I SEMESTER

CH 7112: INORGANIC CHEMISTRY – I

1. CHEMICAL BONDING


2. CHEMISTRY OF THE MAIN GROUP ELEMENTS


Boranes- Classification, preparation of higher boranes by Stock’s method and pyrolysis of diborane, reactions of diboranes with Lewis bases- symmetric and unsymmetric cleavage , types of bonds in higher boranes- the styx number, derivation of the number of 2-centre and 3- centre bonds in boranes. Wades rule as applied to boranes. Geometrical and Lipscomb’s semitopological structures of B$_3$H$_{10}$, B$_4$H$_9$, B$_3$H$_{11}$, B$_5$H$_{10}$ and B$_{10}$H$_{14}$ .

Carboranes- classification, nomenclature, structures of CB$_3$H$_9$, C$_2$B$_4$H$_8$, C$_3$B$_3$H$_7$ and C$_6$B$_2$H$_6$.

Metallocarboranes – Preparation from 1,2-dicarba-closo-dodecaborane, sandwich structure.

Borazines- Preparation, properties, structure. Difference in chemical properties between borazine and benzene, borazine derivatives ( N& B substituted). Preparation of boron nitride.

Phosphazenes-Classification, Cyclophosphazenes-(NPCl$_2$)$_3$ and (NPCl$_2$)$_4$- preparation and structure, Linear polyphosphazenes- preparation and applications.

Sulphur-nitrogen compounds- Preparation and structures of S$_4$N$_4$ and S$_2$N$_2$ , (SN)$_n$,S$_{11}$N$_2$, S$_{15}$N$_2$, S$_{16}$N$_2$, S$_5$N$_6$

Peroxo compounds of boron, carbon and sulphur.

Silicates: classification and structures of ortho, pyro, chain, cyclic, sheet and three dimensional silicates, silica gel, isomorphous replacement, aluminosilicates and their types .

Graphitic compounds – intercalation compounds with heavier alkali metals, halides, oxides, oxygen and fluorine, graphite oxides.
Condensed phosphates – linear polyphosphates, long chain polyphosphates and metaphosphates
Polyhalides – X\textsubscript{Y\textsuperscript{n}} and I\textsubscript{x} types.

3. ACIDS, BASES AND SOLVENTS  10 hrs

Review of acid-base concepts– Bronsted, Lewis and solvent system definitions of acids and bases,
Factors affecting strengths of hydracids, oxoacids and Lewis acids and bases, Drago-Wayland
equation for Lewis acid-base interactions.

HSAB concept- Pearson principle, Theories of hardness and softness. Bronsted acid-base strength
verses hardness and softness, symbiosis in Lewis acid-base interactions, applications and
limitations of HSAB concept.

Non-aqueous media – Classification of solvents, levelling effect, Acid-base reactions in HF, BrF\textsubscript{3},
N\textsubscript{2}O\textsubscript{4} and molten salts, super acids- Hammet acidity function

REFERENCES

1. Inorganic Chemistry – Principles of Structure and Reactivity, 4\textsuperscript{th} edition, J.E. Huheey, E.A.
1. STRUCTURE & REACTIVITY 6 hrs
Resonance, field effects, hyperconjugation, steric effects, steric inhibition of resonance. Quantitative treatment of field and resonance effects – Hammett and Taft treatments.

2. REACTION MECHANISMS 9 hrs

3. STEREOCHEMISTRY 17 hrs

4. ALIPHATIC NUCLEOPHILIC SUBSTITUTION 11 hrs

5. ELIMINATION REACTIONS 6 hrs
The E2, E1, E1cB and E2C mechanisms and the spectrum of elimination mechanisms. Regioselectivity and stereochemistry of E2 and E1 reactions; effect of substrate structure, base,

6. AROMATIC SUBSTITUTION

11 hrs

Resonance and molecular orbital interpretation of aromaticity; aromaticity in benzenoid and non-benzenoid systems and ions.

Electrophilic substitution: Mechanistic interpretations of second substitution, orientation and reactivity, the ortho/para ratio, ipso attack, third substitution, orientation and reactivity of other ring systems like polycyclic aromatic hydrocarbons, heterocyclic systems (5 and 6 membered rings containing one and two hetero atoms), diazonium coupling, Vilsmeir reaction, Gattermann-Koch reaction.

Nucleophilic substitution: S_NAr, S_N1, benzyne and S_RN1 mechanisms.

Reactivity – effect of substrate structure, leaving group and nucleophile; reactivity of heterocyclic systems containing 1 and 2 hetero atoms. The von Richter and Smiles rearrangements.

REFERENCES:

1. CLASSICAL MECHANICS TO QUANTUM MECHANICS  
Expression for wave motion: Concept of progressive and stationary waves.
Expression for stationary wave. (No derivation) Time dependent and Time independent Schrodinger equation and their relations between them with respect to their solutions.
Operators and their properties. Normalization, orthogonality, and orthonormality of wave functions, eigenvalues and eigenfunctions. Postulates of quantum mechanics with explanations for each postulates.

