# M.Sc. CHEMISTRY CBCS PATTERN IN SEMESTER SYSTEM

## DEPARTMENT OF CHEMISTRY

## KAKATIYA UNIVERSITY WARANGAL – 506 009

Department of Chemistry, Kakatiya University introduces Choice Based Credit System (CBCS) for M.Sc. (2 Year course) chemistry for the students admitted in M.Sc. Chemistry course from 2016-17 academic year onwards.

Scheme for CBCS, the workload for each paper, distribution of marks, the number of credits and scheme of examination are attached herewith.

Internal Assessment examination will be conducted twice in every Semester. The main examination (theory and practical) will be conducted at the end of each semester.

One open elective in III semester and one is in IV semester are offered by Department of Chemistry for all the PG-students.

Students joined in M.Sc. Chemistry should choose one open elective offered by Department of chemistry or any other Department of Kakatiya University.

The syllabi of theory and practical papers of I, II III, and IV semesters are enclosed. The syllabi of open elective offered in IV semester will be kept available for the next academic year.

– Prof. Gade Dayakar
Chairperson
Board of Studies in Chemistry

**DEPARTMENT OF CHEMISTRY - KAKATIYA UNIVERSITY**

**[with effect from the academic year 2016-17 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 | Applied Chemistry | 4 | 4 | 80 | 20 | 100 |
| 5 | 1CHP1 | Paper-V | Inorganic Practicals | 6 | 3 | 75 | ---- | 75 |
| 6 | 1CHP2 | 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 |

## Semester –II

| 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 | 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 Practicals | 6 | 3 | 75 | ---- | 75 |
| 6 | 2CHP5 | Paper-VI | Organic Practicals | 6 | 3 | 75 | ---- | 75 |
| 7 | 2CHP6 | Paoer-VII | Physical Practicals | 6 | 3 | 75 | ---- | 75 |
| 8 | ---- | ---- | Seminar | ---- | 1 | ---- | ---- | 25 |
| | Total | ---- | ---- | 34 | 26 | ---- | ---- | 650 |

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Prof. Gade Dayakar, Chairperson, BOS in Chemistry, KU,

## 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 | Spectroscopy | 4 | 4 | 80 | 20 | 100 |
| 2 | 3CHT10 | Paper-II | Synthetic Organic Chemistry-I | 4 | 4 | 80 | 20 | 100 |
| 3 | 3CHT11 | Paper-III | Bioinorganic and Supramolecular Chemistry | 4 | 4 | 80 | 20 | 100 |
| 4 | 3CHT12 | Paper- IV | Inorganic Photochemistry and Chemistry of Materials | 4 | 4 | 80 | 20 | 100 |
| 5 | 3CHP7 | Paper-V | Preparation of Complexes and their characterization by Physiochemical techniques | 9 | 4 | 100 | ---- | 100 |
| 6 | 3CHP8 | Paper-VI | Analysis of Ternary mixtures and Complex materials | 9 | 4 | 100 | ---- | 100 |
| 7 | 3CHOE | Paper-VII | Environmental chemistry (Open elective) | 4 | 4 | 80 | 20 | 100 |
| | | Seminar | | ---- | 1 | 25 | ---- | 25 |
| | Total | | | 38 | 29 | | | 725 |

## 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 | Spectroscopy | 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 |
| 7 | 3CHOE | Paper-VII | Environmental chemistry (Open elective) | 4 | 4 | 80 | 20 | 100 |
| | | Seminar | | ---- | 1 | 25 | ---- | 25 |
| | Total | | | 38 | 29 | | | 725 |

Dean

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## 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 | Spectroscopy | 4 | 4 | 80 | 20 | 100 |
| 2 | 3CHT10 | Paper-II | Synthetic Organic Chemistry-I | 4 | 4 | 80 | 20 | 100 |
| 3 | 3CHT15 | Paper-III | Quantum Chemistry, Kinetics & Electrochemistry | 4 | 4 | 80 | 20 | 100 |
| 4 | 3CHT16 | Paper- IV | Group Theory & Spectroscopy | 4 | 4 | 80 | 20 | 100 |
| 5 | 3CHP11 | Paper-V | Kinetics | 9 | 4 | 100 | ---- | 100 |
| 6 | 3CHP12 | Paper-VI | Instrumentation | 9 | 4 | 100 | ---- | 100 |
| 7 | 3CHOE | Paper-VII | Environmental chemistry (Open elective) | 4 | 4 | 80 | 20 | 100 |
| | | Seminar | | ---- | 1 | 25 | ---- | 25 |
| | Total | | | 38 | 29 | | | 725 |

## 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 | Analytical and 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 | Paper- IV | Organometallic Chemistry | 4 | 4 | 80 | 20 | 100 |
| 5 | 4CHP13 | Paper-V | Ion exchange and Solvent Extraction Methods | 9 | 4 | 100 | ---- | 100 |
| 6 | 4CHP14 | Paper-VI | Instrumental Methods | 9 | 4 | 100 | ---- | 100 |
| 7 | 4CHOE | Paper-VII | Open elective | 4 | 4 | 80 | 20 | 100 |
| | | Seminar | | ---- | 1 | 25 | ---- | 25 |
| | Total | | | 38 | 29 | | | 725 |

## 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 | Analytical and 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 / 4CHT22B | Paper- IVA / Paper- IVB | Natural products (Elective-I) / Medicinal chemistry (Elective-II) | 4 | 4 | 80 | 20 | 100 |
| 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 | | | | | |
| 7 | 4CHOE | Paper-VII | Open elective | 4 | 4 | 80 | 20 | 100 |
| | | Seminar | | ---- | 1 | 25 | ---- | 25 |
| | Total | | | 38 | 29 | | | 725 |

## 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 | Analytical and 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 / 4CHT24B | Paper- IVA / Paper- IVB | Nanomaterials, Macromolecules and Data analysis (Elective-I) / Supramolecular, Material Sciences, Lasers and Computational Chemistry (Elective-II) | 4 | 4 | 80 | 20 | 100 |
| | 4CHP17 | Paper-V | Practicals -Kinetics | 9 | 4 | 100 | ---- | 100 |
| 7 | 4CHP16 | Paper-VI | Practicals-Instrumentation | 9 | 4 | 100 | | 100 |
| 8 | 4CHOE | Paper-VII | Open elective | 4 | 4 | 80 | 20 | 100 |
| | | Seminar | | ---- | 1 | 25 | ---- | 25 |
| | Total | | | 38 | 29 | | | 725 |

## 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 regular octahedral, distorted octahedral, square planar, tetrahedral, square pyramidal and trigonal bipyramidal geometries, Crystal field splitting energy, Pairing energy, High spin and low spin octahedral complexes, Calculation of crystal field stabilization energy (CFSE) in octahedral and tetrahedral complexes, Factors effecting the magnitude of crystal field splitting, Jahn-Teller distortion, general applications and limitations of crystal field theory, Special application of crystal field theory to spinels in site selection.

Molecular orbital theory (MOT): Introduction, 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, Inert and labile complexes, Lability and inertness of complexes in terms of Valence bond theory and Crystal field theory.

Types of substitution reaction mechanism - $SN^1$, $SN^2$, Id (Interchange dissociative) and Ia (Interchange associative).

Nucleophilic substitution reaction in octahedral complexes- Acid hydrolysis , factors affecting acid hydrolysis, Base hydrolysis, Conjugate base mechanism, Evidences in favour of conjugate base mechanism; Anation reactions.

