3CHT11	Paper-III	Bioinorganic Chemistry	4	4	80	20	100
4	3CHT12	Paper- IV	Chemistry of Materials and Inorganic Photochemistry	4	4	80	20	100
5	3CHP7	Paper-V	Preparation of Complexes and their characterization by Physiochemical techniques	9	4	100	----	100
6	3CH**P**8	Paper-VI	Analysis of Ternary mixtures and Complex materials	9	4	100	----	100
		Seminar		----	1	25	----	25
	Total			34	25			625

III Semester-Organic Chemistry

Curriculum						Scheme of Examination		
S. No	Paper Code	Paper no.	Title of the paper	Instruction Hrs/ Week	No. of Credits	Marks		Total marks
						External	Internal	
1	3CHT9	Paper-I	Analytical Chemistry	4	4	80	20	100
2	3CHT10	Paper-II	Synthetic Organic Chemistry-I	4	4	80	20	100
3	3CHT13	Paper-III	General Organic Chemistry-I	4	4	80	20	100
4	3CHT14	Paper- IV	Natural Products	4	4	80	20	100
5	3CHP9	Paper-V	Preparation of organic compounds and Spectral analysis	9	4	100	----	100
6	3CHP10	Paper-VI	Organic mixture analysis (with two component mixture)	9	4	100	----	100
		Seminar		----	1	25	----	25
	Total			34	25			625

III Semester-Physical Chemistry

Curriculum						Scheme of Examination		
S. No	Paper Code	Paper no.	Title of the paper	Instruction Hrs/ Week	No. of Credits	Marks		Total marks
						External	Internal	
1	3CHT9	Paper-I	Analytical Chemistry	4	4	80	20	100
2	3CHT10	Paper-II	Synthetic Organic Chemistry-I	4	4	80	20	100
3	3CHT15	Paper-III	Physical Chemistry-III	4	4	80	20	100
4	3CHT16	Paper- IV	Physical Chemistry-IV	4	4	80	20	100
5	3CHP11	Paper-V	Practicals -Kinetics	9	4	100	----	100
6	3CHP12	Paper-VI	Practicals- Instrumentation	9	4	100	----	100
		Seminar		----	1	25	----	25
	Total			34	25			625

IV Semester-Inorganic Chemistry

Curriculum						Scheme of Examination		
S. No	Paper Code	Paper no.	Title of the paper	Instruction Hrs/ Week	No. of Credits	Marks		Total marks
						External	Internal	
1	4CHT17	Paper-I	Applied Physical Chemistry	4	4	80	20	100
2	4CHT18	Paper-II	Synthetic Organic Chemistry-II	4	4	80	20	100
3	4CHT19	Paper-III	Instrumental methods of analysis	4	4	80	20	100
4	4CHT20 Elective A	Paper-IVA	Organometallic Chemistry	4	4	80	20	100
	4CHT20B Elective B	Paper-IVB	Analytical Techniques and Applied Analysis					
5	4CHP13	Paper-V	Ion exchange and Solvent Extraction Methods	9	4	100	----	100
6	4CHP14	Paper-VI	Instrumental Methods	9	4	100	----	100
		Seminar		----	1	25	----	25
	Total			34	25			625

IV Semester-Organic Chemistry

Curriculum						Scheme of Examination		
S. No	Paper Code	Paper no.	Title of the paper	Instruction Hrs/ Week	No. of Credits	Marks		Total marks
						External	Internal	
1	4CHT17	Paper-I	Applied Physical Chemistry	4	4	80	20	100
2	4CHT18	Paper-II	Synthetic Organic Chemistry-II	4	4	80	20	100
3	4CHT21	Paper-III	General Organic Chemistry-II	4	4	80	20	100
4	4CHT22A	Paper- IVA	Natural products (Elective-A)	4	4	80	20	100
	4CHT22B	Paper- IVB	Medicinal chemistry (Elective-B)					
5	4CHP15	Paper-V	Estimations and Principles of chromatography	9	4	100	----	100
6	4CHP16	Paper-VI	Isolation and purification of natural products and Advanced organic preparations	9	4	100		100
		Seminar		----	1	25	----	25
	Total			34	25			625

IV Semester- Physical Chemistry

Curriculum						Scheme of Examination		
S. No	Paper Code	Paper no.	Title of the paper	Instruction Hrs/ Week	No. of Credits	Marks		Total marks
						External	Internal	
1	4CHT17	Paper-I	Applied Physical Chemistry	4	4	80	20	100
2	4CHT18	Paper-II	Synthetic Organic Chemistry-II	4	4	80	20	100
3	4CHT23	Paper-III	Catalysis	4	4	80	20	100
4	4CHT24A	Paper- IVA	Materials, Computational Chemistry and Data analysis (Elective-A)	4	4	80	20	100
	4CHT24B	Paper- IVB	Molecular Modelling (Elective-B)					
	4CHP17	Paper-V	Practicals -Kinetics	9	4	100	----	100
7	4CHP16	Paper-VI	Practicals-Instrumentation	9	4	100		100
		Seminar		----	1	25	----	25
	Total			34				625

III Semester

Paper-I Analytical Chemistry (3CHT10)

(Common paper for all specializations)

(Marks 100, Total Hours 60)

Unit-I Chromatography:

Chromatographic methods: General discussion, Adsorption and partition chromatography, component identification parameters, Theories of Chromatographic separations – Plate theory and Rate theory; chromatographic process optimization, Retention analysis, Resolution, principles and applications of paper chromatography and thin layer chromatography, Gas-Liquid chromatography, High performance liquid chromatography and supercritical fluid chromatography – Principles, instrumentation, detectors used and applications; Hyphenated techniques – Gas chromatography – Mass spectrometry and liquid chromatography – Mass spectrometry, principles and applications.

Unit-II Thermoanalytical methods:

Introduction to thermoanalytical methods, Thermogravimetric analysis (TGA), Principles, Derivative thermogravimetry (DTG), Comparison and interpretation of TG and DTG curves, Instrumentation of TG, TGA curves of individual compounds and mixtures, Factors affecting TGA curves, Applications of TGA. Differential thermal analysis (DTA) – Principles, Instrumentation, Interpretation of DTA curves, Influence of atmosphere on DTA curves of a sample, complementary nature of TGA and DTA, Applications of DTA in the study of clays, minerals, coals and explosives. Differential Scanning Calorimetry (DSC) – Principles, Methodology, Interpretation of DSC curves, comparison between DSC and DTA, chemical and pharmaceutical applications of DSC.

Unit III Separation techniques:

Solvent Extraction Methods: General discussion, Liquid-liquid systems, Factors favoring extraction of metal ions into organic solvents, quantitative treatment of solvent extraction equilibria, synergistic extraction, Ion association complexes, Some practical considerations in solvent extraction, Determination of Ni as Ni-DMG complex and of Pb as Pb-dithizone complex; solid-liquid systems – Extraction of soluble solid compounds by solvents.

Ion-Exchange Methods: General discussion, Typical synthetic Cation and Anion exchange resins, Action of ion exchange resins, Ion exchange capacity, Determination of cation and anion exchange resin capacities, Column operation and ion exchange chromatography, Separation of Zn and Mg using anion exchange resin; Chelating ion exchange resins, liquid ion exchangers.

Unit-IV CD, ORD and Fluorescence:

Principles and instrumentation of CD and ORD spectroscopy. Cotton effect Use of CD in the conformational studies of metal complexes, DNA and DNA-Metal complexes. Theory and principles of fluorescence spectroscopy. Characteristic of fluorescence emission. Fluorescence life time, quantum yield. Fluorescence polarization and polarization spectra of fluorophore. Application of Fluorescence quenching in general and ligand/drug/metal/ complex DNA binding studies.

Recommended books:

1. Vogel's text book of quantitative chemical analysis- G.H. Jeffery, J. Bassett, J. Mentham and R.C. Denney, 6th ed., Pearson Edn. Ltd.
2. Instrumental methods of analysis- H.H. Willard, L.L. Merritt, J.A. Den and F.A. Settle, 7^{th} ed., CBS Publishers.
3. Principles of instrumental analysis- D.A. Skoog, F.J. Holler and T.A. Nieman, 5^{th} ed., Harcourt Asia PTE Ltd.
4. Analytical chemistry- Gary D christian 6^{th} ed.
5. Principles of Instrumental analysis – Skoog, Nieman, Harcourt.
6. Vogel's text Book of quantitative chemical analysis- A.I Vogel (5^{th} edition).
7. Instrumental methods of Analysis, Willard, Dean & Settle.
8. Principles and practice of Analytical Chemistry, F. W. Fifield & D. Kealy.
9. Automatic methods of analysis, M. Valcarcel, M. D. Luque de Castro.
10. Principles of Instrumental Analysis, Skoog, Holler and Wieman.
11. Principles of fluorescence spectroscopes-Lakowiz.
12. Fluorescence Quenching theory and applications-Maurice R.Eftink.

III Semester

Paper-II Synthetic Organic Chemistry-I (3CHT10)

(Common paper for all specializations)

(Marks 100, Total Hours 60)

Unit-I Organic Photo Chemistry:

Photo excitation of molecules-Electronic transitions and types of electronic transitions, Energies and life times of excited states, Fate of excited molecules, Photophysical processes-Jablonski diagram. Photochemical sensitization and Photochemical quenching.

Photochemistry of carbonyl compounds – Photoreductions (Intermolecular and Intramolecular), Paterno-Buchi reaction (Intermolecular and Intramolecular including stereochemistry) and limitations. Photochemical cleavages–Norrish Type-I and Norrish Type-II reaction (including stereochemistry). Photochemistry of Olefines–Cis-Trans isomerisation, Dimerization, Simple additions and, Inter and Intra molecular cyclo additions. Electrocyclization and Cycloaddition reactions in conjugated dienes. Photochemistry of Aromatic compounds–Ring isomerisation, Photocyclo additions. Photorearrangements-Barton reaction, Zimmermann rearrangement, Photo-Fries rearrangement, and Migration of groups in aromatic compounds.

Unit-II Pericyclic Reactions:

Introduction –Characteristics and classification of pericyclic reactions. Representation of molecular orbitals-Bonding, Non-bonding and Anti bonding, Symmetry properties with special reference to plane of symmetry and two-fold axis of symmetry. FMO, Orbital Correlation Diagram (OCD) approaches and Stereochemistry of Electrocyclic reactions (4n and 4n+2 electron system), Cycloaddition reactions (4n & 4n+2 systems and including **1**,3 Dipolar cycloaddition in ketenes). Detail study of Diels-Alder reaction– Stereochemistry – Cis-rule–Alder's Endo rule and Regioselectivity. Elementary treatment of PMO approach. PMO, FMO approach and Stereochemistry of Sigmatropic rearrangements-[1,3], [1,5], [1,7], Cope, Oxy-Cope, Aza-Cope, Claisen, and Aza-Claisen rearrangements. Sommlet-Hauser reaction, Chelotropic reactions (Additions and Eliminations), Group transfer, Group elimination and Ene reactions. Exercises based on pericyclic reactions.

