### Semester - I

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UNIT I  Structure and Bonding


UNIT II  Coordination chemistry of transition metal ions

Stability constants of complexes and their determination, stabilization of unusual oxidation states, coordination numbers and structures, isomerism, Valence bond theory, molecular orbital theory, (sigma as well as Pi bonding), Crystal field theory, Ligand field theory, Ligand field stabilization energy, Lattice energies and hydration energies, Irving-Williams series, types of ligands (sigma donars, pi donars and pi acceptors) and the spectrochemical series, Jahn-Teller effect, nephelauxetic effect, chelate and macrocyclic effect.

UNIT III  Chromatographic techniques

Column chromatography, Thin layer chromatography, Normal and reversed phase liquid chromatography, Principle, instrumentation and specific applications of Gas Chromatography (GC), High Performance Liquid Chromatography(HPLC), Size-Exclusion Chromatography (SEC); Supercritical Fluid chromatography, Ion Chromatography (IC). Capillary Electrophoresis. Hyphenated techniques: Introduction to interfaces, Principle, instrumentation and applications of GC-MS, LC-MS and GCFT IR.

UNIT IV  Lanthanides and Actinides
Occurrence, properties of the elements, Common and uncommon oxidation states, Absorption and emission Spectra, magnetic properties, Separation of lanthanide elements, lanthanide and actinide contraction, similarities between actinides and lanthanides, Comparison with transition elements, Coordination complexes and Organometallic compounds of lanthanides and actinides, use of lanthanide compounds as shift reagents.

UNIT V Spectroscopy I

**IR and Raman:** Selection rules, predicting number of active modes of vibrations, application of IR and Raman in the study of inorganic structures and coordination compounds. Mode of bonding of ambidentate ligands, application of isotopic substitution, detection of intra and intermolecular hydrogen bonding.

**Mossbauer:** Principle, conditions for Mossbauer spectroscopy, isomer shift, quadrupole interactions, magnetic interactions, interpretation of spectra of iron, tin and gold compounds

**References**

UNIT I Reactive Intermediates and rearrangements


UNIT II Aliphatic Nucleophilic & Electrophilic Reactions


Electrophilic substitution – SE1, SE2 and E1CB mechanism - effect of substrate structure, leaving group, attacking nucleophile and solvent polarity.

UNIT III Aromaticity and Ring system


UNIT IV Study of Organic reaction mechanism

Reaction mechanism – Transition state and intermediate. Kinetic and Thermodynamic requirements of reactions – Hammond Postulate and microscopic reversibility. Kinetic and Thermodynamic control of product formation. Kinetic and Non-kinetic methods of
determination – Primary and secondary isotope effect- Testing and Trapping of intermediates, Isotopic labeling, Cross-over experiments and stereo chemical evidence. LFER: Hammett equation – Physical significance of $\sigma$ and $\rho$ – Applications and Limitations – Taft equation.

UNIT V Stereochmistry

Molecular Symmetry and Chirality - Types of molecules exhibiting optical activity. Configurational nomenclatures of acyclic and cyclic molecules: cis-trans and E,Z - and D, L; R, S; erythro and threo; syn and anti; endo and exo.


Reference:
UNIT I Quantum Mechanics I
Limitation of classical mechanics and success – Plank’s quantum theory – Compton effect – wave particle duality – uncertainty principle, Operators and their algebra, Eigen value and Eigen functions, Quantum mechanical postulates, Schrodinger equations (Time dependent and Time independent), Particle in a box (1D and 3D), Quantum mechanical tunneling and transmission coefficient - rigid rotor and harmonic oscillator.

UNIT II Quantum Mechanics II

UNIT III Electrochemistry I

UNIT IV Electrochemistry II
Polarization and overpotential- Butler-Volmer equation for one step and multistep electron transfer reactions-Tafel equation-significance of $I_c$ and transfer coefficient – polarizable and non-polarizable electrodes- mechanism of metals-hydrogen and oxygen evolution reactions-Corrosion and Polarization of metals-Pourbaix diagrams-Evan’s diagram-fuel cells- electrode deposition –principle and applications

UNIT V Macromolecules

References

2. Castellan.W - Physical chemistry,


11. Antorpcion L, Theoretical Electrochemistry, Mirpublishers, Moscow.


**UNIT I  RESEARCH METHODOLOGY I**

Introduction of research- selection of a research topic- reviewing the literature- including patents- primary source – secondary source – including reviews, treatise and monographs – abstraction of research papers – possible ways of getting oneself familiar with current literature- preparing the proposal and design of study. Experimentation and interpretation of results.- Formation, testing and rejection of hypothesis. Application of microcal origin and Chemdraw.