2. SOLUTIONS OF SCHRODINGER WAVE EQUATION TO SIMPLE SYSTEMS  
For a free particle, Particle on a ring (No derivation only solutions) and particle in a 3D boxes quantum mechanical degeneracy (Cubic Box), quantization effects and electronic spectra of atoms. Quantum Mechanical Tunneling (no derivation) (final equation should be given for finite barrier height) and its application to various systems.
Harmonic oscillator-quantum mechanical treatment- solution of the equation, eigenfunctions and eigenvalues and their plots. Zero point energy and its quantum mechanical significance.
Rigid rotator-quantum mechanical treatment-eigenfunction and eigenvalues of the angular momentum-transition probabilities. Wave mechanical treatment of hydrogen atom-Schrodinger equation in spherical polar coordinates and its solution, the hydrogen- atom-like wave functions.

3. LIMITATION OF SCHRODINGER WAVE EQUATION: APPROXIMATE METHODS  
Variation Principle and its proof and its application to the ground state of the helium atom.
Perturbation Theory (Time-independent )- First order perturbation theory to the ground state of helium atom - comparison of variation results and perturbation results. Symmetric and antisymmetric wave functions—ground and excited states of helium, spin orbitals and Pauli principle, Slater determinants, expression for Slaters’s orbitals for 1s, 2s, 3s,and 3d orbitals (No derivation). Effective nuclear charge based on Slater’s rules. SCF method Introduction to abinitio methods. ( Some Packages to be mentioned foe calculations)

4. THEORY OF ANGULAR MOMENTUM  
Generalized linear and angular momenta; quantum mechanical definition of angular momentum, spin angular momentum, addition of angular momenta. Ladder operators–Rising and Lowering of eigen values-commutative and non-commutative Ladder Operators. Terms, Term Symbols and Molecular Symbols (only representation), spin-orbit interaction, atomic levels, spin multiplicity, L-S coupling (Russel –Saunders-Coupling), and j-j coupling, Hund’s rule of maximum stability.
5. CHEMICAL BONDING

Huckel MO treatment for simple systems - ethylene, butadiene, cyclobutadiene, cyclopropenyl systems, cyclobutadiene.

6. ELECTROCHEMISTRY—I

Debye-Huckel theory of ion-ion interaction, Debye –Huckel limiting law Debye-Huckel equation for appreciable concentration, Hückel and Bronsted equations.
Qualitative verification of the Debye-Huckel equation, ion association-ion pairs and triple ions and conductance minima.

7. ELECTROCHEMISTRY – II

The electrified interface—Surface excess, interfacial tension and its determination, Electrocapillarly curves, Thermodynamics of electrified interface—Lippmann equation, Determination of the electrical capacitance of the interface, Determination of surface excess.
Structure of electrical double layer—Helmholtz-Pern model, Gouy-Chapmann diffuse charge model and Stern model
The structure of the semiconductor-electrolyte interface—comparison between semiconductor and electrolytic solutions, The Garrett-Brattain space charge, differential capacity due to the space charge
Electrodics—Electron transfer under an interfacial electric field, equilibrium and exchange current density, overpotential—dependence of current density on overpotential, The Butler-Volmer equation and its special cases, the symmetry factor, influence of current density, pH and temperature on overvoltage, theories of overvoltage—Bubble formation as the slow process, combination of atoms as the slow process, ion discharge as the slow process and proton transfer as the slow process

8. ELECTROCHEMISTRY – III

Corrosion—local cell theory of corrosion, mechanism of corrosion of ultrapure metals, cathodic reaction in corrosion, thermodynamics and the stability of metals, corrosion in the absence of oxide films, corrosion in terms of Evans diagrams, common example of corrosion or types of corrosion.

REFERENCES

4. Modern electrochemistry 2B by John O’M Bockris , AKN Reddy and others
5. An introduction to Electrochemistry by Samuel Glasstone.
1. GROUP THEORY IN CHEMISTRY

Symmetry elements and symmetry operations, Definition of groups and subgroups, simple theorems in group theory and group multiplication tables. Conjugate relationships, classes of operations and order of a group. Symmetries with multiple higher order axis-symmetry operations in tetrahedral and octahedral point groups. Improper axis of symmetry-operations generated by $S_n$ axis, symmetry conditions for molecular chirality. Point groups, Schoenflies notations for point groups, representation of symmetry operations as matrices, reducible and irreducible representations, characters of representations, great orthogonality theorem (without proof) and its corollaries, properties of irreducible representations. Mulliken’s symbols for irreducible representations. Character tables-character tables of $C_{nv}$, $C_{nh}$ $D_{nh}$ and $C_n$ point groups (derivation of character table only for $C_{nv}$ point group). Applications of character tables in vibrational, electronic spectroscopy and crystalfield splitting.

Group theory & Quantum mechanics: wave functions as basis for irreducible representations, direct products, time dependent perturbation theory, transition moment integral and selection rules in spectroscopy.