Nucleophilic substitution reactions in square planar complexes- Mechanism of substitution, Trans effect, Theories of trans effect -Polarization theory and π–bonding theory, Applications of Trans effect in the synthesis of Pt(II) complexes.

Electron transfer reactions- Inner sphere and outer sphere mechanisms, Cross-reactions and Marcus-Hush theory.

**Unit III Metal-ligand equilibria in solution:**

Solvation of metal ions, Metal complex formation in solution, Types of stability-concentration stability, conditional stability, thermodynamic stability and kinetic stability.

Step-wise stability constants and overall stability constant, Trends in stepwise stability constants. Factors influencing the stability of metal complexes with reference to metal

and the ligand, Chelate effect, and its thermodynamic origin, Macrocyclic effect of crown ethers and cryptates.

Hard and Soft acids and bases (HSAB) rule and its application to stability of complexes and metal-ligand interactions in the biological systems. Methods used for the determination of stability constants of metal complexes (Basic principles only) - Spectro-photometric, $p^H$-metric and polarographic methods.

**Unit IV Magnetochemistry:**

Types of magnetism-paramagnetism, diamagnetism, ferromagnetism and antiferromagnetism, Temperature independent paramagnetism, Behaviour of para, dia, ferro and antiferromagnetic substances with temperature, Magnetic susceptibility measurement by Gouy method. Magnetic properties of metal ions- Origin of paramagnetic moment, spin moment and orbital moment, Quenching of orbital angular momentum by ligand fields; Orbital contribution to magnetic moment, Magnetic properties of metal complexes with A, E and T ground terms, Spin-orbit coupling contribution to magnetic moment, Spin cross-over in complexes.

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

**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. Inorganic Chemistry, D. F. Shriver and P. W. Atkins, 3rd ed., Oxford.
4. Concise Inorganic Chemistry, J. D. Lee, Blackwell Science.
5. Coordination Chemistry, D. Banerjea.
6. Inorganic reaction mechanisms, F. Basolo and R. G. Pearson.
7. Mechanism of reactions in transition metal sites, R. A. Henderson, Oxford Science Publications.
8. Coordination Chemistry, F. Basolo and R. Johnson, Benzamin Inc.
9. Concepts and models of Inorganic Chemistry, B. E. Douglas, D. H. McDaniel and J. J. Alexandar, 3rd ed., John-Wiley.
10. Chemistry of complex equilibria, M. T. Beck, Von Nostrand Reinhold.
11. Metal complexes in aqueous solutions, A. E. Martell and R. D. Hancock, Plenum Press.
12. Inorganic Chemistry, K. F. Purcell and J. C. Kotz, Holt-Saunders International editions.

**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)

**I SEMESTER**

**PAPER-II: ORGANIC CHEMISTRY (1CHT2)**

(Marks-100, Total hrs: 60)

**Unit I Stereochemistry-I:**

Molecular symmetry in organic molecules: Criteria for optical activity - Symmetry elements (Cn, Ci & Sn), symmetry operations; asymmetric and dissymmetric molecules. Racemization, Racemic modifications and methods of resolution. The concept of atropisomerism.

Configuration: R,S and E,Z nomenclature, Concept and determination methods for absolute and relative configurations. Introduction and terminology of stereoselective and stereospecific synthesis: Prostereoisomerism-prochirality, descriptions for prochiral centers, Topos and face differentiation (pro-R and pro-S; Re and Si faces). – Partial and absolute asymmetric syntheses.

**Unit II Reaction Mechanisms-I:**

Study of reaction intermediates: Formation and stability of carbonium ions, carbanions, carbenes, nitrenes, free radicals, and arynes. Kinetic control and thermodynamic control in chemical reactions of organic molecules. Methods of determination of reaction mechanisms: i) Product analysis ii) Intermediate analysis (isolation, trapping) iii) Crossover experiments iv) Isotopic effect and labeling.

Aromatic nucleophilic substitutions: $SN^1Ar$, $SN^2Ar$, and Benzyne mechanisms.

Free radical substitution at paraffinic, aromatic, allylic, and benzylic carbons -auto-oxidation.

Elimination reactions: Mechanistic pathways of eliminations - $E^2$, $E^1$, $E^1CB$, - orientation in eliminations (syn & anti).

Neighboring group participation in nucleophilic substitutions. Factors effecting the reactivity and mechanism of nucleophilic substitutions. Elimination vs Substitution reactions in alkyl halides.

**Unit III Natural products-I:**

Terpenes and Terpenoids: Definition, classification based on isoprene unit, isoprene rule, and special isoprene rule. Isolation, structure elucidation and synthesis of citral, α-terpineol, camphor and α-pinene. Biogenesis of terpenoids.

Alkaloids: Definition, classification – general chemical methods used in the structure elucidation of alkaloids – Isolation, structure determination, and synthesis of atropine, quinine and papaverine and nicotine.

Biogenesis of alkaloids.

**Unit IV Heterocyclic compounds-I:**

Classification and nomenclature of the heterocycles based on the nature of the heteroatom 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, chromone, coumarin, benzofuran, benzothiophene, indole, quinoline and isoquinoline.

**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. A guide book to reaction mechanisms in organic chemistry – Peter Sykes
6. Mechanism and structure in organic chemistry – S.M.Mukherji & S.P.Singh
7. Organic Chemistry – L. G. Wade Jr
8. Advanced Organic Chemistry, Part A: Structure and Mechanisms – Francis A. Carey and Richard J. Sundberg
9. Advanced Organic Chemistry: Part B: Reaction and Synthesis – Francis A. Carey and Richard J. Sundberg
10. Organic Chemistry – Greeves, Warren, and Wothers Clayden
11. Organic Chemistry – Paula Y. Bruice
12. Modern methods of organic synthesis – William Carruthers and Iain Coldham
13. Principles of organic synthesis – Richard O.C. Norman and James M. Coxon
14. Organic Chemistry – Volume-I & II – I.L. Finar
15. Heterocycles – R.K. Bansal
16. An introduction to chemistry of heterocyclic compounds – R.M. Acheson
17. Heterocyclic chemistry – John A. Joule and Keith Mills
18. Heterocyclic Chemistry – Thomas. L. Gilchrist
19. The higher terpenoids – Paul De Mayo
20. Mono- and sesquiterpenoids – Paul De Mayo
21. An introduction to chemistry of terpenoids and steroids – William Templeton
22. The alkaloids – Kenneth Walter Bentley
23. Alkaloids –S. William Pelletier

## 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

**I SEMESTER**

**PAPER-III: PHYSICAL CHEMISTRY (1CHT3)**

(Marks-100, Total hrs: 60)

**Unit I Thermodynamics – I:**

Third law of thermodynamics, calculation of absolute entropies of solids, liquids, and gases – tests and exceptions. Standard entropies and entropy changes in chemical reactions, entropy of mixing, standard entropies of ions. Thermodynamic relations.

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 – Clapeyron and Clausius-Clapeyron equation, Maxwell's relationships and thermodynamic equation of state.

**Non-ideal systems:** Fugacity of a gas, determination (general and graphical methods). Activity and activity coefficients of electrolyte solutions – determination using Debye-Huckel equation and emf method. Vant Hoff's reaction isotherm.

**Non-ideal mixtures:** Concept of partial molar properties – partial molar free energy– chemical potential. Gibbs–Duhem equation – variation of chemical potential with temperature and pressure. Determination of partial molar properties (Direct method, method of intercepts and general method). Properties of non-ideal solutions – vapour pressure curve and their compositions.