Survey of literature

**UNIT II  RESEARCH METHODOLOGY II**

Identification of research problem – assessing the status of the problem guidance from the supervisor – actual investigation and analysis of experimental results – conclusions –
presenting scientific seminar – reporting the results in the form of communication, paper etc- dissertation and thesis writing.

Idea of writing research articles – project proposals to the funding agency- Search engine for locating information and chemical data bases. E-mail operation and online submission of manuscript for publication.

**UNIT III  SPECTROSCOPIC TECHNIQUES**


Principle, instrumentation and data interpretation of TEM, SEM, EDAX, and XRD analysis. Calculation of particle size of nanoparticles from XRD spectra – Debye – Scherrer formula – lattice constant findings.

**UNIT IV  RADIOCHEMICAL METHODS**


**UNIT V  DATA ANALYSIS AND ARTICLE & PROPOSAL WRITINGS**


**References**

UNIT I

Bio-inorganic Chemistry II

Molecular mechanism of ion transport across membranes (Na and K ions), ionophores, transport and storage of iron - Siderophores, transferrin, Ferritin. porphyrins, O₂ binding
properties of heme (haemoglobin and myoglobin) and non-heme proteins (hemocyanin & hemerythrin), their coordination geometry and electronic structure, co-operativity effect, Hill coefficient and Bohr Effect. Electron transfer proteins - structure and functions of ferredoxin, rubidoxin and cytochromes and blue copper proteins. Photosynthesis-PS-I, PS-II, in vivo and in vitro nitrogen fixation.

UNIT II Organometallic Chemistry I

16 and 18 electron rules, synthesis, structure and bonding in mono and polynuclear metal carbonyls, nitrosyls. carbonylate ions, carbonyl hydride complexes, dinitrogen and dioxygen as ligands in organometallic compounds. Wade-Mingos-Lauher rules, Isolobal analogies IR and NMR of carbonyl compounds. synthesis and reactivity of metal alkyls, carbenes, carbynes, carbides, alkenes, alkynes, and arene complexes; metallocenes and bent metallocenes, ionic bond in metallocenes.

UNIT III Bioinorganic Chemistry I

Metalloenzymes-Role of zinc, zinc enzymes (Carboxypeptidase A, Carbonic anhydrase, alcohol dehydrogenase) Cobalt-for-zinc ion substitution. Xanthane oxidase, aldehyde oxidase, Acid phosphatases, Enzymes dealing with H₂O₂ and O₂-catalases, Peroxidases, Oxidases, Oxygenases (cytochrome P₄₅₀), superoxide dismutase(Cu), ceruplasmin(Cu),) Metallothionines. Chlorophyll and Vitamin B₁₂ and their mechanisms of action. Chelation therapy, applications of complexes of Pt, Au and V in medicine

UNIT IV Thermoanalytical and Electroanalytical methods

Thermoanalytical Methods: Principle, instrumentation and applications of Thermogravimetry, Differential Thermal Analysis (DTA), and Differential Scanning Calorimetry: DSC.

**UNIT**

**References**

3. Azaroff L.V., introduction to solids, Tata McGraw Hill publishing Ltd
4. Kittel C., Introduction to solid state physics, Wiley Eastern Ltd, 5th Edn
SEMESTER- II


UNIT – I  Aromatic Electrophilic and Nucleophilic substitution reaction


Aromatic Nucleophilic Substitution - SNAr mechanism- SN1 (Aromatic) mechanism with evidences - Benzyne mechanism - Effect of substrate structure, leaving group, attacking nucleophile and solvent. Selected reactions - Von Richter, Sommelet-Hauser and Smiles rearrangements.

UNIT – II  Addition and Elimination reaction

Addition to C-C and C-O multiple bonds- electrophilic, nucleophilic and free-radical additions- additions to conjugated systems – Birch reduction – hydroboration- Michael condensation- Diels – Alder reactions- carbone addition to double bonds- hydration of olefins.