2. MICROWAVE SPECTROSCOPY

Rotations of molecules, rigid diatomic molecule-rotational energy expression, energy level diagram, selection rules, expression for the energies of spectral lines, computation of intensities, effect of isotopic substitution, centrifugal distortion and the spectrum of a non-rigid rotor. Rotational spectra of polyatomic molecules- linear, and symmetric top molecules. Calculation of bond length of diatomic and linear triatomic molecules. Stark effect.

3. Infrared Spectroscopy


4. RAMAN SPECTROSCOPY

Classical theory of the Raman effect, polarizability as a tensor, polarizability ellipsoids, quantum theory of Raman effect, pure rotational Raman spectra of linear and symmetric top molecules, vibrational Raman spectra, Raman activity of vibrations, rule of mutual exclusion, rotational fine
structure – O and S branches, Polarization of Raman scattered photons, Structure determination from Raman and IR spectroscopy- AB₂ and AB₃ molecules. Techniques and instrumentation.

5. ELECTRON SPECTROSCOPY 13 hrs

Born – Oppenheimer approximation, vibrational coarse structure, intensities by Frank-Condon principle, Dissociation energy, rotational fine structure, Fortrat diagram, Pre-dissociation. Electronic structure of diatomic molecules-basic results of MO theory, Classification of states by electronic angular momentum, molecular orbitals, selection rules, spectra of singlet and triplet molecular hydrogen. Application of group theory and HMO method in the spectra of CH₂ = CH₂, Butadienes and Benzene. Decay of excited states-radiative (fluorescence and phosphorescence) and non-radiative decay, internal conversion.

REFERENCES


CH 7P1: PRACTICAL I – INORGANIC CHEMISTRY

I. QUALITATIVE ANALYSIS: 12 Units

Semi-micro qualitative analysis of a mixture containing two common cations and anions each and one of the less familiar elements: W, Mo, Ce, Th, Zr, V, U and Li.

II. QUANTITATIVE ANALYSIS: 8 Units

Volumetric and gravimetric determination of the following mixtures:
(a) Iron and aluminium (b) Copper and nickel (c) Copper and iron (d) Copper and zinc (e) Barium and calcium

REFERENCES


CH 7P2: PRACTICAL II: ORGANIC CHEMISTRY

I. QUALITATIVE ANALYSIS: 12 Units

Separation, systematic analysis and identification of organic compounds in a binary mixture.

II. QUANTITATIVE ANALYSIS: 8 units

1. Determination of equivalent weight of carboxylic acids.
2. Saponification value of oil/fat.
3. Estimation of glucose.
4. Estimation of phenols by acylation method.
5. Iodine value oil/fat.
8. Estimation of carbonyl group by hydroxylamine-pyridine method.

REFERENCES

II SEMESTER

CH 8112: INORGANIC CHEMISTRY – II 60 HOURS

1. METAL – LIGAND BONDING 13 hrs

Review of basic concepts of co-ordination chemistry. Stereochemistry of complexes with coordination Nos. 2 to 12, crystal field splitting in octahedral, tetrahedral, square planar, square pyramidal and trigonal bipyramidal ligand fields, structural and thermodynamic effects of crystal field splitting- octahedral ionic radii, Jahn – Teller distortion in metal complexes and metal chelates, hydration and lattice energies, site preferences in spinels, octahedral versus tetrahedral co-ordination, Irving-William stability order; spectrochemical series, limitations of crystal field theory, Evidences for metal – ligand orbital overlap from ESR, NMR, electronic spectra and antiferromagnetic coupling, nephelauxetic effect and nephelauxetic series, LFT (ACFT), , MO theory, MO diagrams of octahedral complexes (including \(\pi\)-bonding).

2. METAL – LIGAND EQUILIBRIA IN SOLUTION 13 hrs

Step-wise and overall formation constants and their relationships, trends in step-wise formation constants and exceptions to the trends, factors affecting the stability of metal complexes with reference to the nature of the metal ion and ligand, chelate and macrocyclic effects and their thermodynamic origin, Kinetic and thermodynamic stability of metal complexes.

Determination of composition and stability constants of complexes by spectrophotometry (Job’s method) and potentiometry, stepwise stability constants by Bjerrum’s pH-titration method, Rossoiti and Rossoiti method, Bjerrum,s spectrophotometric method and ion-exchange method.

3. STRUCTURE AND BONDING IN METAL COMPLEXES 15 hrs

Hydride, dihydrogen, isocyanide complexes; mononuclear and dinuclear metal carbonyls and metal carbonyl clusters, Wades rules as applied to metal carbonyl clusters, Nitrosyl, dinitrogen and tertiary phosphine complexes, ligand cone angle in phosphine complexes; complexes containing SO\(_2\) and CO\(_2\).

Metal complexes as liquid crystals, stereochemical non-rigidity, Stereoisomerism – chirality, optical activity, CD, ORD, Cotton effect and absolute configurations.