Unit-III Formation of –C-C- and –C=C- bonds:

C-C (single) bond formation: Alkylation of relatively acidic methylene group-Enolate anions- Alkylation of enolate anions and Stereochemistry of alkylation of enolate anions – Aldol addition reactions of Li, B, Ti enolate anions and Mukaiyama reaction. Conjugate addition of Grignard reagents in presence of copper salts. Synthetic applications of Gilman reagent in C-C bond formation -Reaction with halides, sulfonates, epoxides and α,β-unsaturated carbonyl compounds, esters and epoxides. The enamine reactions in C-C bond formation–Synthetic applications of carbenes and carbenoids.

C=C (double) bond formation: Wittig reaction and related reactions-Phosphonate Modification (Wadsworth-Emmon reaction), Horner-Wittig reaction, Peterson Olefination reaction, Julia-Lythgoe Olefination, McMurray Olefination, Tebbe Reagent, Bamford-Stevens Reaction, and Nickel (II) Catalyzed Cross-Coupling with Grignard Reagents (Kumada Reaction). β-Elimination reactions, Pyrolytic Syn-eliminations in amine oxides (Cope Elimination), Sulphoxides and Selenoxides.

Unit-IV Oxidation and Reductions:

Oxidations: Oxidation of C=C with transition metal oxidants – KMnO4 and OsO4, Epoxidation with peroxy acids, and hydroperoxides and subsequent transformation of epoxides. Stereochemistry of perhydroxylation(cis and trans) – Cleavage of glycols [HIO4 and $Pb(OAc)_4$]. Oxidation of alcohols to carbonyl compounds using Cr^{VI} oxidants-(PCC, PDC, Collins reagent, and Jones reagent) and Swern oxidation. Singlet oxidation– Generation of Singlet oxygen- Reaction of alkenes with Singlet oxygen and their subsequent transformation. Synthetic applications of hypervalent Iodine: 2-Iodoxybenzoic acid (IBX), Dess-Martin oxidation, and Iodobenzenediacetate.

Reductions: Group III-hydride transfer reagents: $NaBH_4$, $NaBH_3CN$, $LiAlH_4$, Lithiumhydrido alkoxyaluminates and DIBAL to reduce carbonyl groups and other functional groups– Reduction of α,β--unsaturated ketones(1,2 and 1,4-additions) Stereochemistry of hydride reductions (Cyclohexanones).

Group IV hydride donors: Trialkylsilanes (R_3SiH and Ar_3SiH) to reduce hindered alcohols and carbonyl compounds, HCOOH -Eschweiler–Clarke reaction and Hydride ion transfer in MPV reduction and Cannizzaro reaction.

Dissolving metal reductions: a) Addition of hydrogen–Metal in liquid NH_3 and alcohol – reduction of carbonyl functional group and α,β--unsaturated ketones, partial reduction of aromatic rings and Birch reduction.

b) Reductive removal of functional groups-reductive removal of halogen, carbonyl group, acetate and sulfonate groups with Li or Na/EtOH, Diethyl phosphorochloridate, Zn-Hg/HCl, Zn-Al/AC_2O and Zn-Al/NH_4Cl.

c) Reductive C-C and C=C bond formation– Formation of diols, cyclic diols, alkenes, cycloalkenes by reduction of carbonyl group with Mg-Hg, Mg-Hg/$TiCl_4$, Na/$TiCl_4$, and Zn or Cu/$TiCl_4$. Reductive coupling of esters with Na/Me_3SiCl in Xylene and Acyloin condensation-construction of small and large ring size cycloalkanes by reduction of diesters.

Recommended Books:

1. Molecular reactions and photochemistry –C. Dupey & O. L. Chapman
2. Molecular photochemistry –Turro
3. Molecular Photochemistry – Gilbert & Baggo
4. Organic Photochemistry – D Coyle

5. Molecular Reactions and Photochemistry – Depuyand Chapman
6. Photochemistry – C W J Wells
7. Some modern methods of organic synthesis –W. Carruthers
8. Guide book to organic synthesis– R. K. Meckie, D. M. Smith, R. A. Atken
9. Organic synthesis –O. House
10. Organic synthesis– M. B. Smith
11. Advanced organic chemistry. Part A Structure & Mechanism –Francis A. Coreyand Richard J. Sundberg
12. March's Advanced Organic Chemistry –Michael B. Smith
13. Conservation of Orbital Symmetry –Woodward and Hoffmann
14. Organic Reactions and Orbital Symmetry, –Gilchrist and Storr
15. Pericyclic Reactions -a problem solving approach– Lehr and Merchand
16. Pericyclic Reactions-A Textbook: Reactions, Applications and Theory –S. Sankararaman, Roald Hoffmann
17. Pericyclic Reactions – Mukherjee S M

III Semester

Paper- III Bioinorganic Chemistry and applications (3CHT11)

(Inorganic specialization)

(Marks 100, Total Hours 60)

Unit-I Metalloproteins and Metalloenzymes:

General principles in metal binding sites – preservation of electroneutrality, selfassembly of metal clusters. Metalloproteins–Electron transfer proteins: Ferridoxins, Rubredoxins, Blue copper proteins, Cytochrome C. Metalloenzymes – Carboxypeptidase A, Carbonic anhydrase, Vitamin B12, Cytochrome P450.

Unit-II Metal ion transport and storage:

Transport of iron by transferring, storage of iron by Ferritin, synthetic iron-oxo aggregates, Transport of iron by siderophores (Hydroxymate and phenolate siderophores), Models for siderophores; Transport of copper by ceruplasmin and serum albumin; transport of Na and K ions across cell membranes by Na+ - K+ ATPase; Transport of Ca across sarcoplasmic Reticulum by Ca^{2+} - AT Pase; storage and transport of Vanadium.

Unit-III Metal complexes and their interaction with nucleic acids:

Structure of nucleic acids, Interaction of metal complexes with nucleic acids – Coordination, Intercalation and Hydrogen bonding; Fundedamental reactions with nucleic acids – Redox chemistry and Hydrolytic chemistry; Nuclease activity of tris (Phenanthroline) metal complexes and their interaction with DNA; Applications of nuclease activity of metal complexes as spectroscopic probes, metallo printing reagents, conformational probes and cleavage probes; Metal-nucleic acid interactions in nature Structural role, Regulatory role and Pharmaceutical role.

Unit-IV: Activation of small molecules:

Aa) Dioxygen complexes: Dioxygen as ligand, supereoxo, peroxo, and Dioxygen complexes of Fe, Co and Ir : Preparation, bonding and structures of dioxygen complexes. Reactions of dioxygen and peroxo complexes. Synthetic applications. Model compounds of oxygen carriers in biological systems.

Bb) Dinitrogen complexes: Isoelectronic species CO, CN^- and N^{2-} comparison and stability of metal complexes of these ligands. Allen'salt, preparation of dinitrogen complexes of Ru, Mo and W. Bonding and structure of dinitrogen complexes. Reactions of coordinated dinitrogen, Biological nitrogen fixation.

Recommended books:

1. Principles of bioinorganic chemistry - S.J. Lippard and J.M. Berg.
2. Inorganic biochemistry, Vols I & II Ed. - G.L. Eichorn.
3. Bioinorganic Chemistry - I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, Viva Books Pvt. Ltd.
4. Bioinorganic Chemistry - K. Hussain Reddy, New Age Internatioal Publishers.
5. Inorganic biochemistry- J.A. Cowan, VCH Publications.

III Semester

Paper- IV Chemistry of Materials and Inorganic Photochemistry (3CHT12)

(Inorganic specialization)

(Marks 100, Total Hours 60)

Unit-I Supramolecular Chemistry:

Concepts and principles, Host-Guest Chemistry, Non-covalent bonds, crown ethers, cryptands and their metal complexes, Molecular recognition for different types of molecules, spherical recognition, Tetrahedral recognition, cooperativity and multivalency, Design and synthesis of co-receptor molecules and multiple recognition, supramolecular reactivity and catalysis, supramolecular devices, supramolecular photochemistry.

Unit-II Nanomaterials – I:

Introduction to nanoparticles, Classification of nanoparticles, Preparation of nanoparticles – Bottom-up approach, Top-down approach, chemical vapour deposition method, Thermolysis method, Pulsed laser method; Optical and electrical properties of nanomaterials, characterization of nanomaterials – X-ray spectroscopy, Scanning electron microscopy, Transmission electron microscopy, Atomic force microscopy, Field ion microscopy; properties and various applications of ZnO, iron and gold nanomaterials.

Unit-III Nanomaterials – II:

Dendrimers–Introduction to dendrimers, synthesis, structure, properties and applications of dendrimers. Fullerenes–Synthesis of fullerenes, chemical properties and nanochemistry of fullerenes, Ligational aspects of fullerenes. Carbon nanotubes–structural aspects of carbon nanotubes, Electrical, mechanical and electromagnetic properties of carbon nanotubes, Applications of carbon nanotubes as metallic and semi-conductors, interconnects and as fibers and films.

Unit-IV Inorganic Photochemistry:

Basics of photochemistry – Absorption of light and molecular excitation, photochemical laws and Quantum yield; Electronically excited states and their life-time measurements, properties of excited states – structure, Acid-base strength and Reactivity; Excited states of metal complexes, comparison with organic compounds, Electronically excited states of metal complexes, charge transfer states; photochemical reactions of metal complexes – photosubstitution (photoaquation and photoexchange), Photoionization, Photoisomerization; Photochemical decomposition of water using CdS and Ru-bipyridyl complex.

Recommended books:

1. Supramolecular Chemistry – concepts and perspectives by Jean-Marie Lehn.
2. Principles and methods in Supramolecular chemistry, Hans-Jorg Schneider and A. Yatsimirsky, John Wiley and Sons.
3. Analytical Chemistry of Macrocyclic and Supramolecular Compounds, S.M.Khopkar, Narosa Publishing House.
4. Inorganic Photochemistry, Journal of Chemical Education, Vol 60. No 10, 1983.

5. Photochemistry of Coordination compounds V.Balzani and Carassiti, academicpresss.
6. Concepts of inorganic photochemistry- Adamson and Fleichner.
7. Elements of inorganic photochemistry- Ferrandi.
8. Materials science and engineering – An introduction - W.D. Callister, Jr. 7th ed. John Wiley & Sons, Inc.
9. Nanochemistry- G.B. Sargeev, Elsevier.
10. Nanochemistry: A chemical approach to nanomaterials - G.A. Ozin and A.C. Arsenault, RSC Publishing.
11. Nanomaterials and nanochemistry - C.Brechigneae, P. Houdy and M. Lahmai (Eds.), Springer.
12. Core concepts in supramolecular chemistry and nanochemistry, J.W. Steed, D.R. Turner and K. Wallace, Wiley.