UNIT – III  Reagents in Organic Reactions

Synthetic applications of the following- Gilman, DDQ, DCC, PCC,1,3-dithiane, Fetizon’s reagent, Lemieux-Johnson reagents, Prevost and Woodword reactions, Jones reagent, Bio- oxidants, Wilkinson’s catalyst, , Ziegler-Natta catalyst.

UNIT – IV  Heterocyclic compounds and Biomolecules

Synthesis and reactions of oxazole, imidazole, thiazole, coumarins, benzopyrones and anthocyanins- synthesis of flavones, flavonol and quercetin. Pyranose and furanose forms of aldohexose and ketohexose- methods used for the determination of ring size-A Detailed study on
the structure of maltose, sucrose and lactose- A brief study on starch and cellulose. Nucleic acids, nucleotides, polynucleotides and nucleosides.

UNIT – V  Molecular rearrangement

Mechanism and application of the following rearrangement: Baeyer- Villiger, Wagner- Merwin, Beckmann, Dienone-Phenol, Pinacol-Pinacolone, Arndt- Eistert synthesis, Darkin, Lossen, Neber, Tiffenev--Demjanov rearrangement.

References
UNIT I Group Theory I: Symmetry Properties Of Molecules And Group Theory
Symmetry elements, symmetry operations. Principles of group theory (point groups) properties of group, symmetry and dipole moment, symmetry and optical activity, symmetry operations as a group, multiplication table. Point group- Schoenflies symbols. Matrix representations of operations. Reducible and irreducible representations. Constructions of character table for point groups (C\textsubscript{2v}, C\textsubscript{3v} and D\textsubscript{2h}). Explanations for the complete character table for a point group.

UNIT II Group Theory II Applications Of Group Theory
Applications of Group theory - Standard reduction formula relating reducible and irreducible representations - Hybridization schemes for atoms in molecules of different geometry - AB\textsubscript{4} tetrahedral, AB\textsubscript{3} triangular planar, AB linear molecules -Symmetries of vibrational modes in non-linear molecules (H\textsubscript{2}O, NH\textsubscript{3} and BF\textsubscript{3}) - Symmetries of vibrational modes in linear molecules (HCN, CO\textsubscript{2}, C\textsubscript{2}H\textsubscript{2}) -Integration method - Selection rules in spectroscopy - Mutual exclusion rule - Symmetry in crystals - Hermann - Mauguin symbols-Space groups of crystals -Translational elements of symmetry – Comparision of crystal symmetry with molecular symmetry.

UNIT – III Nano Chemistry I
Introduction - Importance and characterization of nanomaterials - Stability of nanoparticles in solutions - Synthesis of metal nanomaterials: Physical methods (Laser Ablation, Evaporation, sputtering and solvated metal dispersion) - Chemical methods (Thermolysis, sonochemical approach, reduction of metal ions by hydrogen and methanol) - Biosynthesis (elementary idea only).

UNIT – IV Nano Chemistry II

UNIT V Radiation and Sonochemistry

Radiation Chemistry- Interaction of radiation with matter- primary effect due to charged particle—Radiation tracks , spurs and delta rays- linear energy transfer(LET) Bethe’s equation for LET for charged particles due to collisions with electrons -Radiation dosimetry-units of radiation energy (Rad , Gray , Rontgen , RBE Rem ,Sivert) -Radiolysis of water.

Sonochemistry- Principle and Mechanism- Homogenous systems- initiation of homogeneous catalysis- Heterogenous systems-Applications to heterogenous catalysis- Applications of Sonochemistry-cavitation-Sonoluminescence- Ultrasound reactions- synthetic routes-polymers

References
2. Raman K V, Group Theory and its Applications
Inorganic Chemistry

1. Chemical periodicity
2. Structure and bonding in homo- and heteronuclear molecules, including shapes of molecules (VSEPR Theory).
3. Transition elements and coordination compounds: structure, bonding theories, spectral and magnetic properties
4. Inner transition elements: spectral and magnetic properties, redox chemistry, analytical applications.
5. Organometallic compounds: synthesis, bonding and structure, and reactivity.
6. Analytical chemistry- separation, spectroscopic, electro- and thermoanalytical methods.
8. Characterisation of inorganic compounds by IR, Raman, Mössbauer, UV-vis, MS, electron spectroscopy and microscopic techniques.