Supramolecular chemistry – molecular recognition and self assembly, examples of simple supramolecular systems, metal ions as templates.

4. ELECTRONIC SPECTRA OF TRANSITION METAL COMPLEXES 10 hrs

Spectroscopic ground states, selection rules, term symbols for d\(^n\) ions, Racah parameters, Orgel and Tanabe-Sugano diagrams, Correlation diagram of d\(^2\) configuration, spectra of 3d metal aqua complexes of trivalent V, Cr, divalent Mn, Co, Ni and [CoCl\(_4\)]\(^{2-}\), calculation of Dq, B and \(\beta\) parameters, charge transfer spectra, spectral behaviour of lanthanide ions.

5. MAGNETIC PROPERTIES OF METAL COMPLEXES 9 hrs
Origin and types of magnetic behaviour- diamagnetism, paramagnetism, ferro and antiferromagnetism, magnetic susceptibility and its measurement by the Guoy method, temperature dependence of magnetism – Curie and Curie-Weiss laws, types of paramagnetic behaviour – spin-orbit coupling, magnetic behaviour of lanthanide ions, quenching of orbital contribution and spin only behaviour (explanation based on A, E and T terms), applications of magnetic data, temperature independent paramagnetism, spin-cross over.

REFERENCES

CH 8212: ORGANIC CHEMISTRY – II  

1. ADDITION REACTIONS  
Addition to carbon-carbon multiple bonds: Mechanisms of electrophilic addition reactions; regioselectivity and stereoselectivity; hydrogenation and hydroboration; Nucleophilic addition; Michael addition.
Addition to carbon-hetero atom multiple bonds: Mechanisms of metal hydride reduction of carbonyl compounds, acids, esters and nitriles; addition of Grignard reagents and organolithium reagents to carbonyl compounds; mechanisms of formation of hydrates, acetals, oximes and hydrazones on carbonyl compounds, Wittig reaction.

2. ALIPHATIC ELECTROPHILIC SUBSTITUTION  
S₂, S₁ and Sᵢ mechanisms, hydrogen exchange, migration of double bonds, halogenation of aldehydes, ketones and acids, haloform reaction; aliphatic diazonium coupling; nitrosoation at carbon and nitrogen, diazo transfer reaction, carbene and nitrene insertion, decaboxylation of aliphatic acids; Haller-Bauer reaction.

3. REARRANGEMENTS  
Carbon to Carbon Migrations: Wagner-Meerwein, Pinacol-Pinacolone, Benzil-Benzilic acid, Favorskii and Neber rearrangements; Arndt-Eistert synthesis; expansion and contraction of rings.
Carbon to Nitrogen Migrations: Hofmann, Curtius, Lossen, Schmidt and Beckmann rearrangements.
Nitrogen/Oxygen/Sulfur to Carbon Migrations: Stevens and Wittig rearrangements
Carbon to Oxygen Migrations: Baeyer-Villiger rearrangement
Non-1,2 Rearrangements: Fischer indole synthesis, benzidine rearrangement.

4. PERICYCLIC REACTIONS  
Molecular orbital symmetry; frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system; classification of pericyclic reactions. Woodward – Hoffmann correlation diagrams; FMO and transition state aromaticity approach; selection rules.
Electro cyclic reactions: conrotatory and disrotatory motions; 4n, 4n+2 and allyl systems.
Cycloadditions: suprafacial and antarafacial additions, 4n and 4n+2 systems; [2+2] addition of ketenes, 1,3-dipolar cycloadditions and chelotropic reactions.
Sigmatropic rearrangements: suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 1,3-, 1,5- and 3,3-sigmatropic rearrangements;
Cope and Claisen rearrangements; Sommelet-Hauser rearrangement; Ene reaction.
5. FREE RADICAL REACTIONS AND PHOTOCHEMISTRY  
10 hrs

Generation of free radicals – thermolysis and photolysis of peroxides, peresters and azo compounds, hydrogen abstraction, chain process.
Addition, substitution, elimination, rearrangement and electron transfer reactions; use of free radicals in organic synthesis.
General principles of photochemistry: singlet and triplet state-differences in reactivity, photosensitisation; quantum efficiency, quantum and chemical yields.
Photochemical reactions: Cis-trans isomerisation, di-\(\pi\)-methane rearrangement; Norish type I and type II cleavages; Paterno-Buchi reaction; photoreduction of ketones; photochemistry of arenes.

REFERENCES

8. Introduction to Organic Photochemistry, J.D. Coyle, John Wiley & Sons.
CH 8312: PHYSICAL CHEMISTRY – II  

1. NON-EQUILIBRIUM THERMODYNAMICS  
   Irreversible processes and Steady State. Conservation of mass and energy in open systems.  
   Entropy production – heat flow in chemical reactions.  
   Entropy production and flow in open systems  
   Rate of entropy production – generalized forces and fluxes. Phenomenological equations.  
   Onsagar Reciprocity relation – Electro kinetic and thermoelectric phenomena.  