III Semester –

Inorganic Chemistry Practicals (Specialization)

Paper-V Preparation of Complexes and their characterization by Physiochemical techniques (3CHP7)

(Marks 100, 9 Hours per week)

1. $[Cu(NH_3)_4]SO_4.H_2O$
2. $[Ni(DMG)_2]$
3. $[Mn(acac)_2]$
4. $Na[Cr(NH_3)_2(SCN)_4]$
5. Prussian blue, Turnbull's blue
6. $[Co(NO_2)(NH_3)_5]^{2+}$ and $[Co(ONO)(NH_3)_5]^{2+}$

Paper-VI Analysis of Ternary mixtures and Complex materials (3CHP8)

(Marks 100, 9 Hours per week)

I. Analysis of Ternary mixtures
   1. Ag^+, Cu^{2+}, and Ni^{2+}
   2. Cu^{2+}, Ni^{2+} and Zn^{2+}
   3. Fe^{3+}, Mg^{2+}, and Ca^{2+}

II. Analysis of Complex materials
   1. Brass
   2. Devarda's alloy
   3. Cement

Recommended Books:

1. Vogel's Text Book of Quantitative Chemical Analysis, 6th Edition.
2. Comprehensive experimental chemistry- V.K. Ahluwalia, New publication
3. Analytical Chemistry- Theory and Practice-R.M. Verma, CBS Publishers

Scheme of Valuation

Marks 100	Time: 4Hours
Experiments (2)	80 Marks
Record/ Sample & Viva	20 Marks

III Semester

Paper-III General Organic Chemistry-I (3CHT13)

(Organic Chemistry Specialization)

(Marks 100, Total Hours 60)

Unit-I Heterocyclic Chemistry-II:

Synthetic methods and reactivity of the following heterocyclic systems: Carbazoles, Pyrazoles, Indazoles, Benzimidazoles, Benzoxazoles, Benzthiazoles, Acridines, Pyridazines, Cinnolines, Phthalazines and Pyrimidines.

Unit-II Reaction Mechanisms-III:

Study of the following special mechanistic aspects in organic chemistry:

Principles of microscopic reversibility with reference to esterification – Ester hydrolysis (with H_2SO_4) & hydration of alkenes – Super acids – Long living carbocations – Simultaneous and stereospecifc 1,2 shifts – Cascade of ring expansions – Conversion of aryl iminoesters to diarylamides-Chapmann rearrangement– Cyclodehydration of aldehydes and ketones– Von Ritcher rearrangement – Hofmann–Löffler–Freytag reaction– Knoevenagel condensation, The Darzens-Glycidic ester condensation. Homologation reactions-Seyferth-Gilbert Homologation, Arndt-Eistert Synthesis, Kowalski ester homologation, and Horner–Wadsworth–Emmons reaction.

Unit-III Combinatorial synthesis:

Introduction to combinatorial chemistry, solid phase synthesis of organic libraries, Resins and linkers – Synthesis of peptides libraries, solution phase combinatorial libraries of small organic molecules – Direct deconvolution technique for pool libraries – Encoding techniques – Analytical characterization of synthetic organic libraries – Automation in combinatorial chemistry – High throughput screening.

Unit-IV Green Chemistry:

Introduction, Principles, atom economy- atom economy-calculation of atom economy in substitution reactions, addition reactions, elimination reactions, oxidations, reductions and rearrangement reactions. Introduction to alternative approaches-Solvent free reactions-principle, benefits of solvent free reactions and examples. Phase changes, optimum reaction temperatures, miscibility of reactants and catalysts. Microwave assisted organic synthesis: Solvent free microwave assisted organic synthesis: Introduction, solvent free techniques – Reactions on solid mineral supports, solid-liquid phase-transfer catalysts – Reactions without solvent, support or catalyst. Microwave activation-benefits and limitations. Examples of reactions on solid supports, reactions without support or catalyst.

Recommended Books:

1. Heterocyclic chemistry - R. K. Bansal
2. Heterocyclic Chemistry - T.Gilchrist
3. An introduction to the Chemistry of heterocyclic compounds -R.M.Acheson

4. Heterocyclic Chemistry - J.A.Joule & K.Mills
5. Principles of Modern Heterocyclie Chemistry -A.Paquette
6. Handbook of Heterocyclic Chemistry -A.R.Katritzky
7. Green chemistry, Theory and Practical - Paul T.Anastas and John C.Warner
8. New trends in green chemistry -V.K.Ahulwalia and M.Kidwai.
9. Organic Synthesis: Special techniques - V.K.Ahulwalia and Renu Aggarwal.
10. Analytical Methods in Combinatorial Chemistry (Critical Reviews in Combinatorial Chemistry) - Bing Yan
11. A Practical Guide to Combinatorial Chemistry - Anthony W. Czarnik and Sheila Hobbs DeWitt
12. Advanced organic chemistry. Part B: Reactions and Synthesis -Francis A. Coreyand Richard J. Sundberg
13. Advanced organic chemistry. Part A Structure & Mechanism by Francis A. Corey and Richard J. Sundberg
14. Name Reactions and Reagents in Organic Synthesis - Bradford Mundy, Michael G. Ellerd and Frank G. Favaloro
15. March's Advanced Organic Chemistry -Michael B. Smith

Some modern methods of organic synthesis -W. Carruthers

III Semester

Paper-IV Natural Products (3CHT14)

(Organic Chemistry Specialization)

(Marks 100, Total Hours 60)

Unit-I Classification, Isolation, Separation and Identification of Natural products:

Classification within each type of natural products (classification of alkaloids, terpenoids, steroids, quinonoids, flavanoids...etc.). General techniques of isolation and purification of natural products (with suitable examples representing different types of natural products). General chemical methods used in the structure elucidation of alkaloids. Basic separation techniques used in various types of natural products.

Unit-II Chemistry of Terpenoids:

Structure elucidation and total synthesis of Citral, α-Terpineol, Camphor, Cadinene, Abietic acid**,** Lanosterol and β-Amyrin.

Unit-III Chemistry of Alkaloids:

Structure elucidation and total synthesis of Atropine, Papaverine, Nicotine, Morphine, Codeine, Thebaine, Reserpine and Strychnine.

Unit-IV Chemistry of Steroids:

Structure, stereochemistry and synthesis of Cholesterol, Androsterone, Testosterone, Oestrone, Oestradiol, Oestriol, Progesterone and Cortisone.

Recommended books:

1. Textbook of organic chemistry - I L Finar Vol II
2. An introduction to the chemistry of terpenoids and steroids -William Templeton
4. Steroids - Fieser arid Fieser
6. Alkaloids - Bentley
8. The chemistry of terpenes - A Pinder
9. Terpenoids - Mayo
11. Alkaloids - Pelletier
12. Total synthesis of Natural Products - Apsimon (Vol 1-5)

III Semester

Paper-V Preparation of organic compounds and Spectral analysis (3CHP9)

Organic Chemistry Practicals (Specialization)

(Marks 100, 9 Hours per week)

(A) Two step preparation:

1. *o*-Chlorobenzoic acid form anthranilic acid
2. p-Bromoaniline from acetanilide
3. p-Nitroaniline from acetanilide
4. Tribromobenzene from aniline: (a) Aniline to Tribromoaniline (b) Tribromoaniline to Tribromo benzene
5. Preparation of 2,4-DNP: (a) Chlorobenzene to 2,4-Dinitrochlorobenzene (b) Preparation of 2,4-DNP from 2,4-Dinitrochlorobenzene
6. Preparation of Iosin: (a) Fluorosin from phthalic anhydride (b) Eosin from fluorescein.

(B) Spectroscopic identification of some organic compounds:

A set of spectral analytical data for at least 20 compounds will be analyzed by each student and two out of the same compounds will be chosen for the examination from which the student will analyze and identify one compound.

Scheme of Valuation

Marks 100	Time: 4Hours
Experiments (2)	80 Marks
Record/ Sample & Viva	20 Marks

Paper-VI: Organic Mixture Analysis (with two component mixture) (3CHP10)

(Marks 100, 9 Hours per week)

Organic mixture analysis (With two component mixture): Seperation of the two component mixture of organic compounds in a systematic procedure and systematic identification of each of the component organic compounds by using: Preliminary examination, identification of extra elements, common functional group tests, specific functional group tests, preparation of at least two rational derivatives and finally identifying the given compounds by checking the melting points of its derivatives with those in literature.
Mixture for analysis:

1) Strong Acid + Neutral
2) Base + Neutral
3) Weak acid + Neutral
4) Neutral + Neutral

At least ten mixtures have to be analyzed by the students.

Recommended Books:

1. Practical organic chemistry by Mann & Saunders
2. Text book of practical organic chemistry by Vogel
3. The systematic identification of organic compounds by Ralph L. Shriner, Christine K. F. Hermann, Terence C. Morrill and David Y. Curtin
4. Practical organic chemistry by Mann & Saunders
5. Spectroscopic identification of organic compounds by R M Silverstein and F X Webster

Scheme of Valuation

Marks 100	Time: 4Hour
Separation of mixture	20
*Tests for two components	60
Record/ Sample & Viva	20

*Note: For each component, identification of functional group, extra elements, determination of melting point and preparation of derivatives -30 marks

III Semester

Paper-III Quantum Chemistry, Kinetics & Electrochemistry

(Physical Chemistry-III) (3CHT15)

(Physical Chemistry Specialization)

(Marks 100, Total Hours 60)

Unit-I Group Theory:

Symmetry operations forming a group. Matrix representation of symmetry operations and point groups, isomorphism, Reducible and irreducible representation. The great orthogonality theorem (without proof) and its properties for reducible and irreducible representation.

Character tables – General aspects of character table, construction of character tables for C_2V and C_3V. Point groups- Direct product rule, Group theoretical approach for UV transitions in formaldehyde. IR and Raman active modes of water molecule.

Unit-II Quantum Chemistry – III:

MO diagrams and MO configurations of Homo nuclear diatomic molecules H_2, Li_2, N_2, O_2, F_2 and hetero diatomic molecules HF, BN, CO, NO.

LCAO treatment of H_2^+ and H_2 by VB theory and MO theory wave functions and energy expressions, Comparison of VBT and MOT of Bonding with reference to H_2 molecules. **Angular momentum-**Ladder operators, addition of angular momenta spin, anti-symmetry and Pauli exclusion principle.

Unit-III Quantum Chemistry –IV:

Concept of hybridization, quantum mechanical treatment of SP, SP^2 and SP^3 hybrid orbitals, Wave functions and angles. Hybrid orbitals on oxygen in H_2O. HMO theory of conjugated polyenes. Application to allyl systems, butadiene, cyclopropenyl and cyclobutadiene systems energy and wave functions-Applications of HMO coefficients to calculate electron density, charge density, bond order. HMO theory of hetero aromatic compound of pyrrole.

Unit-IV Kinetics-III

Mechanism of Electron transfer reactions, Oscillatory reactions, conditions and mechanism of oscillatory reactions. Branched Chain reactions – Reactions of H2 and O2 and combustion of hydrocarbons-Decomposition of ozone, acetaldehyde and phosgene. Unimolecular reactions: Rice, Ramspenger and Kassel treatment.