Organic Chemistry

1. IUPAC nomenclature of organic molecules including regio- and stereoisomers.
2. Principles of stereochemistry: Configurational and conformational isomerism in acyclic and cyclic compounds; stereogenicity, stereoselectivity, enantioselectivity, diastereoselectivity and asymmetric induction.
3. Aromaticity: Benzenoid and non-benzenoid compounds – generation and reactions.
5. Organic reaction mechanisms involving addition, elimination and substitution reactions with electrophilic, nucleophilic or radical species. Determination of reaction pathways.
7. **Organic transformations and reagents:** Functional group interconversion including oxidations and reductions; common catalysts and reagents (organic, inorganic, organometallic and enzymatic). Chemo, regio and stereoselective transformations.

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**Physical chemistry**

1. **Basic principles of quantum mechanics:** Postulates; operator algebra; exactly-solvable systems: particle-in-a-box, harmonic oscillator and the hydrogen atom, including shapes of atomic orbitals; orbital and spin angular momenta; tunneling.
2. **Approximate methods of quantum mechanics:** Variational principle; perturbation theory up to second order in energy; applications.
3. **Atomic structure and spectroscopy:** term symbols; many-electron systems and antisymmetry principle.
4. **Chemical bonding in diatomics:** elementary concepts of MO and VB theories; Huckel theory for conjugated π-electron systems.
5. **Chemical applications of group theory:** symmetry elements; point groups; character tables; selection rules.
6. **Chemical thermodynamics:** Laws, state and path functions and their applications; thermodynamic description of various types of processes; Maxwell’s relations; spontaneity and equilibria; temperature and pressure dependence of thermodynamic quantities; Le Chatelier principle; elementary description of phase transitions; phase equilibria and phase rule; thermodynamics of ideal and non-ideal gases, and solutions.
7. **Electrochemistry:** Nernst equation, redox systems, electrochemical cells; Debye-Huckel theory; electrolytic conductance – Kohlrausch’s law and its applications; ionic equilibria; conductometric and potentiometric titrations.
8. **Polymer chemistry:** Molar masses; kinetics of polymerization.
9. **Data analysis:** Mean and standard deviation; absolute and relative errors; linear regression; covariance and correlation coefficient.
1. Qualitative analysis of inorganic mixture containing two familiar and two less familiar cations Pb, Cu, Bi, Cd, Sb, Zn, Co, Ni, Mn, Ca, Ba, Sr, W, Tl, Te, Se, Mo, Ce, Th, Zr, V, U, Ti and Li.

2. Complexometric titrations – Estimation of Cu, Zn and Mg by EDTA titration in presence of either Pb or Ba.

**COURSE WORK**

1. Photocolorimetric estimation of Fe, Ni, Cr, Mn, Cu and NH$_4^+$.

**Reference**
1. Micro Qualitative Analysis of an organic binary mixture
   i. Pilot separation
   ii. Bulk separation
   iii. Determination of melting and boiling points
   iv. Analysis of organic compounds
   v. Derivatization

2. Preparation of Organic compounds
   1. Preparation of Benzoic acid from benzyl Chloride
   2. Preparation of Resacetophenone from resorcinol
   3. Preparation of Iodobenzene from aniline.
4. Preparation of dibenzalacetone from benzaldehyde.

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5. Preparation of 2,4,6-tribromoaniline from aniline
6. Preparation of Tetrahyrocarbazole from cyclohexanone

3. Course work
   Chromatographic techniques
   i) TLC
   ii) Paper chromatography

References

A. DISTRIBUTION
1. DISTRIBUTION OF BENZOIC ACID BETWEEN BENZENE/ TOLUENE AND WATER

B. CONDUCTIVITY
2. DETERMINATION OF SOLUBILITY PRODUCT OF A SPARINGLY SOLUBLE SALT
3. DETERMINATION OF $K_a$ BY USING OSTWALD DISTRIBUTION METHOD
4. TITRATIONS
i) \( HCl + CH_3COOH \) vs NaOH
ii) \( NH_4Cl + HCl \) vs NaOH
iii) \( CH_3COOH + CH_3COONa \) vs NaOH
iv) \( CH_3COOH + CH_3COONa \) vs HCl

C. **Kinetics**

5. **Study of Primary Salt Effect on** \( K_2S_2O_8 \)
6. **Kinetics of** \( K_2S_2O_8 \) **and** \( I_2 \)

D. **Thermometry**

7. **Determination of Solution Enthalpy**
   i) **Oxalic Acid – Water**
   ii) **Ammonium Oxalate – Water**
   iii) **Naphthalene – Toluene**