**Unit II Electro Chemistry - I:**

**Conductance:** 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 $P^H$, $P^{Ka}$ 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 Kinetics – I:**

**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. Thermodynamic formulation of reaction rates–calculation of activation parameters.

Lindemann's theory of unimolecular reactions and Hinshelwood modification–Effect of Solvent and Ionic strength on rates of ion-ion and ion-dipole reactions–Isotopic effect on reaction rates–substrate and solvent isotopic effect.

**Termolecular reactions**: Reactions of nitric oxide with hydrogen, oxygen, and halogens.

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

**Unit IV Quantum Chemistry–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 $\Psi$ and $\Psi^2$ – Normalization and orthogonality of wave function – well behaved functions – Operators like linear momentum (p), angular momentum (L), Energy (E), Hamiltonian (H), operator $\nabla$ and $\nabla^2$. 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-dimensional box, derivation of energy expressions – plots of $\Psi$ and $\Psi^2$ – 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 $\Psi$ and $\Psi^2$

**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.

**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

a. (i) Strong acid and weak acid with Strong base.
(ii) Mixture of strong and weak acids with Strong base.
(iii) Strong acid and weak acid with Weak base.
(iv) Salt with Strong base.

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

| | | |
|---|---|---|
| Experiments (2) | 30 + 30 | 60 |
| 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

**I SEMESTER**

**PAPER-IV: APPLIED CHEMISTRY (1CHT4)**

(Marks-100, Total hrs: 60)

**Unit I Reagents in organic synthesis:**

Preparation and applications of the following reagents in organic synthesis and functional group transformations: 1,3-Dithianes(Reactivity and umpolung effect), Lithium diisopropyl amide (LDA), Dicyclohexylcarbodiimide(DCC), Trimethylsilyl iodide, Tri-n-butyl tin hydride, Dichloro dicyano benzoquinone (DDQ), Chloranil, Selenium dioxide, Lindlar's catalyst and Wilkinson's catalyst Baker's Yeast. Woodward-Prevost hydroxylation, Phase transfer catalysts-Tetra alkyl ammonium halides, and Crown ethers.

**Unit II 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. Structure elucidation and synthesis of Sucrose. Structural features of Maltose, Lactose, Cellobiose, Starch, and Cellulose.

**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 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. Reaction mechanisms – Jerry March
2. Modern methods of organic synthesis – William Carruthers and Iain Coldham
3. Organic Chemistry – Greeves, Warren, and Wothers Clayden
4. Advanced Organic Chemistry: Part B: Reaction and Synthesis – Francis A. Carey and Richard J. Sundberg
5. Organic Chemistry – Volume-I & II – I.L. Finar
6. Carbohydrate chemistry – Davidson
7. Reagents for organic synthesis – Louis Fieser and Mary Fieser
8. Reactions Rearrangements And Reagents – S.N. Sanyal
9. Essential reagents for organic synthesis – Philip L. Fuchs, Andre B. Charette, Tomislav Rovis and Jeffrey W. Bode
10. Modern textbook of organic chemistry – Furguson
11. Principles of Instrumental analysis – Skoog, Nieman, Harcourt.
12. Principles of polarography- Kapoor
13. Principles of polarography- Heyrovsky
14. Modern electroanalytical methods – C. Charlot
15. Principles of physical chemistry – Gurudeepraj
16. Vogel's text Book of quantitative chemical analysis- A.I Vogel ($5^{th}$ edition)
17. Analytical Chemistry, Gary D. Christian ($6^{th}$ edition)
18. Instrumental methods of Analysis, Willard, Dean & Settle.
19. Principles and practice of Analytical Chemistry, F. W. Fifield & D. Kealy,
20. Automatic methods of analysis, M. Valcarcel, M. D. Luque de Castro,
21. Principles of Instrumental Analysis, Skoog, Holler and Wieman,

## 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:**

Classification and nomenclature of organometallic compounds, Principles of synthesis of organometallic compounds. Synthesis, structure and properties of organometallic compounds of **Al** and **Sn.** 18-electron rule and stability of organotransition metal compounds. Synthesis, structure and bonding of olefin, allyl and cyclopentadienyl organometallic compounds of **Fe, Pd** and **Pt**. 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, Physiological significance of hemoglobin, Role of globin chain in haemoglobin.

**Metals/ Metal compounds in medicine –** Introduction, Metal deficiency and disease, Iron deficiency, Zinc deficiency, and Copper deficiency; Metals used for diagnosis and radiodiagnosis; Lithium, Gold and Platinum compounds used in therapy.

**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, Electron counting methods i) Neutral atom method and ii) Oxidation state method, Structural and bonding aspects of $Ni(CO)_4$, $Mn_2(CO)_{10}$ and $Fe_2(CO)_9$.

**Metal carbonyl clusters**- Factors favouring metal-metal bond, Classification of metal carbonyl clusters, Structures of $Fe_2(CO)_9$, $Co_2(CO)_8$, $Fe_3(CO)_{12}$, $Ru_3(CO)_{12}$, $Co_4(CO)_{12}$, and $Rh_6(CO)_{16}$.

**Metal nitrosyls:** General methods of preparing metal nitrosyls, 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 $[RuCl(PPh_3)_2(NO)_2]^+$.

**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.

**Recommended books:**


1. Inorganic chemistry, J. E. Huheey, E. A. Keiter and R. L. Keiter, 4th ed., Harper Collins College Publishers.
2. Introduction to ligand fields, B. N. Figgis, Wiley.
3. Concise Inorganic Chemistry, J. D. Lee, Blackwell Science.
4. Organometallic Chemistry, R. C. Mehrotra and A. Singh, New age international.
5. Metalorganic Chemistry, A. J. Pearson, Wiley.
6. Bioinorganic Chemistry, L. Bertini, H.B. Gray, S. J. Lippard and S. J. Valentine, Viva Low-Priced Student edition.
7. Principles of Bioinorganic Chemistry, S. J. Lippard and Berg.
8. Bioinorganic Chemistry, K. Hussain Reddy, New Age international Publishers.
9. Structure and bonding Vol. 55 H. J. Clark.
10. Modern inorganic Chemistry, W. L. Jolly, McGraw-Hill.
11. 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, Record and samples | – | 15 |

**Recommended Books:**

1. A Text Book of quantitative inorganic analysis (3rd and 6th editions)

## II SEMESTER
## PAPER-II: ORGANIC CHEMISTRY (2CHT6)

(Marks-100, Total hrs: 60)

**Unit I Named reactions in organic synthesis:**

Beckmann rearrangement, Mannich reaction, Michael addition, Dienone-Phenol rearrangement, Robison annulation, Favorski reaction, Baylis-Hillman reaction, Shapiro reaction, Ugi reaction, Grubbs reaction, Heck reaction, Suzuki coupling, Stille coupling, Sonogashira coupling, and Buchwald reaction.

**Unit II Stereochemistry II:**

Conformational analyses of Cycloalkanes: Conformations of small and medium sized rings and conformations of mono and disubstituted cyclohexanes. Factors governing the reactivity of equatorial and axial substituents attached to the cyclohexane ring – Relative stability and reactivity of conformational diastereomers –Stereochemistry of bicyclic systems involving five and six numbered rings. Conformations of cyclohexanone – Stereochemistry of addition to the carbonyl group in rigid cyclohexanone system.