Solvent-Solute interactions- Solvation parameters- effect of solvent on reactivity.

Kinetics of fast reactions: Flow methods – Stopped-flow and continuous flow methods– Relaxation methods – Relaxation time and its relation to rate constant. Flash photolysis.

Recommended books:

1. Chemical applications of Group theory - F. A. Cotton, Wiley, New York,1990.
2. Quantum chemistry - Ira N. Levine, Prentice - Hall & India. New Delhi.
3. Introduction to Quantum chemistry -A. K. Chandra. Tata Mc. Graw-Hill Publishers Company Ltd., New Delhi
4. Quantum chemistry - D. A. Mcquarrie, Viva Books Pvt., Ltd.,
5. Quantum chemistry - R. K. Prasad, New Age International (P) Ltd.
6. Advanced physical chemistry by Gurudeep raj Goel Publishers House, Meerut
7. Chemical kinetics-K.J.Laider-Mcgraw Hill,3rd Edition
8. Kinetics and Mechanism of chemical transformations-J.Rajaraman and J.C.Kuriacose-MacMillian.
9. Physical organic chemistry-E.M.Kosower-Johnwiley& Sons.
10. Text book of physical chemistry -Puri& Sharma
11. Text book of advanced physical chemistry – Gurudeepraj

III Semester

Paper-IV Non-Equilibrium Thermodynamics, Materials, Lasers & Solid State (Physical Chemistry-IV) (3CHT16)

(Physical Chemistry Specialization)

(Marks 100, Total Hours 60)

Unit-I Non-Equilibrium Thermodynamics:

Thermodynamic criteria for non-equilibrium states, entropy production and entropy flow, entropy balance equations for different irreversible processes (e.g., heat flow, chemical reaction etc.) transformations of the generalized fluxes and forces, non-equilibrium stationary states, phenomenological equations, microscopic reversibility and Onsager's reciprocity relations, irreversible thermodynamics for biological systems, coupled reactions.

Unit-II Material Science:

Classification of materials – ceramics, polymers, composites, semiconductors and biomaterials.

Ceramics – criteria for determining the crystal structure of ceramic materials – examples. Composites – particle reinforced and fibre reinforced composites. Preparative methods of solid materials - Ceramic method (Solid State method), co-precipitation and sol - gels process (Zeolite synthesis).

Techniques of single crystal growth – growth from solutions – growth from melts – growth from vapour. Non-linear optical (NLO) behavior – basic concepts, second and third harmonic generation, examples of organic, inorganic and polymer NLO materials.

Unit-III Lasers in Chemistry:

General principles of laser action. Stimulated emission. Rates of absorption and emission. Einstein coefficients. Population inversion. Three-level and four-level laser systems. Pumping. Laser cavity-resonant modes. Characteristics of laser light. Laser pulses and their characteristics. Pulse production, - switching. Pulse modification, mode-locking. Practical of lasers. Solid-state lasers, chemical and excimer lasers. Examples. Application of lasers in chemistry. Femtochemistry. The pump-probe technique. Time-resolved spectroscopy. Photodissociation of ICN. Formation and dissociation of CO-hemoglobin complex. Conversion of ethylene to cyclobutene. Bond selectivity in chemical reactions-the reaction between hydrogen atoms and vibrationally excited HDO molecules. Lasers and multiphoton spectroscopy-underlying principles. Two-photon spectra of diphenyl octatraene. Lasers in fluorescence spectroscopy and Raman spectroscopy.

Unit IV Solid State:

Bonding in metals: Crystal structures, Molecular orbital approach to the Band theory of solids– classification of solids – Insulators, conductors, and semiconductors, types of semiconductors. **Defects in crystals:** Point defects, colour centers, line defects and plane defects. **Superconductivity:** Superconductivity and types of superconductors – Theories of

superconductivity – BCS theory – Applications of superconductors. High temperature superconductors - Structure of defect perovskites. High superconductivity in cuprates. **Specific heats of solids:** Dulong and Pettit's law, Einstein theory and Debye theory of specific heats.

Recommended books:

1. Advanced physical chemistry - Gurudeep raj Goel Publishers House, Meerut.
1. Advanced physical chemistry -Guru & Singh, Pragati Prakashan.
2. Kinetics and Mechanism of chemical transformations-J. Rajaraman and J.C. Kuriacose-MacMillian.
3. Material Science and Engineering- An introduction, Willian D. Callister, Jr., John Wiley & Sons
4. Material Science & Engineering –A First Course, V. Raghavan, Prentice Hall. Principal of Physical chemistry by Puri & Sharma.
5. Chemical Engineering Kinetics, J. M. Smith, McGraw Hill.
6. The physics and chemistry of solids. Stephen Elliot, John Wiley & Sons.
7. Molecular Modelling: Principles and Applications by Andrew Leach, Longman publications
8. Lasers in Chemistry and Biological Sciences, S. Chopra & H.M. Chawla, Wiley Eastern Ltd.
9. Solid State Chemistry -D.K. Chakravarty
10. Solid state chemistry and Applications - A.R. West, Plenum Press.
11. Solid State physics - S.O. Pillai, New Age Publishers.

III Semester

Paper-V –Kinetics (3CHP11)

Physical Chemistry - Practicals (Specialization)

(Marks 100, 9 Hours per week)

1. Persulphate -Iodide reaction -Determination of
   a. Order b. Solvent Effect
   c. Salt effect d. Temperature effect
   e. Catalytic effect using Ferric in presence of copper.

Paper-VI Instrumentation (3CHP12)

(Marks 100, 9 Hours per week)

I. Potentiometry / P^H Metry

1. Titration involving dibasic and tribasic acids.
2. Redox reactions and mixture of metal ions.
   a. (V^{5+} + Mn^{7+}) by Fe^{2+}
   b. (V^{5+} + Ce^{4+}) by Fe^{2+}
3. Single Electrode potential
4. Precipitation titration
   a. KCl Vs $AgNO_3$ **b.** (KCl +KI) Vs $AgNO_3$
   c. (KCl + KBr + KI) Vs $AgNO_3$
5. Isoelectric point of Glycine.
6. Verification of Gibbs- Helmholtz equation.
7. P^{ka} of Chloroacetic acid.

II. Colorimetry:

1. Estimation of Cu^{2+} by EDTA (Mono and bivariation methods)
2. Estimation of Ni^{2+} by EDTA (Mono and bivariation methods)
3. Estimation of Fe^{2+} by complexing with (1,10 phenanthrolin)
4. Determination of Cu^{2+} and Fe^{3+} in the given mixture by EDTA

Scheme of Valuation

Marks 100	Time: 4Hours
Experiments (2)	80 Marks
Record/ Sample & Viva	20 Marks

Recommended books:

1. Practical physical chemistry by A.Findlay,Longman-London
2. Practical physical chemistry by B.Vishwanthan and P.S. Raghavan.
3. Practical physical chemistry by B.D. Khosla and V.C.Gard, R.Chand or Co. Delhi.
4. Systamatic experimental physical chemistry by S.W.RajNhoj and Dr.T.K.Chondhekar, Anjali Publications,Aurangabad.

IV Semester

Paper – I Applied Physical Chemistry (4CHT17)

(Common paper for all specializations)

(Marks 100, Total Hours 60)

Unit-I Photo Chemistry:

Photophysical processes - Radiationless processes (Vibrational relaxation, internal conversion, intersystem crossing) and their rate constants-Radiative processes (fluorescence emission, phosphorescence emission). Kinetics of photophysical unimolecular processes. Delayed fluorescence. Quantum yield and its determination, fluorimetry, phosphorimetry.

Bimolecular processes-quenching –Stern-Volmer relationship derivation and deviations. Kinetics - photolysis of HI, formation of HCl and HBr reactions. Photodimerization of anthracene. Photosensitized reactions and photochromism.

UNIT-II Nuclear Chemistry:

Introduction- The atomic nucleus-elementary particles, quarks, and classification of nuclides. Nuclear stability- mass defect, packing fraction, binding energy, average binding energy per nucleon and magic numbers. Radioactivity, nuclear emissions, nuclear transformations, The kinetics of radioactive decay, half-life, average life and radioactive equilibrium. Nuclear reactions- Fission and fusion, efficiency of fission and fusion, bombardment of nuclei by high-energy α-particles and neutrons, bombardment of nuclei by slow neutrons, theories of α, β-, β+ and γ-decay, internal conversion, Auger effect. Detection of radiations and measurement techniques. Nuclear models - shell model-salient features, forms of the nuclear potential, filling of orbitals, nuclear configuration, liquid drop model, fermi gas model, collective model and optical model. Nuclear reactors - General aspects of reactor design, thermal, fast and intermediate reactors, reactor fuel materials. Types of research reactors. Radio isotopes - The separation of radioactive isotopes - Chemical separation the preparation of Radioisotopes - The Szilard-Chalmer's effect. Applications of radio isotopes - kinetic isotope effects, Radiocarbon dating, Analytical applications

UNIT-III X-ray Diffraction:

Bragg condition. Miller indices, d-spacing formula, Lattice planes and number of d-spacings, experimental methods of X-ray diffraction. Laue method and Debye-Scherrer method. Primitive and non-primitive unit cells. Indexing the reflections. Identification of unit cells from systematic absences in diffraction pattern. Structure factor and its relation to intensity and electron density. Description of the procedure for an X-ray structure analysis. Typical examples. Electron diffraction. Scattering intensity versus scattering angle. Wierl equation. Measurement technique. Elucidation of structure of simple gas phase molecules. Indexing of planes cubic systems.

<u>Unit IV</u> Electro Analytical Techniques:

a) Polarization and over-voltage, applications of over-voltage, over-potentials exchange current density, derivation of Butler –Volmer equation, Tafel plot.

b) Polarography: Dropping mercury electrode- Instrumentation - polarogram. Types of Currents: Residual, Migration, and Limiting - Likovie equation. Types of limiting Currents: Adsorption, Diffusion, Kinetic. Polarographic maxima and suppressors. Half –wave potentials (derivation). Applications of polarography in qualitative and quantitative analysis. Analysis of mixtures. Application to inorganic and organic compounds. Determination of stability constants of complexes.

c) Amperometric titrations: Principle and instrumentation. Types and application of amperometric titrations. Determination of SO_4^{2-} metal ions viz., Mg^{2+}, Zn^{2+} Cu^{2+} and other substances.

d) Cyclic Voltammetry: Principle, instrumentation, reversible and irreversible cyclic voltammograms-applications. Cyclic voltammetric study of insecticides (ex. Parathion)

e) Optical measurements: Refractometers, polarimeters, and colorimeters: Basic principles, instrumentation, and qualitative applications

Recommended books:

1. Fundamentals of photochemistry-K.K.Rohatgi, Mukharjee, Wiely-Eastern Ltd-1978
2. Photochemistry-R.P.Wayne-Oxford University Press.
3. Essentials of nuclear chemistry, 4th edition; H. J. Arniker, NAIL publishers (1995); Chapters 1, 3 and 4.
4. Nuclear and Radioactive chemistry; Friedlander, Kennedy and Miller; Chapters 8 and 9.
5. X-ray diffraction procedures for polycrysralline and amorphous materials, H. P.
6. Klug & L. E. Alexander, John Wiley
7. Automatic methods of analysis, M. Valcarcel, M. D. Luque de Castro,
8. Principles of Instrumental Analysis, Skoog, Holler and Wieman.