References

5. Yadav. J.P , Physical Chemistry Practicals
UNIT I

I Solid state I

Electronic structure of solids - band theory, free electron theory, Insulators and semiconductors and its types. Electrical properties (Thomson effect, Peltier effect, Seebeck effect, Hall effect) optical and magnetic properties of semiconductors. p - n junction and n-p-n junction and their applications. Dielectric, Ferroelectric, Piezoelectric and Pyroelectric Materials
and their and applications. solid electrolytes, superconductors, High-temperature superconductors, BCS theory, cooper electrons Meissner effect and levitation

UNIT II  Acids and Bases


UNIT III  Solid state II

Types of close packing - hcp and ccp, packing efficiency, radius ratios; Powder x-ray diffraction, electron and neutron diffraction, solid-state reactions, Methods of Single Crystal Growth- Bridgeman, Czochralski, Verneuil; Chemical Vapour Transport, Hydrothermal method Dislocations in solids, Point defects - Schottky and Frenkel defects Line defects, Surface Defects - Dislocations, Grain Boundary and Stacking Fault. Crystal structures of common ionic compounds NaCl, Na₂O, zinc blende, wurtzite, nickel arsenide, CsCl, rutile, CdI₂, CdCl₂, and Cs₂O, perovskite, K₂NiF₄, spinels.

UNIT IV  Nuclear Chemistry

Radioactive decay and equilibrium, Nuclear Reactions - Types, Q value, Cross Section of reactions, Chemical effects of nuclear transformation, Nuclear Fission - theory of nuclear fission, Fission Products, Fission Yield, Nuclear Fusion and stellar energy, Nuclear Reactors, Nuclear waste management, nuclear reactors in India – Radioactive techniques: i) Countering Techniques such as G.M Ionization and Proportional counters. ii) Tracer techniques (neutron activation analysis).
UNIT V Spectroscopy II


PES : UPS - principle, spin-orbit coupling, XPS - Principle, spin-spin splitting chemical shift in XPS. Koopmans' theorem and applications of XPS and UPS to inorganic spectra. Auger electron spectroscopy.

References

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<th>SEMESTER- III</th>
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<td>Core VIII</td>
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UNIT – I Spectrosopy – I
UV – Visible and IR- Spectroscopy - Absorption laws -types of electronic transitions – Instrumental and Sampling – Solvent effect – Application of Woodward fieser rule to calcualte $\lambda_{max}$ values of conjugated diene, triene ,polyenes, $\alpha$ and $\beta$ unsaturated carbonyl compound. Optical rotatory dispersion and circular dichroism, octant rule, $\alpha$-haloketone rule and their applications.

IR instrumentation- characteristics of IR absorption of different functional groups- factors influencing vibrational frequencies-Hydrogen bonding- Inter and intra molecular hydrogen bonding.

UNIT – II Spectrosopy – II
PMR spectroscopy-Basic principle-number of signals- chemical shift- factors influencing chemical shift- spin–spin coupling AX, ABX- geminal, vicinal and long range coupling. NOE in stereochemistry - FT-NMR- $^{13}$NMR-2D NMR-COSY, NOESY, INADEQUATE, DEPT- broad and off resonance decoupling application

UNIT – III Spectrosopy – III
Mass spectrometry-instrumentation- basic Principles- techniques of Ion production – EI, CI, FD, FAB, ESI-MS, MALDI-MS- Base peak- molecular ion-nitrogen rule-metastable ion- isotope ion-daughter ion--calculation of molecular formula-fragmentation pattern of various classes of organic compounds- hydrocarbons, alcohols, amines, aldehyde, ketone, ether, ester, acids and phenols- Mc-Lafferty rearrangement. Problems on combined applications of UV -Visible, IR, NMR and mass spectrometric methods to structural elucidation of organic compounds.
UNIT – IV Conformational Analysis
Conformations of mono and disubstituted cyclohexanes- effect of hydrogen bonding, dipole and steric effects on the disubstituted cyclohexanes- conformation and reactivity of acyclic and cyclic compounds (6 members)- conformation of decalin and perhydrophenanthrene- Curtin- Hammett principle.

Unit-V Alkaloids and terpenoids

Terpenoids Introduction-general methods to elucidate the structure of terpenes, structural determination of camphor, zingiberine, α-pinene, squalene.