Use of physical methods (dipole moment, IR and NMR) in determining the preferred conformers of simple organic molecules such as 1,2-dihalo ethanes, halohydrins and vicinal diols.

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

**Unit III P**

**rotection of functional groups and Nucleic acids:**

P**rotection of functional groups:** Principles of (1) protection of alcohols – Ether formation: methyl, benzyl, allyl, methoxy ethoxy methyl (MEM), 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 – Amide and Carbamate formation with formyl, acetylation, benzoyl, benzyloxy carbonyl (CBZ), *tert*-butyloxycarbonyl (BOC), tert-butyl azido formyl, phthaloyl, di-tert-butyl pyrocarbonyl, Fluorenylmethyloxycarbonyl (FMOC), and triphenyl methyl groups (5) protection of carbonyl groups – acetal, ketal, 1,3-dioxolane, 1,3-dioxane, 1,3-dithiolane, 1,3-oxathiolane and 1,3-dithiane formation.

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

**Unit IV Nonbenzenoid aromatic compounds:**

Concept of aromaticity, Robinson's sextet theory, Huckel's rule, basis for the Huckel's rule, limitations of the Huckel's rule- Alternant and Non-alternant hydrocarbons Craig's rule – Various Nonbenzenoid aromatic molecules – Synthesis and properties of aromatic 3,4,5,6,7,8-membered rings, metallocenes, annulenes, heteroannulenes, azulenes, fullerenes($C_{60}$), Sydnones – Antiaromatic compounds,

Recommended Books:


1. Reaction mechanisms – Jerry March
2. Organic Chemistry – Volume-I & II – I.L. Finar
3. Carbohydrate chemistry – Davidson
4. Textbook of organic chemistry – Morrison and Boyd
5. Organic reagents – Fieser and Fieser
6. Modern textbook of organic chemistry – Furguson

**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), Maxwell–Boltzmann distribution law–partition function and types. 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.

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

**Unit II Solid State:**

**Bonding in metals:** Valence bond theory of metallic bond, Free electron Theory-Molecular orbital approach to the Band theory of solids–classification of solids–Insulators, conductors, and semiconductors–types of semiconductors, temperature effect on conductivity, photoconductivity and photovoltaic effect–p and n junctions.

**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. **Solid state reactions:** Classification and theory of solid state reactions Δ-Wagner's theory – examples.

**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 (θ) parts of wave functions–total wave function of rigid rotator.

**Hydrogen atom:** Separation of (r), (φ) and (θ) 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 Donal D; Mcquarrie & John D Simon.
2. Atomic Structure and the Chemical Bond including Molecular Spectroscopy –Manas Chanda ($4^{th}$ edn)
3. Physical Chemistry - Peter Atkins and de Pulpa Oxford University Press.
4. Principles of Physical Chemistry - Samuel H.Maron and Carl F. Prutton.
5. Advanced Physical Chemistry -Gurdeep Raj Goel Publishers House, Meerut.
6. Quantum Chemistry - R.K.Prasad
7. Thermodynamics - Samuel Glasstone
8. Chemical Kinetics by K.J. Laidler
9. Chemical Kinetic Methods–Principles of Relaxation techniques & Applications - C. Kalidas.
10. Principles of Chemistry by Paul Ander Anthony J. Sonnessa.
11. Solid State Chemistry -D.K. Chakravarty
12. Solid state chemistry and Applications - A.R.West, Plenum Press.
13. Solid State physics - S.O. Pillai, New Age Publishers.

**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 molar extinction coefficient of $KMnO_4$, $CuSO_4$, $K_2Cr_2O_7$, 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)
5. Determination of partial molar volume of methanol in aqueous methanol.

## Scheme of valuation

Marks: 75 Time: 4Hrs

| | | | | |
|---|---|---|---|---|
| Experiments (2) | – | 30+30 | – | 60 |
| Viva, Record and samples | | | – | 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, Anjali Publications, Aurangabad.

**II SEMESTER**

**Paper-IV: Spectroscopy (2CHT8)**

(Marks-100, Total hrs 60)

**Unit I Symmetry & Group Theory:**

Introduction- concepts of symmetry in molecules, symmetry elements, symmetry operations, mathematic rules of a group – abelian and non-abelian groups. Point groups-classifications of point groups- Exercises on molecular point groups -$H_2O$, o-$C_6H_4X_2$, $C_5H_5N$, $CH_3Cl$, $H_2O_2$, $CH_4$, $B(OH)_3$, $C_2H_2Cl_2$,$[PtCl_4]^{2-}$, $C_3H_4$(Allene), $[FeCl_6]^{3-}$, Metallocenes (Eclipsed and Staggered). Descent in symmetry of molecules with substitution ($H_2O$, HOD, $CH_4$, $CH_3X$). Symmetry criteria of optical activity, Symmetry restrictions of dipole moment, group multiplication table – subgroups.

**Unit II Microwave & Electronic Spectroscopy:**

**Microwave spectroscopy:** Types of molecular energies and molecular spectroscopy. Classification of molecules based on moment of inertia. Rigid rotator model, energy levels and selection rules of rotational spectra – Calculation of bond lengths of heteronuclear diatomic molecules, Intensity of spectral lines – Boltzmann distribution law-degeneracy of energy states, Effect of isotopic substitution-abundance of isotopes. Nonrigid–rotator, energy levels and its spectrum, Stark effect, Centrifugal distortion constant, Rotational spectra of linear triatomic (like OCS and HCN) molecules.

**UV & Visible (Electronic) Spectroscopy:** Origin of electronic spectra, Lambert-Beer's absorption law, Types of electronic transitions. Effect of solvent, substituent, conjugation on electronic transitions. Benzene and its substituted derivatives. Applications of UV-visible spectroscopy in analysis (qualitative/quantitative) of polyenes/aromatic (hetero & homo) systems, geometrical isomers, keto-enol tautomers, components of a mixture, ionization constants of acids and bases. Woodward-Fieser rules for calculating absorption maximum in dienes, trienes and α,β-unsaturated carbonyl compounds. Charge transfer spectra of complexes. Photometric titrations. Determination of composition of complexes by Job's slope ratio method. UV spectra of Mesityl Oxide, Phenol and Benzoic acid.

**Unit III Infrared and Raman Spectroscopy:**

**Infrared spectroscopy:** Vibrational energy of a diatomic molecule-an harmonic oscillator –Selection rules- Overtones-hot bands. Zero-point energy-Calculation of force constant of diatomic molecules. Rotational –Vibrational spectra of diatomic molecules-P,Q,R branches. Instrumentation–sources-sampling techniques. Normal modes of

vibrations for linear and non-linear molecules (stretching, bending, scissoring, rocking, twisting, wagging). Functional group frequencies-Factors influencing vibrational frequencies-Coupled vibrations and Fermi resonance-combinational bands. Applications of infrared spectroscopy-structure elucidation of simple organic molecules-benzene and its substituted derivatives-cis-trans isomers and keto-enol tautomers. Hydrogen bonding, isotopic effect – study of metal-ligand bonding in complexes. IR spectra of Ethyl alcohol, Acetophenone, Mesityl oxide, Benzaldehyde, Aniline, and Acetaldehyde.