2. REACTION KINETICS  
   Theories of Reaction rates – Review of Arrhenius and Bimolecular Collision theories. Activated  
   complex theory – derivation. Thermodynamic method and partition function method)  
   Reactions in solutions – factors affecting reaction rates in solution  
   Diffusion controlled reactions – influence of solvation, internal pressure and dielectric constant on  
   reaction rates. Ionic reactions – double sphere model for effect of solvent on ionic reaction rates.  
   Primary and secondary salt effects.  
   Kinetic and thermodynamic control of reactions.  
   Unimolecular Reactions – Quantitative treatment of Lindemann and Hinshelwood theories.  
   Qualitative treatment of RRK and RRKM theories. Comparison of these theories.  
   Kinetics of Chain reactions – H₂ and O₂ reaction – Explosion limits. Dehydrogenation of ethane,  
   pyrolysis of acetaldehyde – Rice – Herzfeld mechanisms.  
   Kinetics of fast reactions – Features of fast reactions. Study of fast reactions by flow method,  
   relaxation method, flash photolysis and NMR method.  

POLYMERISATION AND KINETICS OF POLYMERIZATION  
   Kinetics and mechanism of free radical polymerization, kinetic chain length and chain transfer.  
   Kinetics of cationic and anionic polymerization.  
   Co polymerization – free radical mechanism and copolymer composition  

CHEMICAL THERMODYNAMICS  
   Introduction –Review of thermodynamic laws. Thermodynamics of open systems-- Partial molar  
   quantities, Chemical potential, effect of temperature and pressure, Gibbs-Duhem equation,  
   chemical potential of a pure substance, fugacity and its determination—graphical and  
   compressibility factor, chemical potential in ideal gas mixture, partial molar volume and its  
   determination-method of intercept, thermodynamics of mixing;  
   Activity and activitycoefficients, and determination by solubility and emf methods .Chemical  
   potential in ideal solution, Mixing properties of ideal liquid solution, Henry’s law; Raoult’s law;
Validity of Raoult’s and Henry’s law-thermodynamic deduction; Chemical potential of non-ideal solutions; thermodynamic functions of mixing of non-ideal solutions. Excess thermodynamic functions; Gibbs-Duhem-Margules equation; Application of Gibbs-Duhem-Margules equation-Konovalov’s first law and second law.

**STATISTICAL THERMODYNAMICS**

Different types of ensembles, ensemble averaging, Stirling’s approximation, distribution law (Boltzmann statistics), partition function and thermodynamic parameters—energy, heat capacity, free energy, chemical potential, pressure entropy and equilibrium constant translational partition function, monoatomic gases, State functions in terms of partition function—energy, pressure, Sackur-tetpde equation, free energy functions, rotational partition function and vibrational partition function, electronic partition function, the partition function of system—Thermodynamic properties of molecules from partition function of system, Application of statistical thermodynamics: Equipartition theorem, heat capacity behaviour of crystals.Introduction to quantum statistics: Distribution law for fermions (Fermi-Dirac statistics) and forbosons (Bose-Einstein statistics).

**References:**

5. Principles of Physical Chemistry, Late B.R. Puri, L.R.Sharma and M.S. Pathania
CH 8409: SPECTROSCOPIC METHODS OF ANALYSIS – II

60 Hours

1. UV AND VISIBLE SPECTROSCOPY
7 hrs

2. INFRARED SPECTROSCOPY
11 hrs
Technique and instrumentation, Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides). Effect of solvent and hydrogen bonding on the vibrational frequencies in alcohols. IR spectra of metal complexes involving ammine, aquo, hydroxo and carbonyl ligands.

3. NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY
15 hrs

4. CARBON–13 NMR SPECTROSCOPY
4 hrs
5. ADVANCED NMR TECHNIQUES

Pulse sequences, spins and magnetization vectors. The DEPT experiment. Determining the number of attached hydrogens.

Introduction to two – dimensional spectroscopic methods. The COSY technique. An overview of the Cosy Experiment.

6. MASS SPECTROMETRY


7. ELECTRON SPIN RESONANCE SPECTROSCOPY

Theoretical principles, ‘g’ factor, hyperfine splitting, Illustration of hyperfine splitting using examples, cyclopentadienyl radical, radical anions of benzene, naphthalene, p-benzo semiquinone. Isotropic spectra of some transition metal complexes and compounds, bis(salicylaldimine)Cu(II), [VO(glycolate)2]−2, [(NH3)5Co-O-O-Co(NH3)5]+, Mn2+ as a substitutional impurity in MgO.

8. MOSSBAUER SPECTROSCOPY

Mossbauer effect and Mossbauer nuclei, isomer shift, quadrupole splitting and magnetic hyperfine interactions, elucidation of electronic structures of Fe(II) and Fe(III) systems

References:

CH 8P1: Practical III – Physical Chemistry

**Chemical Kinetics**
1. Determination of the velocity constant, catalytic coefficient, temperature coefficient, energy of activation and Arrhenius parameters for the acid hydrolysis of an ester.
2. Evaluation of Arrhenius parameters for the reaction between potassium persulphate and potassium iodide (1 order)
3. Kinetics of reaction between \( \text{K}_2\text{S}_2\text{O}_8 \) and KI (salt effect).