References
UNIT I Surface Chemistry

UNIT II Statistical Thermodynamics

UNIT III Applications of Statistical Thermodynamics
Unit IV  Introduction of spectroscopy and Rotational spectra
Characterization of electromagnetic radiation - Regions of Spectrum - transition probability - width and intensity of spectral transitions.
Classification of molecules according to their moment of inertia - Rotational spectra of rigid and non rigid diatomic molecules - The intensities of spectral lines-The effect of isotopic substitution - Polyatomic and symmetric top molecules - stark effect.

Unit V  Infrared spectroscopy and Raman spectroscopy:
Infrared spectroscopy : Polyatomic molecules-Fundamental vibrations and their symmetry , overtune and combination frequencies ,concept of group frequencies ,Fermi resonance and FTIR.

References
1. Arthur W.Adamson , Physical Chemistry of Surfaces , John Wiley and Sons , INC


UNIT I  Inorganic reaction mechanism:


UNIT II  Inorganic photochemistry

Laws of photochemistry, Photo physical processes, Prompt and delayed reactions, d-d and charge-transfer reactions, bimolecular deactivation and energy transfer, Transitions in metal-metal bonded systems. Photo substitution, Photo aqutation, Photo anation Adamson’s rules, Photo rearrangement, Photo redox reactions, Photochemistry of Cr(III), Co(III), Rh(III) and Pt(II) complexes. Photochemistry of ruthenium polypyridyls, Photo chemistry of organo metallic compounds. Applications in semiconductor electrodes.
UNIT III  Organometallic Chemistry II

Reactions of organometallic complexes: Substitution, oxidative addition, reductive elimination, nucleophilic and electrophilic displacement of coordinated ligands, insertion (1,1 and 1,2) and elimination cyclometallation. Homogeneous Catalysis - Hydrogenation, Hydroformylation, Monsanto process, Wacker process, Alkene metathesis, heterogeneous catalysis - Fischer-Tropsch process, Ziegler Natta polymerization.

UNIT IV  Inorganic chains, rings, cages and clusters

Homocyclic and heterocyclic inorganic ring systems, isopoly and heteropoly anions, Silicates, polysilicates and aluminosilicates, sulphur nitrides, borazines, Phosphazenes, phosphazene polymers. Synthesis, properties and structure of boranes, [styx notation] heteroboranes, metalloboranes and metallo carboranes, silicones, metal - metal bonds, clusters - carbonyl clusters, anionic and hydrido clusters, carbide clusters, sulphur metal clusters, Wade’s rule. Isolobal relationships between main-group and transition metal fragments.

UNIT V  Chemistry of Non-transition Elements

General discussion on the properties of the non-transition elements, special features of individual elements, synthesis, properties and structure of their halides and oxides, polymorphism of carbon, phosphorus and sulphur, oxyacids of nitrogen, phosphorus and sulphur, halogen oxides and oxo compounds, Interhalogens, polyhalides, basic properties of the halogens, pseudohalides and xenon compounds.

Spectroscopy III

NMR : Principle, 31P, 19F and 15N NMR, Application of spin spin coupling to structure determination, nuclei with quadrupole moment, double resonance, NMR of fluxional molecules, applications in biological systems.

NQR : Principle, energies of the quadrupole transitions, Structural information from NQR spectra.

EPR : Principle, Interaction between nuclear spin and electron spin (hyperfine coupling) Hyperfine splitting in isotropic systems, Zero field splitting, Kramer's degeneracy, anisotropy in the g value, interpretation of g values, anisotropy in hyperfine coupling, Application to transition metal complexes, Jahn - Teller distortion.
References
8. Gurdeep Raj, Advanced Inorganic chemistry II, Goel publishing house, Krishna prakashan media (P) Ltd.
UNIT- I  Photochemistry and Pericyclic reactions


Atomic and molecular orbitals- Woodward – Hoffmann rules, FMO and MO correlation diagram approaches: Electrocyclic reaction- con and dis rotatory motions for 4n and 4n+2 system (butadiene and 1,3,5-hexatriene)- Stereochemical course of electrocyclic reaction in terms of conservation of orbital symmetry.  Cycloaddition- suprafacial and antarafacial additions, [2+2] and [4+2] reactions (ethylene and butadiene) – Sigmatropic rearrangements- [i,j] shift of C-H and C-C bonds (1,3, 1,5 and 3,3 system).