**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 $CH_4$.

**Unit IV NMR Spectroscopy and ESR Spectroscopy:**

**Nuclear magnetic resonance spectroscopy (NMR):** Theory of NMR-Nuclear energy levels-Instrumentation-Relaxation phenomenon, spin-spin and spin-lattice relaxations. Shielding and deshielding mechanism-chemical shift. Factors affecting the chemical shift. Isotropic and anisotropic effects-alkanes, olefins, acetylenes and aromatic systems. Low and High resolution of NMR spectrum of ethyl alcohol. Spin-spin coupling of strongly and weakly coupled systems-coupling mechanism, types of coupling constants. Factor affecting coupling constants-hybridization-dihedral angle and steric effects. NMR spectra of vinyl chloride, acetophenone, monosubstituted benzenes (benzaldehyde, ethylbenzene, p-chlolroaniline and benzoic acid). Applications of NMR spectroscopy-hydrogen bonding, keto-enol tautomers, cis-trans isomers, conformational analysis and deuterium exchange reactions.

**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 and its significance. ESR spectra of organic radicals like methyl, ethyl, isopropyl, benzene (anion and cation radicals), 1,4-benzosemiquinone and naphthalene anion.

**Recommended Books:**


1. Chemical Applications of Group Theory – F. A. Cotton.
2. Atomic structure and chemical bonding – Manas Chanda (Tata McGraw Hill).
3. Fundamentals of Molecular spectroscopy-Banwell & McCash (Tata McGraw Hill).
4. Molecular spectroscopy-Patel and Patel (Sardar Patel University Press).
5. Spectroscopy organic compounds-P. S. Kalsi (New Age International).
6. Organic Spectroscopy-Jag Mohan (Narosa)

7. Elementary Organic Spectroscopy-Y.R. Sharma (S.Chand & Company).
8. Organic spectroscopy-W. Kemp (ELBS).
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. Spectroscopy - Donald L. Pavia, Gary M. Lampman, George S. Kriz.
12. Instrumental methods of chemical analysis-G. R. Chatwal & S. K. Anand (Himalaya).
13. Group Theory and Molecular spectroscopy-K. Veera Reddy.
14. Spectrometric Identification of organic compounds, 6th Ed. Rober M. Silverstein & Francis Webster.
15. Applications of spectroscopy-J. Dyer.

**III Semester**

**Paper-I SPECTROSCOPY (3CHT9)**

(Common paper for all specializations)

(Marks 100, Total Hours 60)

**Unit-I NMR spectroscopy:**

Applications of spin-spin coupling in determination of structure and stereochemistry of organic molecules, NOE and its applications, and Lanthanide shift reagents. Recording of $^{13}C$ NMR spectra (PFT technique), Types of $^{13}C$ NMR spectra: Undecoupled, proton decoupled, selective proton decoupled spectra 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 and alkynes. Applications of $^{13}C$ NMR spectra in structure determination of organic molecules. Editing techniques: INEPT and DEPT methods.

**2D NMR techniques**: 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), Homonuclear and Heteronuclear 2D-J-resolved spectroscopy, NOESY and 2D– INADEQUATE experiments.

**Unit-II Mass Spectroscopy:**

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. Salient features of fragmentation pattern of organic compounds– α-cleavage, β-cleavage, McLafferty rearrangement, Retro-Diels-Alder fragmentation and ortho effect. Fragmentation pattern of individual heterocyclic systems viz., Furan, Pyrrole, Thiophene and Pyridine. Preliminary account of chemical ionization.

**Unit-III Photoelectron, AUGER Electron & Mössbauer spectroscopy**

A) Photoelectron spectroscopy – Principles, Koopman's theorem, Block diagram of photoelectron spectrometer. Ultraviolet photoelectron spectroscopy (UPS), Applications of UPS to $O_2$ and $N_2$ molecules. X-ray photoelectron spectroscopy (XPES/ESCA), Chemical shift, Applications of XPES in qualitative analysis, Structural analysis and surface studies.

B) AUGER electron spectroscopy – Principles, Instrumentation and Applications

C) Mössbauer Spectroscopy–Principles, Block diagram for experimental set-up. Recording Mössbauer spectrum, Isomer shift, Quadrupole interactions and Magnetic interactions, Applications of Mössbauer spectroscopy in the study of iron and tin compounds.

**<u>Unit-IV</u> Combined application of UV, IR, $^{1}$H-NMR, $^{13}$C -NMR and Mass spectra:**

Introduction to the analytical approach towards the structure elucidation of simple organic molecules by combined application of UV, IR, $^{1}$H-NMR $^{13}$C-NMR and Mass spectra.

**Recommended Books:**


1. Instrumental methods of Analysis– Willard, Dean & Settle.
2. Principles of Instrumental Analysis – Skoog, Holler and Wieman
3. Introduction to photoelectron spectroscopy – P. K. Ghosh
4. Applications of Mössbauer Spectroscopy – Green Wood
5. Structural inorganic chemistry-Mössbauer spectroscopy – Bhide
6. Spectroscopic identification of organic compounds– Silverstein, Basseler and Morril
7. Application of absorption spectroscopy – John R. Dyer
8. NMR in chemistry -A multinuclear introduction – Willam Kemp
9. Organic Spectroscopy – William Kemp
10. Spectroscopic methods in Organic chemistry – DH Williams and I Fleming
11. Modern NMR techniques for chemistry research – Andrew B Derome
12. Introduction to organic spectroscopy – Pavia
13. Carbon-13 NMR for organic chemists – GC Levy and O L Nelson
14. Nuclear Magnetic Resonance Basic principles – Atta-Ur-Rahman
15. Applications of Mössbauer spectroscopy –N.N. Greenwood and T.C. Gibb, Chapman & Hall
16. Principles of Mössbauer spectroscopy–T.C.Gibb, Chapman & Hall.
17. Physical methods for chemists– R.S. Drago, 2nd ed. (Saunders College Publishers)
18. Spectroscopy of organic compounds- P. S. Kalsi

**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, Dimerisation, Simple additions and, Inter and Intra molecular cyclo additions. Electrocyclisation 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), Cyclo addition 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-Inorganic Chemistry (Specialization)**

**Paper–III Bioinorganic and Supramolecular Chemistry (3CHT11)**

(Marks 100, Total Hours 60)

**Unit-I Metalloproteins and Metalloenzymes:**

General principles in metal binding sites – preservation of electroneutrality, self-assembly of metal clusters. Metalloproteins–Electron transfer proteins: Ferridoxins, Rubredoxins, Blue copper proteins, Cytochrome C. Metalloenzymes – Carboxypeptidase A, Carbonic anhydrase, Vitamin $B_{12}$, 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 albubin; transport of Na and K ions across cell membranes by $Na^+$ - $K^+$ ATPase; Transport of Ca across sareoplasmic 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; Funde\amental reactions with nucleic acids – Redox chemistry and Hydrolytic chemistry; Nuclease activity jof 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 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.

**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.
6) Supramolecular Chemistry- J.M. Lehn.

**III Semester -Inorganic Chemistry (Specialization)**

**Paper – IV Inorganic Photochemistry and Chemistry of Materials (3CHT 12)**

(Marks 100, Total Hours 60)

**Unit-I 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.

**Unit-II Chemistry of Materials:**

Ceramics – Introduction, structures, classification and Applications of ceramics Dielectrices – Types and mechanism of polarization, Ferroelectrics, Hysteresis loop of ferroelectrics, Pyroelectrics, Piezoelectrics, Relation between ferroelectricity, pyroelectricity and piezoelectricity, Applications of ferro-, Pyro- and piezoelectrics.