**Colorimetry**
4. Determination of the Fe/ Cu in different matrices by colorimetry.
5. Determination of percentage titration error of ferrous ammonium sulphate with potassium permanganate or an acid base titration colorimetrically.
6. Kinetics of reaction between \( \text{K}_2\text{S}_2\text{O}_8 \) – KI colorimetrically.
8. Simultaneous estimation of Mn and Cr by spectrophotometric method

**Partial Molal Volume**
10. Determination of PMV by apparent molar volume method, NaCl-H₂O system.

**Conductivity**
11. Titration of a mixture of strong and weak acids and salt against a strong base.
12. Determination of dissociation constant of a weak acid or weak base by conductometry.
14. Estimation of weak acid like phenol
15. Estimation of urea by enzyme hydrolysis using conductance method

**Potentiometry**
17. Titration of silver nitrate against potassium chloride/bromide/ iodide, calculation of the solubility product of silver chloride/bromide/iodide.
18. Titration of a weak acid against a strong base using quinhydrone electrode and calculation of pKa values of the weak acid.
19. Titration of a mixture of HCl and CH₃COOH potentiometrically and the determination of the composition of the mixture.
20. Estimation of a weak acid in a given sample using sodium hydroxide by differential potentiometry.
21. Determination of dissociation constant of phosphoric acid by potentiometric titrations
23. Evaluation of I order rate constant by potentiometry.
24. Determination of activity coefficient of an electrolyte by potentiometry.
25. Construction and application of liquid membrane electrode.

References

CH 8P2: Practical IV – Synthesis and Characterization of Compounds

Inorganic Compounds:
1. Preparation and quantitative analysis of hexamminecobalt(III) chloride – 2 sessions.
2. Preparation of potassium trioxalatoferrate(III) trihydrate and its characterization by quantitative analysis and IR studies– 2 sessions.
3. Preparation of a variety of complexes (5 Nos.) and their characterization by UV-Visible and IR techniques– 4 sessions.
4. Preparation of a nano material and their characterization by UV spectroscopy (band gap) and XRD (particle size) – 2 sessions.
5. Synthesis of spinels and its characterization by XRD studies – 2 sessions.

**Organic Compounds:**
6. Preparation of anthrone from anthracene.
7. Preparation of anthranilic acid from phthalic acid.
8. Preparation of benzanilide from benzophenone.
9. Preparation of benzilic acid from benzoin.
10. Preparation of NBS from succinic acid and its application in allylic bromination.
12. Resolution of a racemic mixture by fractional crystallization
13. Preparation of an organic compound (one step preparation) by 2 or 3 different methods and comparison/evaluation of the methods with respect to the following parameters:
   (i) Ease of preparation, problems in handling chemicals, toxicity and flammability of chemicals
   (ii) Yield and cost effectiveness
   (iii) Product purity/quality
   (iv) Environmental costing (from the point of view of Green chemistry)
Characterisation of the organic compounds (experiments 8 –14) by: TLC, column liquid chromatography, fractional crystallization, UV, IR and NMR spectroscopic techniques.

**References**
2. Practical Inorganic Chemistry, Marr and Rocket
III SEMESTER

CH 9112: PRINCIPLES OF CHEMICAL ANALYSIS 60 HOURS

1. ERRORS IN CHEMICAL ANALYSIS, STATISTICAL DATA TREATMENT AND EVALUATION 10 hrs

Significant Figures: Rounding of numerical expression. Addition and subtraction; multiplication and division- numerical problems on above concepts.

Errors: Some important terms Replicate, outlier, Accuracy and precision. Errors affecting precision and accuracy; Systematic errors: Sources and types of systematic errors with examples. Ways of expressing accuracy: Absolute and relative errors; Constant and proportional errors. Detection of systematic instrument and personal errors. Identification and compensation of systematic method errors. Terms used to describe precision of a set of replicate measurements. Mean and median. Problems. Deviation and average deviation from the mean.

Statistical treatment of random errors; Spread, sample and population; sample mean and population mean. Standard deviation and variance of Population; area under Gaussian curve
Sample standard deviation, sample variance, standard error of the mean, Relative standard deviation, coefficient of variation, pooled standard deviation. Confidence interval; Problems.

Student - t statistics; Significance testing, null hypothesis, one and two tailed significance tests. Comparing measured results with a known value.


Method validation. Determination limits, calibration sensitivity. Limit of quantization and Linear dynamic range.