UNIT – II  Some typical reactions and their applications in organic synthesis


UNIT – III Retrosynthetic Analysis

Synthon- synthetic equivalent –Functional group interconversions- use of protecting groups for alcohols, amines, acids, carbonyl compounds- use of activating and blocking groups- Robinson annulations reaction- carbon skeletal complexity- Role of key intermediates in organic synthesis. Reterosynthetic analysis of the following compounds: Twistane, cis – Jasmone, Baclofan,Brufen, Trihexylphenyldyl, Bisabolene, a-onocerin, isonootkatone, cascarillic acid, camphor and 2,4-dihydroxy pentanoic acid.
UNIT – IV Steroids

Classification – Structural elucidation of cholesterol and ergosterol – structural elucidation of androsterone, testosterone, progesterone, Oestrone.

Conversion of Cholesterol into androsterone, progesterone, testosterone, 5α- and 5β-Cholanic acid, Conversion of Oestrone to Oestriol.

Unit V Green Chemistry

Twelve principles, atom economy- addition and rearrangement reaction, substitution reaction, elimination reaction- Green solvents- Supercritical CO₂, H₂O, Ionic liquids.

Solid state and non solid state microwave assisted reaction – Stille reaction, suzuki reaction – Krohnka reaction – Huyama reaction- sonogashira reaction.

References

UNIT I Chemical Kinetics

UNIT II Chemical Kinetics
Reaction in solution - Comparison between gas phase and solution reactions - Cage effect - The influence of the solvent on the reactions between ions and reaction between ions and neutral molecules - Influence of ionic strength on rates of reactions in solution - Significance of volume and entropy of activation - Secondary salt effect - Kinetic treatment of complex ion - Parallel reactions of the same order (first or second, parallel first and second order reactions) - Reversible reaction of the same order (first or second order) - First order forward and second order backward - Consecutive first order reactions, steady state and rate determining step (or equilibrium) approximation of complex reactions - Chain reactions and explosions.

UNIT III Electronic Spectroscopy
Electronic spectroscopy of diatomic molecules - Born-Oppenheimer approximation - Sequences and progressions - The vibrational course structure and rotational fine structure of electronic band - The Frank-Condon principle - Dissociation energy and dissociation products - Birje-Sponer extrapolation - The fortrat diagram - Predissociation


**Unit IV NMR and ESR**

**Nuclear Magnetic Resonance Spectroscopy** : The theory of PMR spectra, Chemical shift, factors affecting chemical shift, relaxation times and spin-spin interactions - NMR of simple AX and AMX type molecules - Calculation of coupling constants, C$^{13}$, P$^{31}$ NMR, 2D-NMR spectra - Principle and applications.

**Electron Spin Resonance Spectroscopy** : Basic principles, factors affecting “g” value, hyperfine splitting - Dueterium, methyl, benzene, naphthalene, anthrazene, xylene (o,m,p-), p-benzosemiquinone radicals, calculation of electron density - McConnel equation - Fine structure in ESR - Zero field shifting and Kramer’s degeneracy - Double resonance – ELDOR and ENDOR, study of unstable paramagnetic species, spin labeling studies of bio-molecules.

**Unit V Quadrupole resonance and Mossbauer Spectroscopy**

**Nuclear quadrupole resonance**: Basic principle - comparison with NMR - Splitting of quadrupole energy levels, Asymmetry parameter - Applications – Hydrogen bonding - Phase transition - Substituent effect and Pi-bond character.

**Mossbauer parameters**: Isomer shifts, quadrupole splitting - Magnetic hyperfine interaction - Doppler effect/shift - Applications of Mossbauer Spectroscopy - (i) covalent bonded compounds (ii) oxidation states of metal ion in compounds (iii) structural determination (iv) magnetically ordered compounds (i.e. Ferromagnetic & antiferromagnetic compounds).