IV-SEMESTER

Paper-II Synthetic Organic Chemistry-II (4CHT18)

(Common paper for all specializations)

(Marks 100, Total Hours 60)

Unit-I Synthetic methodology-I:

Introduction, Terms and definitions – Target molecule, Retrosynthesis, Disconnection, Synthon, Reagent, Transform and Synthetic equivalents. Criteria for selection of target molecule, Functional group interconversion (FGI), Disconnection or Synthon approach for organic synthesis, Synthetic tree, Linear and convergent synthesis. One-group C-X disconnections-Carboxylic acid derivatives (acid halides, esters, amides etc.), alcohols, ethers alkyl halides and sulphides. One-group C-C disconnections -Alcohols and carbonyl compounds, Reterosynthetic analysis involving chemo, regio and stereoselectivities.

Unit-II Synthetic methodology-II:

Introduction to Two-group C-C and C-X disconnections–Two-group C-X disconnections: 1,2-difunctionalised and 1,4-difunctionalised compounds with suitable examples. Two-group C-C disconnections: Diels-Alder reaction, 1,3-difunctionalised and 1,5- difunctionalised compounds- Michael addition and Robinson annulation. Control in carbonyl condensations (ex: Mevalonic acid). Rearrangements in synthesis strategy -Strategy in ring synthesis. Strategic bond approach, rules for Strategic bond approach, Application of the strategies to the synthesis of Multistriatin (+) Disparlure, and Longifolene.

Unit-III Stereoselective Synthesis-I:

Introduction, terminology and principles of stereoselective synthesis – Categories of stereoselective synthesis: Introduction to diastereoselective synthesis, enantioselective synthesis and double stereo differentiating reactions – Diastereomeric excess (de) and enantiomeric excess (ee). Strategies for stereo control in diastereoselective synthesis (preliminary conceptual treatment): Small ring templates, molecular walls, ring forming reactions pericyclic reactions, co-ordination metal centers, use of π-donar complexes, chiral auxiliaries, achiral auxiliaries, intra annular and extra annualr stereo control. Nucleophilic additions to cyclic and acyclic carbonyl compounds: Cram's rule, Felkin's model: addition to chelated carbonyl compounds, Prelog's rule, addition to chelated carbonyl compounds, addition of –H and –R to cyclic ketones (Formation of axial and equatorial alcohols) Aldol reations: (a) Achiral enolates with achiral aldehydes, (b) Achiral enolates with chiral aldehydes, (c) Chiral enolates with achiral aldehydes and (d) chiral enolates chiral aldehydes.

Unit-IV Stereoselective synthesis-II:

Stereoselective transformation of C=C (double) bond: Diastereoselective synthesis involving catalytic hydrogenation, Hydroboration, Simmons-Smith reaction, Prevost reaction. Enantioselective synthesis with chiral non racemic reagents: Hydroborations with chiral

boranes; Reductions with chiral complex hydrides and chiral organometallic compounds. Enantioselective synthesis with chiral non racemic catalysts: Catalysis by chiral transition metal complexes with reference to Sharpless enantioselective epoxidations and Jacobsen asymmetric epoxidations enantioselective hydrogenations. Enzyme mediated enantioselective synthesis. Enantioselective Iminium catalyzed reactions- Diels – Alder reaction, Michael addition and 1,4-reduction of α, β-unsaturated aldehydes, Enamine asymmetric aldol reaction. Techniques for determination of enantiomeric excess- specific rotation and Chiral NMR.

Recommended Books:

1. Stereochemistry of organic compounds -Principles & Applications by D Nasipuri
2. Stereochemistry of Carbon compounds - Ernest L Eliel & Samuel H. Wilen
3. Stereochemistry: Conformation & Mechanism -P SKalsi
4. The third dimension in organic chemistry-Alan Bassendale
5. Stereo selectivity in organic synthesis- R S Ward.
6. Asymmetric synthesis-Nogradi
7. Asymmetric organic reactions -J D Morrison andH S Moschcr
8. Principles in Asymmetric synthesis -Robert E. Gawley & Jeffreyaube
9. Stereo differentiating reactions - Izumi
10. Enantioselective organocatalysis-Peter I Dallco
11. Organic Synthesis-The disconnection approach -S Warren
12. Organic Synthesis - C Willis and M Willis
13. Problems on organic synthesis - Stuart Warren
14. Organic synthesis-R. E. Ireland
15. Organic synthesis-Michael Smith
16. Principles of organic synthesis 3rd Ed. R O C Norman and J M Coxen
17. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
18. Organic synthesis by Michael B Smith
19. Some modern methods of organic synthesis - W Carruthers
20. Catalytic asymmetric synthesis- Iwao ojima (Third Edition Wiley publication)

IV Semester

Paper- III Instrumental methods of Analysis (4CHT19)

(Inorganic specialization)

(Marks 100, Total Hours 60)

Unit-I Spectrophotometry and Atomic absorption spectroscopy:

Spectrophotometry: Beer-Lambert Law, Deviations from Beer-Lambert law, photometric accuracy, Block diagram of a spectrophotometer, simultaneous spectrophotometric determination of metals, Determination of ratio of metal complexes – Job's method of continuous variation, slope ratio method.

Atomic absorption spectroscopy: Principles, Instrumentation, sources of radiation (Hollow cathode lamp and Electrodeless discharge lamp), Interferences and methods of minimization, Applications.

Unit-II Inductively coupled Plasma-related techniques and Molecular fluorescence spectroscopy:

Inductively coupled plasma-atomic emission spectroscopy (ICP-AES) and ICP-Mass spectrometry (ICP-MS) – Principles, Instrumentation, AES detectors, Quadrupole mass spectrometer, Difference between the two detectors, Applications in the analysis of trace and toxic metals in water, geological and industrial samples. Molecular fluorescence spectroscopy Principles, theory of fluorescence, phosphorescence, Relation between intensity of fluorescence and concentration, correlation of fluorescence with molecular structure, Fluorescence quenching, instrumentation, Applications.

Unit-III Combined methods in structural characterization of compounds:

Importance of structural characterization of compounds, selection and application of various methods in structural characterization of inorganic, coordination and organometallic compounds. Case studies of (1) Diborane (2) $Ni(DMG)_2$ (3) $Ni(CO)_4$ (4) $[Co(en)_2F_2]^+$ (5) $Cu(Salen)_2$ (6) $Fe(CO)_5$ (7) $Fe_2(CO)_9$ (8) $Fe_3(CO)_{12}$ (9) Ferrocene (10) $[Cr(CH_3COO)_2.H_2O]_2$.

Unit-IV Physical Methods for Inorganic Chemistry:

Electronic and Photoelectron Spectroscopy: Excitation and ejection of electrons- Core level and valence- electron level photoelectron spectroscopy- Valence electron excitation spectroscopy- Electronic spectra of transition metal complexes.

Vibrational Spectroscopy: Applications to Inorganic systems.

NMR Spectroscopy- Time scale- Multinuclear and Organometallic NMR spectroscopy –More common spin-1/2 nuclei, ^{19}F, ^{31}P, ^{29}Si, ^{119}Sn, ^{195}Pt - Quadrupolar nuclei, e.g. ^{6}Li, ^{11}B, ^{14}N, ^{17}O and their characteristics and applications

Diffraction methods: Distinction among X-ray, neutron and electron diffraction techniques Single crystals and interpretation of results from X-ray crystallography.

Recommended books:

1. Vogel's text book of quantitative chemical analysis, G.H. Jaffery, J. Bassett, J.Mentham and R.C. Denney, 6th ed., Pearson Edn. Ltd.
2. Principles of instrumental analysis, D.A. Skoog, F.J. Holler and T.A. Neiman, 5th ed., Harcourt Asia PTE Ltd.
3. Instrumental methods of analysis, H.W. Willard, L.L. Merritt, J.A. Dean and F.A. Settle, 7th ed., CBS Publishers.
4. Physical methods for chemists, R.S. Drago, 2nd ed., Saunders College Publishing.
5. Infrared and Raman spectra of inorganic and coordination compounds, K. Nakamoto.
6. Structural methods in inorganic chemistry, E.A.V. Ebsworth, D.W.H. Rankin and S. Craddock, ELBS.
7. Inorganic Chemistry – Principles of structure and reactivity, J.E. Hubeey, E.A. Keiter and R.L. Keiter, 4th ed., Addison-Wesley Publishing Co.
8. Concepts and models of inorganic Chemistry, B.Douglas, D. McDaniel and J. Alexander, 3rd ed., John-Wiley & Sons, Inc.
9. E. A. V. Ebsworth, D. W. H. Rankin and S. Cradock, Structural methods in Inorganic Chemistry, ELBS, (Blackwell), 1987.
10. R. S. Drago, Physical Methods in Chemistry (Saunders publishing)
11. R. A. Scott and C. M. Lukehart (Editors) Applications of Physical Methods to Inorganic and Bioinorganic Chemistry, 2007 [also available as Encyclopaedia of Inorganic Chemistry, 5 Volume Set].

IV Semester

Paper- IVA Organometallic Chemistry (Elective-A) (4CHT20A)

(Inorganic specialization)

(Marks 100, Total Hours 60)

Unit-I Organometallic Compounds –II:

Organometallic compounds of transition metals: Classification of transition metal organometallic compounds based on the nature of the ligands. η^1 bonded complexes of transition metals – Alkyls and aryls, types and routes of synthesis, stability and decomposition pathways, organocopper compounds in organic synthesis. Alkylidenes, alkylidynes, low valent carbenes and carbines – synthesis, nature of bond, Structural characteristics, nucleophilic and electrophilic reactions on the ligands, role in organic synthesis.

Unit-II Organometallic Compounds –III:

Organotransition metal compounds with – donor and – acceptor ligands – η^2, η^3, η^4 organic groups. Preparation, structures and properties of olefin complexes of iron and nickel groups Preparation, structures and properties of π-allyl complexes of nickel and palladium complexes. Exo/endo conformers, η^4 – Butadiene complexes of cobalt, rhodium and iron. **Organophosphines:** Preparation and properties of organophosphines, organophosphines as ligands. Synthesis, structures and properties of organophosphine complexes of Rh and Pd.

Unit-III Organometallic Compounds – IV:

Organotransition metal complexes of the cyclic n-perimeter: CnHn: Preparation, Structure and reactions of – Fe, Co, and Ni complexes with cyclic η^{4}-C_4H_4(R4) ligands. Fe, Ru, and Os complexes with η^{5}-(C5H5) ligands, Ti, V and Cr complexes with η^{6}-(C6H6) ligands and their carbonyl derivatives.