2. ACID – BASE TITRATIONS 5 hrs

Basic principles: K\textsubscript{w}, pH scale, dissociation of acids and bases Titration curves for mono functional acids and bases, pH calculations, theory of indicators,. Titration curves for di, tri and polybasic acids ,polyamines and amino acid systems. Fractions of phosphoric acid species as a function of pH.
3. REDOX TITRATIONS

Nernst equation, Standard & formal potentials. Titration curves, end point signals, Indicators, criteria for the selection of indicators. Feasibility of redox titration. Titration of multicomponent system. Adjustment of analyte’s oxidation state. Applications: Oxidants such as Permanganate, dichromate, Ce (IV), bromate, Iodates Reductants such as Ferrous ammonium sulphate and Ascobic acid.

Karl-Fischer titrations: Stoichiometry of the reaction, preparation of the reagent, titration method, standardization of the reagent using water-in-methanol, determination of water in samples, interference and their elimination, application to quantitative analysis of some organic compounds- alcohols, carboxylic acids, acid anhydrides and carbonyl compounds.

4. PRECIPITATION TITRATIONS


5. COMPLEXOMETRIC TITRATIONS

Complexometric titrations with particular reference to EDTA titrations, suitability of polydentate ligands as titrants, expressions for the different forms of EDTA in solution as a function of pH, conditional stability constants, derivation of titration curve, effect of pH and second complexing agent on the conditional stability constant and titration curve. Selectivity by pH control, masking and demasking, metal ion indicators, types of EDTA titrations, titrations involving monodentate ligands.

6. NON-AQUEOUS TITRATIONS

Acid–base titrations in non-aqueous solvents- classification of solvents, leveling and differentiating solvents, acidic and basic titrants, methods of titration. Titrations in glacial acetic acid and ethylene diamine, applications of non-aqueous titrations.

7. GRAVIMETRIC ANALYSIS

Formation and treatment of precipitates, co-precipitation, post precipitation homogeneous precipitation, important precipitating agents and their significance in inorganic analysis
8. KINETIC METHODS OF ANALYSIS  
4 hrs
Rate laws, pseudo first order kinetics, types of kinetic methods, fixed time methods. Applications of catalytic and non-catalytic kinetic methods.

9. RADIOCHEMICAL TECHNIQUES  
5 hrs
Measurement of radioactivity, Principle, methodology and applications of isotope dilution analysis, Neutron activation analysis, PGNAA and principle of Radioimmunoassay.

10. ABSORPTION AND EMISSION TECHNIQUES  
7 hrs
Quantitative aspects of spectrochemical Measurements. Nephelometric and turbidimetric methods Instrumentation; turbidimetric titrations.
Molecular luminescence- Quantitative aspects of fluorescence. Fluorescence and structure, Effects of temperature, dissolved oxygen and solvent on quantum efficiency of fluorescence.
Atomic absorption methods- principle and Instrumentation (single and double beam) Light sources of AAS; atomization (flame and electrothermal) Interferences. Atomic emission method (AES) Plasma – DCP and ICP techniques; Advantages of plasma over flame.

11. THERMAL METHODS OF ANALYSIS  
2 hrs
Thermogravimetric analysis- Differential thermal analysis; differential scanning colorimetry- thermometric analysis.

References:
1. SOLVENT EXTRACTION  5 hrs
Partition coefficient-equation for batch extraction & multiple extraction, Extraction efficiency- pH effects, Extraction with metal chelator and crown ethers.

2. CHROMATOGRAPHY  6 hrs
Types of chromatography –Theoretical principles; Retention time, retention volume, adjusted retention time, relative retention, capacity factor (retention factor) –Relation between retention time and partition coefficient –Scaling up, scaling rules-Efficiency of separation, resolution -Ideal chromatographic peaks (Gaussian peak shape)- Factors for Resolution-diffusion, diffusion coefficient - Plate Height- Plate Height as a Measure of Column Efficiency-Number of theoretical plates-asymmetric peaks- Factors Affecting Resolution Band Spreading- van Deemter equation, Optimum Flow Rate, A Term – multiple paths, longitudinal diffusion, Mass Transport, Extra column contributions to zone broadening -advantages of open tubular columns- isotherms and the resulting band shapes.

3. GAS CHROMATOGRAPHY  7 hrs
Separation process in gas chromatography –schematic diagram-open tubular columns, Comparison with packed columns, Effect of column inner diameter and length of the column, choice of liquid stationary phase, chiral phases for separating optical isomers-molecular sieves as stationary phase-packed columns-Retention index-Temperature and pressure programming -Carrier gas-Guard columns and retention gaps-sample injections, split injection and split less injection, solvent trapping and cold trapping, on column injection- Detectors : thermal conductivity detector, flame ionisation detector, electron capture detector, Mention about other detectors like nitrogen phosphorous detector, flame photometric detector, photoionisation detector, sulphur chemiluminescence detector -GC-MS- Element specific plasma detectors. sample preparation-solid phase micro extraction, purge and trap, thermal desorption-Derivatisation in GC-Method development in GC.