**References**

3. Atkins.P.W, Physical Chemistry
1. Preparation of Single Stage inorganic complexes. (a minimum of 6 complexes)

   1. cis potassiumdiaquadioxalatochromate(II) dihydrate
   2. trans potassiumdiaquadioxalatochromate(II) dihydrate
   3. trithioureacopper(I)chloride dihydrate
   4. hexathiourealead(II)nitrate
   5. pentaamminenitritocobalt(III) nitrate
   6. hexaamminecobalt(III)chloride
   7. aquapentamminecobalt(III)chloride
   8. pentakisthioureadicopper(I) nitrate trihydrate

2. Quantitative estimation of a mixture containing two metal ions (Volumetric and Gravimetric estimations).

   1. Estimation of Cu$^{2+}$ and Ni$^{2+}$ ions.
   2. Estimation of Cu$^{2+}$ and Zn$^{2+}$ ions.
   3. Estimation of Fe$^{2+}$ and Cu$^{2+}$ ions.
   4. Estimation of Fe$^{2+}$ and Ni$^{2+}$ ions.
   5. Estimation of Ca$^{2+}$ and Mg$^{2+}$ ions.
   6. Estimation of Ca$^{2+}$ and Ba$^{2+}$ ions.
3. Analysis of ores and alloys (Course work only).

Note: For examination, a mixture may be given from which one cation is to be estimated volumetrically and the other gravimetrically.

References


1. Quantitative Analysis
   i. Estimation of ethyl methyl ketone
   ii. Estimation of glucose-Lane Eynon method
   iii. Estimation of glucose- Bertrand’s method
   iv. Determination of saponification value of oil.
   v. Estimation of iodine value of oil.

2. Preparation of Organic compounds (Double stage)
   i. Preparation of p-bromoaniline from acetanilide
   ii. Preparation of m-nitrobenzoic acid from ethylbenzoate
   iii. Preparation of p-nitro aniline from acetanilide
   iv. Preparation of 1,3,5-tribromobenzene from aniline
   v. Preparation of benzpinacolone from benzophenone
Each student is expected to submit recrystallised samples of the preparation during her regular practical for evaluation during practical examinations.

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3. Course work
i. Estimation of phenol
ii. Estimation of aniline.
iii. Estimation of Ascorbic acid

References

1. Potentiometry
   1. Determination of solubility product of sparingly soluble salts.
   2. Determination of dissociation constant of a weak acid.

3. Potentiometric titrations
a) Redox titrations
   i) Fe$^{2+}$ Vs Cr$_2$O$_7^{2-}$
   ii) I$^-$ Vs MnO$_4^-$
   iii) Fe$^{2+}$ Vs Ce$^{2+}$

b) Precipitation titrations
   i) Cl$^-$ Vs AgNO$_3$
   ii) I$^-$ Vs AgNO$_3$
   iii) Mixture of Cl$^-$ and I$^-$ Vs AgNO$_3$

4. Spectroscopy
   a) Verification of Beer-Lambert’s law. Determination of [Mn$^{2+}$] and [Cr$^{3+}$] by using UV-Visible spectrophotometer.

5. Adsorption:
   Adsorption of acetic acid/oxalic acid on activated charcoal-verification of Freundlich isotherm-determination of unknown concentration.

6. Conductivity method
   Study of Kinetics of ester hydrolysis and comparison of acid strength by conductivity method.

References
5. Yadav. J.P, Physical Chemistry Practicals
Inorganic Chemistry

2. Main group elements and their compounds: Allotropy, synthesis, structure and bonding, industrial importance of the compounds.
3. Transition elements and coordination compounds: reaction mechanisms.
4. Organometallics in homogeneous catalysis.
5. Cages and metal clusters.
7. Characterisation of inorganic compounds by NMR, EPR, NQR, and microscopic techniques.
8. Nuclear chemistry: nuclear reactions, fission and fusion, radio-analytical techniques and activation analysis.

**Organic Chemistry**

1. Concepts in organic synthesis: Retrosynthesis, disconnection, synthons, linear and convergent synthesis, umpolung of reactivity and protecting groups.
4. Synthesis and reactivity of common heterocyclic compounds containing one or two heteroatoms (O, N, S).
6. Structure determination of organic compounds by IR, UV-Vis, $^1$H & $^{13}$C NMR and Mass spectroscopic techniques.

**Physical Chemistry**

1. Molecular spectroscopy: Rotational and vibrational spectra of diatomic molecules; electronic spectra; IR and Raman activities – selection rules; basic principles of magnetic resonance.
3. Chemical kinetics: Empirical rate laws and temperature dependence; complex reactions; steady state approximation; determination of reaction mechanisms; collision and transition state theories of rate constants; unimolecular reactions; enzyme kinetics; salt effects; homogeneous catalysis; photochemical reactions.
4. Colloids and surfaces: Stability and properties of colloids; isotherms and surface area; heterogeneous catalysis.
5. Solid state: Crystal structures; Bragg’s law and applications; band structure of solids.