**Unit-III Nanomaterials – I:**

Introduction to nanoparticles, Classification of nanoparticles, Preparation of nanoparticles – Bottom-up approach, To-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-IV 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.

**Recommended Books:**


1. Concepts of inorganic photochemistry- Adamson and Fleichner
2. Elements of inorganic photochemistry- Ferrandi.
3. Materials science and engineering – An introduction - W.D. Callister, Jr. 7th ed. John Wiley & Sons, Inc.
4. Nanochemistry- G.B. Sargeev, Elsevier.
5. Nanochemistry: A chemical approach to nanomaterials - G.A. Ozin and A.C. Arsenault, RSC Publishing.
6. Nanomaterials and nanochemistry - C.Brechigneae, P. Houdy and M. Lahmai (Eds.), Springer.
7. Core concepts in supramolecular chemistry and nanochemistry, J.W. Steed, D.R. Turner and K. Wallace, Wiley.
8. The most beautiful molecule – The discovery of the Buckyball, H.A. Williams, John Wiley & Sons, Inc.

**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 -Organic Chemistry (Specialization)**

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

(Marks 100, Total Hours 60)

**Unit-I Heterocyclic Chemistry-II:**

Synthetic methods and reactivity of the following five membered heterocyclic systems: Carbazoles, Pyrazoles, Indazoles, Imidazoles, Benzimidazoles, Oxazoles, Benzoxazoles, Isoxazoles, Thiazoles and Benzthiazoles.

**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, Corey-Fuchs Reaction 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
16. Some modern methods of organic synthesis –W. Carruthers

**III Semester -Organic Chemistry (Specialization)**

**Paper-IV Natural Products (3CHT14)**

(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, classification of terpenoids, steroids, quinonoids, flavanoids...etc.) –General techniques of isolation and purification of natural products (with suitable examples representing different types of natural products) – Color reactions, spot tests and other basic identification techniques in natural products (with reference to flavanoids, terpenoids, alkaloids, quinine pigments, steroids etc.) –Basic separation techniques used in various types of natural products.

**Unit-II Chemistry of Terpenenoids:** Structure elucidation and total synthesis of Farnesol, Zinziberene, Cadinene, Abietic acid**,** Lanosterol and β-Amyrin.

**Unit-III Chemistry of Alkaloids:**

Structure elucidation and total synthesis of Ephedrine, Cocaine, Narcotine, 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 -Organic Chemistry practicals (Specialization)**

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

(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) Iosin from fluorosin.

**(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-Physical Chemistry (Specialization)**

**PAPER-III Quantum Chemistry, Kinetics & Electrochemistry (3CHT15)**

(Marks 100, Total Hours 60)

**Unit-I Quantam Chemistry – III:**

MO diagrams and MO configurations of Homo nuclear diatomic molecules $H_2$,$Li_2$,$N_2$,$O_2$,$F_2$ and hetro 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, Comparision 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-II Quantam 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 allylsystems, 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-III Kinetics:**

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 effect:** Solvent-solute interactions solvation parameters-effect of solvent on reactivity-solvolysis and nucleophilic substitution reactions. Grunwald–Winstein equation, Swain-Scott equation, Edward equation.

**Unit-IV Electro Chemistry:**

Batteries. Battery parameters. Energy density and power density. Measure of battery performance Primary and secondary batteries. $Zn/MnO_2$ ,lead –acid Ni-Cd batteries. Zinc –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. photovoltaic cells. Semiconductor based photochemical energy from solar energy.

Electro kinetic phenomenon, electrical double layers,(Helmholtz and stern potential),Zeta potential and its determination – Electro osmosis and streaming potential, electro capillary phenomena.

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

**Recommended books:**


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

**III Semester-Physical Chemistry (Specialization)**

**PAPER-IV Group Theory & Spectroscopy (3CHT16)**

(Marks 100,Total Hours 60)

**Unit-I Group Theory:**

Symmetry operations forming a group. Matrix representation of symmetry operations and point groups, isomorphism, Reducibleand irreducible representation.The great orthogonality theorm (without proof) and its properties for reducible and irreducible representation. Relation between reducible and irreducible representation. Character tables – construction of character tables for $C_2V$ and $C_3V$ groups- Direct product rule,Group theoretical aprroach for UV tranissions in ethylene and formaldehyde. IR and Raman active modes of water molecule.

**Unit-II Diffraction Studies:**

**X–Ray diffraction** : Bragg condition . Miller indices. Expermentel methods of x - ray diffraction laue method and Debye - Scherrer method. Primitive and non primitive unit cell. Index reflextion. Identification of unit cells from systamatic absences in diffraction pattern for cubic crystals. Structre factor and its relaton to intensity and electron density. Description of the procedure for an X- ray structure analysis . Tipical examples.

**Electron diffraction:** Scattering intensity versus scattering angle. Wierl equation. Measurement technique. Elucidation of structure of simple gas phase molecules.

**Neutron diffraction** : Scatterring of nuetrons, magnetic scattring, Elucidation of structure of magnetically ordered unit cell. Application and limitations.

**Unit-III Spectroscopy –I:**

**Photoelectron spectroscopy :** Basic principles, photo-electric effect, ionization process, Koopmans theorem, PES of Simple molecules , XPES , Chemical shift applications and ESCA.

**Photo acoustic spectroscopy :** Basic Principles of PAS-PAS of gases and condensed systems chemical and surface applications.

**Electron-Spin resonance spectroscopy:** Zero-field splitting- kramer's degeneracy – Mcconnell relationship , double resonance technique (ENDOR). ESR spectra of transition metal complexes

**ORD and CD Spectroscopy :** Basic concepts of optical rotatory dispersion (ORD) and circular dichroism (CD), Deduction of absolute configuration–Cotton effect–Octant rule for ketones. Applications of ORD and CD spectroscopy.

**Unit-IV Spectroscopy –II:**

**13C-NMR:** General considerations 13C-NMR & 1H-NMR- Chemicalschift (aliphatic, olefinic,alkyne, aromatic and carbonyl carbon). Coupling constant and factors affecting it. Splitting of 13C-NMR signals and simplication of signals by decoupling methods. Examples of 13C-NMR spectra.

**ATR spectroscopy:** Basic principle, total internal reflection instrumentation and applications.

**Emission spectra:** Frank-Condon principle, electronic spectra of polyatomic molecules. Radiative and non – radiative decay, Internal conversion and intersystem crossing. Excimers. Excited dimmers and Exciplex. Charge transfer and energy transfer mechanism. Properties of electronically excited species in comparision with ground state molecules. Electronic spectra of transition metel complexes.

**Recommended books:**

1. Chemical applications of Group theory-F.A.Cotton,Wiley,New York,1990.
2. Molecular Spectroscopy Patel and Patel.
3. Physical methods for chemistry-R.S.Drago,Saundes,1992
4. H.H.Jaffe and M.Orchin,Symmetry,Orbitals and spectra,Wiley,Newyork,1971.
5. Raman,K.V.,Group theory and its application to chemistry,Tata McGraw Hill,New Delhi.
6. P.K.Ghosh,Introduction to photoelectron spectroscopy,Wiley.
7. Chang,R:Basic principle of spectroscopy ,McGraw Hill.
8. Symmetry and spectroscopy of molecules,K.VeeraReddy,New Age International,1998.
9. X-ray diffraction procedures for polycrystalline and amorphous materials, H.P.Klug & L.E.Alexander, John Wiley.