Organometallic compounds of lanthanides**:** Comparison of organometallic chemistry of *d*- and *f*-block metals. Homoleptic organolanthanides, cyclopentadienyl and pentamethyl cyclopentadienyl complexes of trivalent and divalent lanthanides – Structures and Applications in organic synthesis.

Unit-IV Homogenous Catalysis:

Stoichiometric reactions for catalysis, catalytic reactions and the valence electron (16/18) rule, Oxidative addition reactions (H-H, H-X and R-X); Reductive elimination reactions: α-and β-elimination reactions and cyclometallation reactions. Asymmetric hydrogenation; Olefin oxidation (Wacker's process), Oligomerization & Polymerization (Ziegler-Natta Catalysis), Water gas shift reaction and Fischer-Tropsch reaction.

Recommended books:

1. Principles and applications of Organotransition metal chemistry, Collman.
2. The Organometallic chemistry of transition metals, Crabtree.
3. Metalloorganic Chemistry, Pearson.
4. Homogenous catalysis, Vol I & II, M.M. Taqui Khan & A.E. Martell.

IV Semester

Paper- IVB Analytical techniques and Applied Analysis (Elective-B) (4CHT20B)

(Inorganic specialization)

(Marks 100, Total Hours 60)

Unit-I Analysis of industrial materials:

A) Composition and Analysis of Coal: Classification of coal, role of sulphur and ash in coal, coal chemicals, proximate analysis, ultimate analysis, calorific value of coal, chemical processing of solid fuels.

B) Composition and Analysis of Cement: Composition of Portland cement, Determination of CaO, MgO, AL_2O_3, Fe_2O_3, and sulphide in cement. Determination of AL_2O_3, by polarography.

C) Analysis of pesticides: Determination of methyl parathion residues in food grains and vegetables by solvent extraction and volumetric analysis Determination of organochlorine pesticides (cypermethrin) by GC. Determination of malathion and DDT residues by spectrophotometry.

Unit-II Analysis of Air and Water Pollutants:

Air quality standards, sampling, analysis of air pollutants-SO_2 (UV-Vis, IR), H2S (Spectrophotometry and Non-dispersive IR Spectrophotometry), NO-NOx (Chemiluminescence technique, Colorimetric technique- Saltzman method), CO & CO_2 (IR, AAS & GC), Hydrocarbons (GC, GC-MS), Aromatic hydrocarbons in automobile exhaust, petrol, air, O_3 (Chemiluminescence & Spectrophotometry), particulate matter analysis. Objectives of analysis, sampling, preservation and pre-concentration methods,

physical analysis - colour, odour, temperature, pH, EC, redox potential, total dissolved solids (turbidimetry), Chemical analysis of anions – CN-, Cl-, F-, NO_2-, NO_3 - (spectrophotometry), SO_4, PO_4.

Determination of BOD, COD, TOC & DO. Analysis of Toxic Metals: Hg, As, Pb, Cd, Be, Al, Cr (Atomic Absorption Spectroscopy and Spectrophotometry)

Unit-III Food and Pharmaceutical analysis:

Analysis of Chemical additives**:** Division of colour additives (Coal-tar dyes, vegetable colours and mineral colours). Chemical preservatives and synthetic sweetening agents (organic-ether extractable and non-ether extractable) Antioxidants: Types of Antioxidants used in foods, Analysis of Butylated hydroxy toluene (BHT), Food adulteration: Common adulterants in food, contamination of food stuffs. Microscopic examinations for food adulterants. Pharmaceutical analysis: Determination of Diclofenac (non-aqueous titration), Calcium in vitamin and Calcium formulations (Complexometry), Sulphanilamide(potentiometry), Pethidine Frusemide (UV-Vis), hydrochloride(UV-Vis), Aspirin, paracetamol, and codein in APC

tablets(NMF) Phenobarbitone in tablets(IR), atropinr in eye drops(GC), Paracetamol and aspirin in tablets(HPLC) Impurity profiling of Propranolol(GC-MS),famotidine(LC-MS).

Unit-IV Analysis of Drinking Water and Sewage Water and Treatment:

Hardness: causes, measurement of hardness, units- types of hardness, estimation of temporary and permanent hardness, Alkalinity of water and its estimation. Treatment of Water for Municipal Supply: Characteristics of potable water/Domestic water, WHO standards, and Indian Standards. Aeration, Sedimentation with coagulation, Filtration, Sterilization and Disinfection: Physical Methods-Boiling, Exposure to Sunlight, Disinfection with UV light, Chemical Methods – Ozonization, Chlorination, Breakpoint chlorination and Dechlorination Desalination of Brackish Water: Treating saline water: distillation, electrodialysis, reverse osmosis (RO). Mineral Water and Purified Water: Typical Manufacturing Process, Flow Sheet Diagram of Mineral Water Manufacturing Process, Purified Water-Purification methods-Distillation, Double distillation, Deionization - Co-current deionization, Counter-current deionization, Mixed bed deionization, Demineralization, Uses of purified water- Laboratory use, Industrial uses and other uses; Health effects of drinking purified water Sewage Water Treatment: Domestic sewage - Physical, Chemical, and Biological Characteristics of Domestic Sewage, Municipal sewage, Sewage Composition and Contaminants, Sewage Treatment – On-Site Sewage Treatment Systems and Off-Site Sewage Treatment System.

Recommended books:

1. Analytical Chemistry, G. D. Cristian, 6th Edition, John Wiley & Sons, New York. id
2. Industrial Chemistry, B. K. Sharma, Goel Publishing House, Meerut.
3. Analytical Chemistry, S. L. Chopra, J. S. Kannan.
4. Principles of Instrumental Analysis, Skoog, Holler and Wieman, Harcount Asia, PTE Ltd.
5. Instrumental methods of Analysis, Willard, Dean & Settle.
6. Automatic Methods Environmental Pollution Analysis, S M Khopkar, Wiley Eastern Ltd 1995.
7. Environmental Analytical Chemistry, F W Fifield, P J Haines, Blackie Academic& Professional.
8. Environmental Chemistry, B K Sharma, Goel Publishing House, Meerut.
9. Handbook of Analysis and quality control for fruit and vegetable products, S Ranganna, Tata Mc Graw Hill Publishers Ltd, 1986.
10. Introduction to chemical analysis of foods, S Suzanna & Nielsen, CBS Publishers & Distributors.

IV Semester

Paper-V Ion exchange and Solvent Extraction Methods (4CHP13)

Inorganic Chemistry practicals (Specialization)

(Marks 100, 9 Hours per week)

Ion exchange and Solvent Extraction Methods

I. Ion exchange Methods

1. Determination of capacity of an anion exchange resin
2. Determination of capacity of a cation exchange resin
3. Separation and determination of Zinc and Magnesium using a cation exchange resin
4. Separation and determination of Chloride and Bromide using an anion exchange resin
5. Determination of the total cation concentration in a water sample.

II. Solvent Extraction Methods

1. Determination of Ni as anion NiDMG complex
2. Determination of Chloride ion and Iodide ion by $AgNO_3$
3. Determination of Pb as Pb-dithiazone complex

Paper-VI Instrumental Methods (4CHP14)

(Marks 100, 9 Hours per week)

III. Analysis of Ternary mixtures

4. Ag^{+}, Cu^{2+}, and Ni^{2+}
5. Cu^{2+}, Ni^{2+} and Zn^{2+}
6. Fe^{3+}, Mg^{2+}, and Ca^{2+}

IV. Analysis of Complex materials

4. Brass
5. Devarda's alloy
6. Cement

Recommended Books:

4. Vogel's Text Book of Quantitative Chemical Analysis, 6^{th} Edition.
5. Comprehensive experimental chemistry- V.K. Ahluwalia, New publication
6. Analytical Chemistry- Theory and Practice-R.M. Verma, CBS Publishers

Scheme of Valuation

Marks 100	Time: 4Hours
Experiments (2)	80 Marks
Record/ Sample & Viva	20 Marks

IV Semester

Paper-III General Organic Chemistry-II (4CHT21)

(Organic specialization)

(Marks 100, Total Hours 60)

Unit-I Heterocyclic Chemistry-III:

Methods of synthesis, aromatic character and reactivity of the following six membered heterocyclic systems: quinazolines, pyrazines, quinoxalines, 1,2,3-triazoles, 1,2,3-triazines, azepines, diazepines, rearrangements of 1,2-diazepines and benzodiazepines-Structure determination and synthesis of uric acid and caffeine.

Unit-II Molecular Rearrangement in organic transformations:

Mechanisms and synthetic applications of rearrangement reactions- Beckmann rearrangement, Curtius rearrangement, Hofmann rearrangement, Lossen rearrangement, Schmidt rearrangement, Fries rearrangement, Wagner–Meerwein rearrangement, Wolff Rearrangement, Baker-Venkataraman Rearrangement, [1,2]-Wittig Rearrangement, [2,3]-Wittig Rearrangement, Benzidine rearrangement Brook rearrangement and Stevens's rearrangement. Favorskii, Quasi-Favorskii Rearrangement

Unit-III Chemistry of Vitamins and nonsterodial hormones:

(a) Chemistry and synthesis of the following vitamins: A_1, A_2, B_1, B_2, B_6, H, K and C.

Chemistry and synthesis of non-steroidal hormones: Oxytocin, Thyroxin and Adrenalin. Structure determination of Insulin (synthesis is not required).

Unit-IV Drugs:

Synthesis and pharmacological applications and adverse effects of Nifedipine, Acyclovir, Warfarin, Fluconazole, Cefalexin, Sulfadoxine, Cycloserine, Chloroquine, Norfloxacin, Levocetirizine, Sulfamethoxazole and Nateglinide.

Recommended Books:

1. Bioorganic chemistry,-Herman Dugas
2. Organic Drug synthesis - Ledneiser Vol 1-6
3. Strategies for organic drug synthesis and design - Daniel Ledneiser
4. Top Drugs: Top synthetic routes - John Saunders
5. Organic chemistry -Vol. 1 and Vol. 2, Finar
6. March's Advanced Organic Chemistry -Michael B. Smith
7. Heterocyclic chemistry - R. K. Bansal
8. Heterocyclic Chemistry - T.Gilchrist
9. Heterocyclic Chemistry - J.A.Joule & K.Mills

IV Semester

Paper-IVA – Natural products (Elective-A) (4CHT22A)

(Organic specialization)

(Marks 100, Total Hours 60)

Unit-I Chemistry of Flavanoids:

Classification of Flavanoids, General methods of synthesis of Anthocyanins, Flavones, Flavonols and Flavanones. Chemistry of Pelargonidin, Cyanidin, Delphinidin chloride, Chrysin, Quercitin and Diadzein.