**III Semester Physical Chemistry-Practicals (Specialization)**

**Paper-V –Kinetics (3CHP11)**

(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.

**III Semester Physical Chemistry-Practicals (Specialization)**

**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- Helmohltz equation.
7. $P^{Ka}$ of Chloro acetic 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

**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.

**Scheme of Valuation**

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

**III Semester**

**Environmental Chemistry (Open elective)** (3CHO1)

(Marks-100, Total hrs: 60)

**Unit-I Enviroment and Natural cycles:**

Enviroment – Introduction to enviroment and enviromental chemistry, Enviromental segments– 1) Atmosphere: Structure and composition of atmosphere, Earth's radiation balance; particles, ions and radicals in the atmosphere 2) Hydrosphere: Water resources and distribution of water, solubility of gases in water 3) Lithosphere: Composition of lithosphere, process of soil formation and 4) Biosphere: Natural cycles – Hydrologic cycle, Oxygen cycle, Nitrogen cycle, Carbon cycle, Phosphorous cycle and Sulphur cycle.

**Unit-II Air pollution and its control measures:**

Air pollution and sources of air pollution, Air pollutants, Chemical and photo chemical reactions in the atmosphere, Acid rain, Green house effect; Major sources of green house gases, Emission of carbon dioxide, Correlation of rise in temperature with increasing atmospheric carbon dioxide concentration, Impact of green house effect on global climate, Other consequences of green house effect, Control and remedial measures of green house effect; Ozone depletion, Causes and consequences of ozone depletion, Mechanism of ozone depletion by chemicals, Control and remedial measures of ozone depletion; Photochemical smog.

**Unit-III Water pollution and its control measures:**

Water quality parameters: Dissolved oxygen demand and Chemical oxygen demand; water pollution, Signs of water pollution, water pollutants; Sources of water pollution: Domestic wastes and their harmful effects, Industrial wastes and their harmful effects; Sewage treatment: Domestic sewage treatment, Industrial sewage treatment; Treatment of drinking water: Sedimentation, Coagulation, Filtration, Disinfection, Removal of colour and odour, Destruction of algal and fungal growth, Deflouridation by adsorption process.

**Unit-IV Soil pollution and Radio active pollution and their control:**

Soil pollution and Soil pollutants, Adverse effects of soil pollution, Mining and soil pollution, Sources and adverse effects of solid waste. Solid waste disposal methods: Open dumping, Ocean dumping, Land filling, Recycling and Composting.

Radioactive Pollution: Sources of radioactive pollution, Adverse effects of radioactive pollution, Control measures of radioactive pollution, Disposal methods of radioactive wastes.

**Recommended books:**

1. Environmental chemistry, A.K.De
2. Environmental chemistry, B.K. Sharma and H. Kaur
3. Environmental chemistry, J.W. Moore and E.A. Moore

**M.Sc Chemistry-IV Semester**

**Paper – I Analytical and Physical Chemistry (4CHT17)**

(Common paper for all specializations) (Marks 100, Total Hours 60)

**Unit-I Chromatography:**

Chromatographic methods**:** Geneal 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 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. Photodimerission of anthracene . Photosensitized reactions and photochromism.

**<u>Unit-IV</u> 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, electro kinetic phenomena, diffusion, electric conduction, irreversible thermodynamics for biological systems, coupled reactions.

**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, 7th ed., CBS Publishers.
3. Principles of instrumental analysis- D.A. Skoog, F.J. Holler and T.A. Nieman, 5th ed., Harcourt Asia PTE Ltd.
4. Fundamentals of photochemistry-K.K.Rohatgi, Mukharjee, Wiely-Eastern Ltd-1978
5. Photochemistry-R.P.Wayne-Oxford University Press.
6. Text book of physical chemistry - Puri& Sharma.
7. Advanced physical chemistry - Gurudeep raj Goel Publishers House,Meerut.
8. Photochemistry - Calvert,J.G.and J.N.,Wiely 1996.
9. Advanced physical chemistry -Guru & Singh, Pragati Prakashan.
10. Kinetics and Mechanism of chemical transformations-J.Rajaraman and J.C.Kuriacose-MacMillian.

**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 steroselective 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: Diastereo selective 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 enantio selective 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-Inorganic specialization**

**Paper-III Instrumental methods of analysis (4CHT19)**

(Marks 100, Total Hours 60)

**Unit-I Electroanalysis methods:**

Potentiometry – Theory of potentiometry, calculation of electrode potential at the equivalence point, Finding of equivalence volume – Linear and derivative titration plots, Ion-sensitive electrodes – Metal-based cation and anion sensitive electrodes, solid membrane electrodes, Glass electrodes, Liquid ion-exchange electrodes, Gas-sensing membrane electrodes.

Stripping voltammetry: Anodic stripping voltammetry, cathodic stripping voltammetry – Basic principles and applications.

**Unit-II 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-III 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.

**<u>Unit-IV</u> 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) $[Cr(CH_3COO)_2.H_2O]_2$

**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.

**IV Semester-Inorganicspecialization**

**Paper-IV Organometallic Chemistry (4CHT20)**

(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. ?$^1$ 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 – ?$^2$, ?$^3$, ?$^4$ organic groups. Preparation, structures and properties of olefin complexes of iron and nickel groups Preparation, structures and properties of ?-allyl complexes of nickel and palladium complexes. Exo/endo conformers, ? $^4$ –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: $C_nH_n$: Preparation, Structure and reactions of – Fe, Co, and Ni complexes with cyclic ?$^4$ $C_4H_4(R_4)$ ligands. Fe, Ru, and Os complexes with ?$^{5-}$ ($C_5H_5$) ligands, Ti, V and Cr complexes with ?$^6$ ($C_6H_6$) ligands and their carbonyl derivatives.

Organometallic compounds of lanthanides**:** Comparison of organometallic chemistry of *d*- and *f*-block metals. Homoleptc 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: □-and □-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-Inorganic Chemistry practicals (Specialization)

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

(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, 6th 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-Organic specialization**

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

(Marks 100, Total Hours 60)

**Unit-I Heterocyclic Chemistry-III:**

Methods of synthesis and reactivity of the following six membered heterocyclic systems: Acridines, pyridazines, cinnolines, phthalazines, pyrimidines, quinazolines, pyrazines, quinoxalines, - 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-Organic specialization**

**Paper-IVA – Natural products (Elective-I) (4CHT22A)**

(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-Organic specialization**

**Paper IVB Medicinal chemistry (Elective-II) (4CHT22B)**

(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.

**<u>Unit-IV</u> 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-Physical chemistry specialization**

**Paper III Catalysis (4CHT23)**

(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 SO2 and Fisher - Tropsch method for the synthesis of methanol. Gibbs adsorption equation.

**Unit-II Phase-Transfer catalysis:**

Classification , charactertiscs and criterion for P.T.C.catalysis. Mechanism and types of P.T.C catalysed reactions. Preparation of P.T.C.catalysts like quaternary salts, tetrahexyl ammonium bromide and crown ethers.Application to hydrolysis, oxidation, reduction, esterification and formation of ethers.

**Metal ion catalysis:** Molecular activation, proximity, interaction and catalytic cycle. Application to hydrogenation, isomerization, oxidation and hydroformylation.

**Micellarcatalysis**: Micellization and types of surfactants-critical micellar concentration(CMC)and its determination-factors effecting CMC. Solubilization in surfactant solutions. Emulsion polymerization mechanism.