Unit-II Antibiotics:

Classification of Antibiotics–Isolation, Structure determination, Synthesis and Stereochemistry of Tetramycin, Pencillin-G, Cephalosporin-C, Streptomycin and Chloramphenicol.

Unit-III Prostaglandins, Porphyrins and Carotenoids:

Prostaglandins– Occurrence, Nomenclature, Classification and Physiological activity. Structure determination and synthesis of PGE_2 and $PGF_{2\alpha}$ – Porphyrins: Structure and synthesis of HAemoglobin and Chlorophyll.

Carotenoids: Structure determination and synthesis of α-Carotene, β-Carotene, γ-Carotene and Lycopene.

Unit-IV Biosynthesis of Natural products:

Introduction, Major biosynthetic pathways: (a). Acetate hypothesis and its use in construction of Aromatic rings and Polyphenolic compounds (b). Mevalonic acid pathway-Ruzicka biogenetic isoprene rule, Biosynthesis of mono, sesqui and diterpenes – formation of the Presqualene alcohol and biosynthesis of triterpenes. (c) Shikimic acid pathway: Biosynthesis of essential amino acids (Phenyl alanine, Tyrosine and Tryptophan), Flavonoids, Porphyrins and Alkaloids-(Morphine and Indole group alkaloids).

Recommended Books:

1. Biosynthesis - Geismann
2. Biosynthesis - Bernfeld
3. Chemistry of natural products, Vol 12, by Atta-Ur-Rahman
4. Organic chemistry - Vol. 2, Finar

IV Semester

Paper IVB Medicinal chemistry (Elective-B) (4CHT22B)

(Organic specialization)

(Marks 100, Total Hours 60)

Unit-I Basic concepts in Medicinal Chemistry:

Definition of Drug (WHO), Stereo chemical aspects of drugs, Classification of drugs based on chemical structure, pharmacological action and mechanisms at molecular level. Mechanism of drug action-Physical and Chemical action. Explanation of Quantal dose, Graded dose, Efficacy, Potency, LD_{50}, ED_{50} Therapeutic index and Margin of safety. Targets of Drug action: a) Receptors: Concept, Types of receptors, Agonist, Antagonist, Partial and Inverse agonist. b) Ion channels c) Enzyme : Specific and non specific Enzymes d) Carrier molecules.

Unit-II Drug Discovery:

1). a) Drug Discovery without Lead b) Lead discovery: Random screening, Non-random screening and Drug metabolism studies. Clinical observations, Rational approaches to Lead discovery. 2). Drug development: Lead modification- a) Identification of active part-Pharmacophore b) Fundamental group modification c) Structure activity relationship d) Structure modification to increase potency and therapeutic index i) Homologation ii) Chain branching iii) Ring chain transformations iv) Bioisoterism.

Drug development process: a) Pre-formulation and Product development. B) Preclinical studies; Acute toxicity, Sub acute toxicity, Chronic toxicity, Mutagenecity and Reproductive studies c) Clinical Research: Phase –1, Phase –2 and Phase –3 d) Regulatory approval process. Cost of drug development. 3). Intellectural property in drug discovery: Introduction of Patents, Concept of Patent, Requirements for Patentability and Patent restrictions.

Procedure to obtain Patent.

Unit-III Pharmaco dynamic agents:

Definition, Mechanism of action at molecular level, synthesis, Medicinal uses and Adverse effects of the following classes of compounds with special reference to specific drugs mentioned under each class. 1) Anti-Inflammatory – Ibuprofen and NSAIDS. 2) Anti-Emetic-Metoclopramide (5 HT-receptor antagonist). 3) Anti-Histamines –Pheniramine and H1-Antagonist 4) Anti-Ulcer – Ranitidine, H2-Antagonist Omeprazole- H^+K^+ Atpase inhibitor. 5) Anti-Hypertensives: a) α-Blocker- Prozosine b) β-Blocker:-Atenolol c) Ca^{+2} channel blockers-Nefedipine d) ACE-inhibitor - Enalapril e) Centrally active - Methyl Dopa. 6) Anti-Anginal Drugs- Isorsorbide dinitrate 7) Bronchodilator-Salbutamol. 8) Anti-Depressants- Fluxetine. 9). Drugs used in Schizophrenia - Chlorpromazine 10) Anxiolytic-Sedative -Diazepam.

Unit-IV Chemotherapeutatic agents:

Introduction to Chemotherapy, Differences between Pharmacodynamic agents and Chemotherapeutatic agents. 1). Inhibition of cell wall biosynthesis: Structures of Methicillin, Ampicillin, Amoxicillin, Carbenicillin and Cloxacillin. Synthesis of Phenoxy Methyl Penicillin. and Cephalosporin. New β-Lactam Drugs -Structures of Imipenem and Nocardicin.

Mechanism of Inhibition of cell wall biosynthesis by β-Lactam antibiotics 2). Inhibitors of protein biosynthesis: Structures of Streptomycin, Gentamycin-A, Tetracycline, Oxy-tetracycline, Doxycycline, Chlorotetracycline, Erythromycin and synthesis of Chloramphenicol. 3) Inhibition of RNA synthesis: Mechanism of action, Structure and uses of Rifampicin. 4) Inhibition of DNA synthesis: Mechanism of action, Structures and uses of Norfloxacin, Ofloxacin, Nalidixic acid, Synthesis of Ciprofloxacin. 5). Inhibition of DNA by polymerase: Mechanism of action, uses and synthesis of AZT. Bacterial resistance to Chemotherapeutic agents.

Recommended Books:

1. An introduction to Medicinal chemistry, G. L. Patrick, Oxford Press
2. Burger's Medicinal Chemistry and Drug Discovery, Vol. 1-5, Wiley
3. Medicinal Chemistry, Ashutoshkar, New Age International Ltd
4. Principles of Medicinal Chemistry, W. O. Foye, Varghese Pub. House
5. Essentials of Medical Pharmacology, K. D. Tripathi, Jaypee Brothers
6. A text book of medicinal chemistry, P. Primo, CBS Publishers & Distributors
7. Text book of pharmaceutical organic chemistry, Md. Ali, CBS Publishers
8. A Text book of pharmaceutical chemistry, Jayasree Ghosh
9. The organic chemistry of drug design and drug action, Silvermann R. Academic press.

Paper-V Organic Chemistry practicals (4CHP15)

(Marks 100, 9 Hours per week)

(A) Estimations:

1) Estimation of acetone /ethyl methyl ketone
2) Estimation of asprin
3) Estimation of acid value
4) Estimation of amino acid
5) Estimation of unsaturation
6) Estimation of glucose

(B) Principles of chromatography:

Determination of RF value – Ascending and descending techniques – Circular paper chromatography – Selection of solvents in paper chromatography – Location of spots in paper chromatography.

Experiments in chromatography:

(a) Separation of leaf pigments – chlorophyll-'a' & 'b' xanthophylls
(b) Separation of amino acids by paper chromatography
(c) Determination of RF value of glycine by ascending paper chromatography
(d) Determination of various impurities by thin layer chromatography
(e) Purification of commercial anthracene by column chromatography using benzene

Paper-VI -Organic chemistry practicals (4CHP16)

(Marks 100, 9 Hours per week)

(A) Isolation and purification of the following natural products:

1) Caffeine 2) Embelin 3) Piperine 4) Lycopine 5) Nicotine 6) Rutin
7) Lachnolic acid 8) Mangiferin

(B) Advanced organic preparations:

1) 2-methyl indole
2) 2,5-dihydroxyacetophenone (Fries reaction)
3) Photoreduction of benzophenone
4) Glucose to glucose penta acetate
5) Ammonium thiocyanate to urea
6) 1,2,3,4-Tetrahydrocarbazole.
7) Antipyrin
8) Benzocaine
9) Benzimidazole
10) Paracetamol

Scheme of Valuation

Marks 100	Time: 4Hours
Experiments (2)	80 Marks
Record/ Sample & Viva	20 Marks

IV Semester

Paper III Catalysis (4CHT23)

(Physical chemistry specialization)

(Marks 100, Total Hours 60)

Unit-I Heterogeneous Catalysis:

Adsorption and types of adsorption-classification of adsorption isotherm-Heat of adsorption and its determination - Freundlisch adsorption isotherm-Derivation of Langmuir adsorption isotherm- B.E.T. equation derivation and its limitation. Determination of surface area of solids Mechanism of heterogeneous catalysis. Langmuir-Hinshelwood mechanism and Langmuir Reidel mechanism. Examples of SO_2 and Fisher - Tropsch method for the synthesis of methanol. Gibbs's adsorption equation.

Unit-II Acid-Base Catalysis:

General catalytic mechanism-Specific acid base catalysis-Arrhenius and Van't Hoff intermediates – Activation energies for catalyzed reactions. Mechanism of general acidbase catalysis-Bronsted realationships types of acidity functions and their determinations. Zucker-Hammett's hypothesis and its application. Bunnett's and Olsons criteria of acidbase catalyzed reactions with examples.

Anchord catalysis: Concept of anchored catalysis and types. Montemorillorite anchored catalysis and its reactions.

Unit-III Enzyme and Micellar Catalysis:

Kinetics and mechanism of single substrate reaction. Michaelis-Menton law-Brigg's Haldane modification -Line weaver-Burk plots. Bi-substrate reaction mechanism. Temperature effect and influence of PH on the nature of active site. Inhibition of enzyme catalyzed reactions. Competitive inhibition-uncompetitive inhibition, non-competitive.

Micellar catalysis - Micellization and types of surfactants-critical micellar concentration (CMC)and its determination-factors effecting CMC. Solubilization in surfactant solutions.

Unit-IV Environmental and Photocatalysis:

Environmental Catalysis: Introduction, Automotive Exhaust Catalysis, the Three-way Catalyst and Catalytic Converter-Demonstration Experiments. Catalyst Deactivation, Catalytic Reactions in the Three-way Catalyst: Mechanism and Kinetics, CO Oxidation Reaction, CO + NO Reaction, Reactions Involving Hydrocarbons. NOx Storage–Reduction Catalyst for Lean-burning Engines, Selective Catalytic Reduction: The SCR Process and Catalyst for the SCR Process. Catalysts for Renewable Energy and Chemicals, the thermal Conversion of Biomass.

Photocatalysis: Electronic structure: from basic principles of photocatalysis, Photodegradation Processes using dyes for evaluating photocatalytic properties, Band gap energy and its determination.

Primary Processes in Photocatalysis, Solar Photocatalytic Processes: Water Decontamination and Disinfection, Current Heterogeneous Catalytic Processes for Environmental Remediation of Air, Water, and Soil, Principle of photocatalysis and Design of Active Photocatalysts,

Photocatalytic Water Splitting for hydrogen generation, Photocatalytic Reduction of CO_2 in Hydrocarbon: A Greener Approach for Energy Production.

Recommended books:

1. Chemical kinetics-K.J.Laider-McGraw-Hill
2. Enzyme catalysis –K.J. Laider-McGraw-Hill
3. Principle of biochemistry- A.L.Lehninger-Butterworth Publishers
4. Micelles, Theoretical and applied aspects-V.Moroi-Plenum.
5. Biochemistry,Voet and Voetjohn Wiely
6. Catalysis-J.C.Kuriacose-Macmillan-India Ltd.
7. Kinetics and mechanism of chemical transformations,J.Rajaramam&J.Kuriacose.
8. Adamson,A.W; Physica chemistry of surfaces.5th edition,Wiley,1992.
9. Catalytic Science Series Volume 1-Environmental Catalysis Edited By: F J J G Janssen (*Eindhoven University of Technology, The Netherlands*) and R A van Santen (*Eindhoven University of Technology, The Netherlands*).
10. Environmental Catalysis. G. Ertl, H. Knözinger, J. Weitkamp, WilleyVCH Verlag GmbH 1999.
11. Photocatalysis: Fundamental Processes and Applications, Volume 32 of Interface Science and Technology, ISSN 1573-4285, Ed: Mehrorang Ghaed, Elsevier Science, 2021.

IV Semester

Paper IV(A) Nanomaterials, Macromolecules, Computational Chemistry and Data analysis (Elective-A) (4CHT24A)

(Physical chemistry specialization)

(Marks 100, Total Hours 60)

Unit-I Nanoparticles and their applications:

Introduction to nanoparticles – preparation of nanoparticles-like Chemical methods, thermolysis and Pulsed laser methods. Optical and electrical properties of nanoparticles Characterization of nanoparticles-Experimental techniques: Scanning electron microscopy (SEM), Transmission electron microscopy (TEM), field ion microscopy (FM), and X-rays spectroscopy.

Carbon nanotubes: - electrical, mechanical and electromagnetic properties. Use of nanotubes in fuel cells and catalysis.

Unit-II Characterization of Macromolecules:

Polydispersion - Concept of average molecular weight, Number, Weight and Viscosityaverage molecular weights. Polydispersity and molecur weight distribution. The practical significance of molecular weight. Measurement of molecular weights. End group, viscocity, light scattering, osmotic and ultracentrifugation methods.

Kinetics and mechanism of free radical polymerization. Degree of polymerization, kinetic chain length and chain transfer coefficient. Kinetics and mechanism of linear stepwise polymerization, cationic, anionic polymerization. Copolymerization reactions and copolymer composition.

Unit-III Computational Chemistry:

Introduction to Molecular Modeling, Single molecule calculations, assemblies of molecules and reactions of molecules-Co-ordinate systems, Cartisian and internal co ordinate, Z-matrix, Potential energy surface- Conformational search-Global minimum. Local minima, Conformational analysis of ethane. Force field-Feature of Molecular Mechanics-Bonded and Non bonded interctions. Bond stretching-Angle Bending, Torsonal Terms-Improper Torsions and out of plane Bending, Motions-CrossTerms. NonBonded interaction- Electroststic Interctions-VanderWall's interctic Hydrogen Bonding, Miscellaneous interactions.

Unit-IV Data Analysis:

Types of errors, Accuracy and precision, methods of expressing them. Least square analysis-average and standard deviations, correlation coefficient Normal (Gaussian) distribution, significant figures, comparision of results Student t-test, F-test, Chi square test. Electric properties of molecules (Dipole moments), The Clausius – Mosotti equation - Debye equation, polarizability volume. Dipolements and molecular structure determination.

Phase rule and its derivation. Application of phase rule to three component systems.

Recommended books:

1. Nanomaterials and Nanochemistry, C.Brechigneae, M.lahmai (Eds) Spinger 2007.
2. Nanochemistry, G.B.sergeev, Elsevier
3. Nanochemistry: A chemical approach to nanomaterials, G.A.Ozin & A.C.Arsenault, RSC Publishing.
4. principles of polymerization- George Odian (John Wiley)
5. Polymer science, V.R. Gowarikar, N.V. Viswanatthan & J.Sreedhar , Wiley Eastern
6. Quantitative Inorganic Analysis, A.I.Vogel
7. Computational chemistry,GuyH.Grant & W.GrahamRichards,OxfordUniversity press.
8. Computational chemistry: Introduction to the theory and Applications to Molecular and Quantum Mechanics- Errol Lewars, (Springer).
9. Introduction to Computational chemistry - Jensen,Wiley publishers.
10. Quantum chemistry – Ira N. Levine, Prentice-Hall & India. New Delhi.
11. Systamatic experimental physical chemistry, S.W.Raj Bhoj,T.K.Chondhekar, Anjali Publication, Aurangabad.

IV Semester

Paper IV(B) Molecular Modelling and its Applications (Elective-B)

(4CHT24B)

(Physical chemistry specialization)

(Marks100, Total Hours 60)

Unit-I Molecular Modelling – I:

Introduction to Molecular Modeling, Single molecule calculations, assemblies of molecules and reactions of molecules - Co-ordinate systems: Cartesian and Internal Co-ordinates, Z-matrix - Potential energy surface - Conformational search; Global minimum, Local minimum, Conformational analysis of ethane.

Force field; Features of Molecular Mechanics, Bonded and Non-bonded interactions, Bond Stretching, Angle Bending, Torsional Terms (Improper Torsions, out of Plane Bending Motions, Cross Terms), Non - Bonded Interactions (Electrostatic Interactions, Van-der Waals interactions), Hydrogen Bonding Interactions.

Unit-II Molecular Modelling – II:

Force Field Equation in Energy minimization (Energy as function of r, θ, ω) - Introduction to Derivative Minimization Methods (First Order Minimization), Types of energy minimization Methods; Steepest Descent, Conjugate Gradient, Conformational Search procedures – Geometry optimization procedures - Molecular Dynamics: Introduction, description of Molecular Dynamics, basic elements of Monte-Carlo method, differences between Molecular Dynamics and Monte-Carlo method, Qualitative exposure to Molecular Dynamics Simulations.

Unit-III Drug Design Methods I - Ligand Based:

Lead Molecule - Structure Activity Relationship (SAR), Quantitative Structure Activity Relationship (QSAR), Distinguish between SAR and QSAR - Physicochemical parameters ; Electronic effects, Hydrophobicity, Steric Factors Taft's Steric function, Molar Refractivity, Verloop Steric factor - Molecular Descriptor analysis: Craig plot, Topliss scheme, Bioisosteres -Hansch model, Free-Wilson model for QSAR equations - Regression analysis: Multi Linear Regression and Partial Least Square(terms: n, SD, r, r_2, r_2%, F) -Examples for linear and nonlinear equations - 3D QSAR: CoMFA and CoMSIA - Differences between 2D and 3D QSAR.

Unit-IV Drug Design Methods II - Structure Based:

Database similarity searches - Pair-wise alignment: Global sequence analysis (Needleman-Wunsch), Local Sequence Alignment (Smith Waterman), Multiple Sequence Alignment - Homology Modeling: Query sequence, Template selection, Alignment, Backbone Modeling, Loop Modeling, Side chain Modeling, Model optimization, Energy minimization – Model Evaluation: Ramachandran Plot, Verify 3D, Errata and ProSA - Active site Identification - Docking, Docking Algorithms: Genetic Algorithm, Incremental construction – Molecular Interactions, Scoring functions - Virtual Screening: Ligand Based and Structure Based. De novo ligand design and its limitations.

Recommended books:

1. Molecular Modelling: Principles and Applications, by Andrew Leach, Longman Publications.
2. Computational Chemistry, Guy H. Grant & W. Graham Richards, Oxford University Press.
3. Computational Chemistry: Introduction to the theory and Applications of Molecular and Quantum Mechanics, Errol Lewars, Springer Publications.
4. Recent advances in Bioinformatics by I. A. Khan and A Khanum Ukaaz publications, 2003.
5. Molecular modelling – Basic Principles and Applications by Hans Dieter Holtje and Gerd Folkers, Wiley-VCH, 1996
6. Introduction to Computational Chemistry by Jensen, Wiley Publishers, second edition
7. Bioinformatics – A Primer by P. Narayanan, New Age International, (PC) Ltd, 2005.
8. Introduction to Bioinformatics by Arthur M. Lesk, Oxford University Press (Indian. Edition), 2002
9. Principles of Medicinal Chemistry Vol. II by Dr. SS Kadam Pragati books Pvt. Ltd; 2007
10. An Introduction to Medicinal Chemistry by G L Patrick, Oxford University Press
11. Bioinformatics: Methods and Applications: Genomics, Proteomics and Drug Discovery. S.C. Rastog, Namita Mendiratta, Parag Rastogi, PHI Larning Pvt. Ltd; 2006
12. Pharmacy Practice Vol.I and II by Remington, Pharmaceutical Press
13. Burger's Medicinal Chemistry and Drug Discovery, 5th Edition, Wiley-Interscience, New York
14. Text book of Drug design and Vol.1 discovery 3rd Edition by POVL krogsgaard- Larsen Tommy liljefors and ULF Madsen.

IV Semester

Physical chemistry Practicals

Paper-V Kinetics experiments (4CHP17)

(Marks 100, 9 Hours per week)

1. Kinetics of i) Acetone - Iodine reaction: Determination of

a) Order b) Acid effect

c) Solvent effect d) Temperature effect.

ii) Inversion of sucrose-Effect of acidity functions.

Scheme of Valuation

Marks 100	Time: 4 Hours
Experiments (2)	80 marks
Record/Samples &Viva	20 marks

Paper–VI Instrumentation (4CHP18)

(Marks 100, 9 Hours per week)

Instrumentation:

I. Conductometry:

1. Mixture of acids and CuSO4 vs NaOH
2. Mixture of chloroacetic acids vs NaOH
3. Replacement Reactions
4. Verification of Onsagers euations with KCl
5. Determination of composition of complex (Cu(II) Vs EDTA)
6. Kinetics of Saponification of ethylacetate.

II. Potentiometry /P^H Metry:

1. Determination of dissociation constants of monobasic / dibasic acids by Albert-Serjeant method.
2. Determination of dissociation constant of acetic acid in DMSO, acetone and dioxane.
3. Determination of thermodynamic constans, ΔG, ΔS and ΔH for the following reaction by e.m.f. method.

$$Zn + H2SO4 \rightarrow ZnSO4 + H_2$$

III. Polarography:

1. Estimation of Pb^{2+}, Cd^{2+}, and Ni^{2+} separately and in a complex.

Scheme of Valuation

Marks 100	Time: 4 Hours
Experiments (2)	80 marks
Record/Samples &Viva	20 marks

Recommended books:

1. Practical physical chemistry - A. Findly, Longman – London
2. Practical physical chemistry - B. Vishwanthan and P.S. Raghavan.
3. Practical physical chemistry - B.D. Khosla and V. C. Gard, R. Chand or Co. Delhi.
4. Systematic experimental physical chemistry - S.W. RajBhoj and Dr. T. K. Chondhekar
5. Instrumental methods of analysis - Skoog and West.
6. Instrumental methods of analysis - Willard, Merritt, Dean Seatle.