**Unit-III Acid-Base Catalysis:**

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

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

**Unit-IV Enzyme 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 $P^H$ on the nature of active site. Inhibition of enzyme catalyzed reactions. Competitive inhibition-uncompetitive inhibition, non-competitive

inhibition. Enzymatic catalytic mechanism by Acid-base catalysis, Covalent catalysis, Metal ion catalysis, Catalysis through proximity and orientation effects, catalysis by preferential transition state binding.

**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. Advanced Inorganic Chemistry –F.A. Cotton & G. Wilknson.
6. Organicmetallic Chemistry-R.C. Mehrothra
7. Biochemistry,Voet and Voetjohn Wiely
8. Catalysis-J.C.Kuriacose-Macmillan-India Ltd.
9. Phase transfer catalysis by E.V.Dehmlow O.S.S. DehmlowVerlagChemie,Weinheim.
10. Kinetics and mechanism of chemical transformations,J.Rajaramam&J.Kuriacose.
11. Adamson,A.W; Physica chemistry ofsurfaces.5th edition,Wiley,1992.

**IV Semester-Physical chemistry specialization**

**Paper IV(A)- (Elective-I)**

**Nanomaterials, Macromolecules and Data analysis (4CHT24A)**

(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 technique: Transmission electron microscopy (TEM), fieldin microscopy (FM), Scanning microscopy (SM) and X-ray spectroscopy Carbon nanotubes- electronic, mechanical and other properties. Use of nanotubes in fuel cells and catalysis.

**Unit-II Characterization of Macromolecules:**

Polydispersion- Concept of average molecular weight, Number, Weight and Viscosity average 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. Analysis and testing of polymers-chemical analysis of polymers, spectroscopic methods, X-ray diffraction study. Thermal analysis and physical testing-tensile strength.Fatigue, impact, Tear resistance. Hardness and abrasion resistance.

**Unit-III Kinetics –IV:**

Kinetices and mechanisam of free radical polymerization. Degree of polymerization, kinetic chain length and chain transfer coefficient.

Kinetics and mechanisam of linear stepwise polymerization, cationic, anionic polymerization. Copolymerization reactions and copolymer composition. Reactivity ratios and their determination. Significance of alfrey and price Q-e scheme for monomer and radical reactivity. Block and graft copolymers.

Bulk, solution, suspension and emulsion polymerizations.

**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. Dipole moments and its measurements .Its application to 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.Polymer Chemistry, B.Vollmert.
8.Systamatic experimental physical chemistry, S.W.Raj Bhoj,T.K.Chondhekar, Anjali Publication, Aurangabad.

**IV Semester-Physical chemistry specialization**

**Paper IV(A)- (Elective-II) (4CHT24B)**

**Supramolecular, Material Sciences, Lasers and Computational Chemistry**

(Marks 100,Total Hours 60)

**Unit-I: Supramolecular Chemistry:**

Molecules, super molecules and supra molecular chemistry. Molecular recognition and factors involved .Ionophores-molecular receptors . Design principles-Types of interactions between host and guest molecules. Molecular receptors for alkali metal ions, ammonium ion, anions and neutral molecules. Crownethers, cryptands, spherands and cyclodextrains, Thermodynamics of host-guest complexation. Enthalpy and entropy contribution-complexation free energies. Supra molecular catalysis with examples.

**Unit-II Types of materials and liquid crystals:**

Classification of materials: Ceramics, polymers, composites, semiconducters, super conductors and bio materials. Ceramics: criteria of determining the crystal structure of ceramics materials.-examples; Mechanical propertics of ceramics. Composites: Particle-reinforce dardfibre-reinforced composites, pre-perative methods of solid materials. Ceramic methods-Co precipatatio and sol-gelprocess. Techniques of single crystal growths, growth from solutions, grouth from melts and growth from vapour.Liquid crystals: Themesophase ,thermotropic liquid crystals. Nematic and smectic mesophases. Typical applications.

**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.Laer 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 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.

**Recommended books:**


1. Core concepts in Supramolecular Chemistry and Nanochemistry- J.W. Steed, D.R.Turner,K.Wallace (Wiley, 2007)
2. Supramolecular Chemistry ,J.M. Lehn.
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.
5. Principal of Physical chemistry by Puri & Sharma.
6. Molecular Modelling: Principles and Applications by AndrewLeach,Longman publications
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. A Guide to Lasers in Chemistry ,G.R.Van Hecke & K.K.Karukstis,Jones and Bartlett Publishers.
11. Lasers in Chemistry and Biological Sciences,S.Chopra & H.M.Chawla,Wiley Eastern Ltd

**IV Semester-Physical chemistry Practicals**

**Paper-V Kinetics experiments (4CHP17)** (Marks 100, 9 Hours per week)

**1. Kinetics of** i) Actone- Iodine reaction: Determination of

a) Order b) Acid effect

c) Solvent effect d) Temperature effect.

ii) Inversion of sucrose-Effect of acidity functions.

**Paper–VI Instrumentation (4CHP18)**

(Marks 100, 9 Hours per week)

**Instrumentation:**

**I. Conductometry:**

1. Mixture of acids and $CuSO_4$ vs NaOH
2. Dibasic acids Vs NaOH
3. Mixture of chloroacetic acids vs NaOH
4. Replacement Reactions
5. Determination of $p^{Ka}$ of chloroacetic acid
6. Verification of Onsagers euations with KCl
7. Determination of composition of complex (Cu(II) Vs EDTA)
8. Kinetics of Saponification of ethylacetate.

**II. Potentiometry /$P^H$ Metry:**

1. Determination of dissociation constants of moaobasic / dibasic acids by Albert-Serjeant method.
2. Determination of dissociation constant of acetic acid in DMSO, acetone and dioxane.
3. Determination of thermodynamic constans, $\Delta G$, $\Delta S$ and $\Delta H$ for the following reaction by e.m.f. method.

$$Zn + H_2SO_4 \rightarrow ZnSO_4 + 2H$$

**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

– Prof. Gade Dayakar
Chairperson
Board of Studies in Chemistry
Kakatiya University - Warangal

*Mobile*: +91- 9849777797
*Email*: gadedayakar@yahoo.co.in

**Model paper** **M.Sc CHEMISTRY**

## Internal examination

## Scheme of examination:

**Internal examination: [Best of 2** –Internal exam-I, Internal exam-II]

In each exam – No. of questions –10 Total marks–20 Duration of exam –1Hr

**(**Internal exam-I from Unit I and Unit II; Internal exam-II from Unit III and Unit IV)

**MODEL PAPER**

**FACULTY OF SCIENCE**

**M.Sc (-Semester examination)**

**CHEMISTRY**

**Time: 3Hrs** **Paper-** **Max Marks: 80**

***Answer ALL questions in serial order***
**All questions carry equal marks**

1. Answer the following (4x4=16M)
   a) Unit-I
   b) Unit-II
   c) Unit-III
   d) Unit-IV

2. a) Unit-I (16M)
   b) Unit-I
   Or
   c) Unit-I
   d) Unit-I

3. a) Unit-II (16M)
   b) Unit-II
   Or
   c) Unit-II
   d) Unit-II

4. a) Unit-III (16M)
   b) Unit-III
   Or
   c) Unit-III
   d) Unit-III

5. a) Unit-IV (16M)
   b) Unit-IV
   Or
   c) Unit-IV
   d) Unit-IV