4. HIGH-PERFORMANCE LIQUID CHROMATOGRPHY  8hrs
The chromatographic process-effect of small particles, scaling relation between columns, relation between number of theoretical plates and particle size, column pressure-The column, stationary phase, monolithic silica columns-Bonded stationary phases-solute column interactions-shape selectivity-The elution process, isocratic and gradient elution, selecting the separation mode, solvents, Maintaining symmetric band shape, dead volume – Injection and detection in HPLC, Detector characteristics, signal to noise ratio, detection limits, Linearity- Spectro photometric detectors, refractive index detector, Evaporative
Light scattering detector, Method development in reverse phase separation-Criteria for adequate separation-Optimisation with one solvent, optimization with two or three different solvents-choosing a stationary phase-Gradient separations- Dwell volume and Dwell time-developing a gradient separation. Chiral separation.- derivatives for HPLC.

5. LIQUID CHROMATOGRAPHIC METHODS 12hrs

Reversed phase chromatography for neutral samples. Reverse phase retention process-selectivity- Solvent type selectivity and column selectivity-isomer separations.

Normal phase Chromatography- Retention mechanism -solvent strength-use of TLC data for predicting NPC retention- Solvent type selectivity and column selectivity-isomer separations.

Ion Exchange chromatography- ion exchangers, resins-ion exchange selectivity, selectivity coefficient, Donnan Equilibrium- Conducting ion exchange chromatography, Gradient elution, Application of ion exchange.

Ion Chromatography-Suppressed ion –anion and Cation chromatography-Ion chromatography without suppression-detectors-Ion pair chromatography

Molecular exclusion chromatography-the elution equation, stationary phase, molecular mass determination.

Affinity chromatography.-Principle-Matrix, ligand, spacer arm-properties required for efficient and effective chromatographic matrix-partial structure of agarose-Types of ligands- need of spacer arm. -Immobilized metal affinity chromatography.

Hydrophilic interaction chromatography (HILIC).

Sample Preparation: 2 hrs

Statistics of sampling-choosing a sample size-choosing the number of replicates. dissolving samples for analysis., dissolving inorganic material, dissolving organic material, decomposition of organic substances, sample preparation techniques and derivatisation.

6. ELECTROANALYTICAL TECHNIQUES 20 hrs

Electrophoresis and Electrochromatography 3 hrs

General introduction to electrophoresis. Important terms- Basis of electrophoretic separation. Expression for distance traveled on application of electrode potential. Role of buffer in electrophoresis.

Capillary gel electrophoresis, capillary isoelectric focusing; capillary isotachophoresis. Capillary electrochromatography (basic principle) Micellar electrokinetic capillary electrophoresis.

**Ion Selective Electrodes**

4 hrs


**Voltammetric Techniques:**

13 hrs

References for separation techniques:


References for electroanalytical techniques:

## CH 9312: CHEMISTRY OF MATERIALS 60 HOURS

<table>
<thead>
<tr>
<th>Topic</th>
<th>Hours</th>
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<tbody>
<tr>
<td><strong>1. INTRODUCTION</strong></td>
<td>3 hrs</td>
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<tr>
<td>Nanodomine; properties of nanomaterials-optical, electrical, mechanical and redox properties</td>
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<tr>
<td><strong>2. SYNTHETIC STRATEGIES</strong></td>
<td>15 hrs</td>
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<tr>
<td>Principles and Preparation of bulk materials by precipitation (including co-precipitation, homogeneous precipitation), impregnation and hydrothermal synthesis.</td>
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<td>Preparation of nanoparticles</td>
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<td>Thin film deposition methods – pulsed laser deposition electrodeposition and chemical vapour deposition.</td>
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<td>Synthesis of organic-dispersible uniform magnetic nano particles.</td>
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<td><strong>3. SURFACE MODIFICATION AND FUNCTIONALIZATION OF METAL, METAL OXIDE AND SEMICONDUCTOR NANO PARTICLES, BIOLOGICAL APPLICATIONS</strong></td>
<td>4 hrs</td>
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<td><strong>4. NANOPARTICLES IN ENERGY STORAGE-BATTERIES, FUEL CELLS AND SUPER CAPACITORS</strong></td>
<td>3 hrs</td>
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<td><strong>5. NANO COMPOSITE MATERIALS</strong></td>
<td>4 hrs</td>
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<td>Metal-metal nanocomposites, metal-ceramic nanocomposites, ceramic-ceramic nanocomposites, polymer based nanocomposites- polymer-ceramic composites, inorganic-organic polymer nanocomposites, polymer-polymer nanocomposites.</td>
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<td><strong>6. NANO TOXICITY</strong></td>
<td>1 hr</td>
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<td><strong>7. STRUCTURE, SYNTHESIS, SPECIAL PROPERTIES (INCLUDING MODIFICATIONS) AND APPLICATION OF MATERIALS</strong></td>
<td>15 hrs</td>
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<td>Zeolites, zeotypes including ALPOS, SBM, MCM types, Heteropoly anions and acids; carbon nano tubes; graphenes; zirconia and modified zirconia, Layered solids (clays and DH), conducting polymers, fly ash.</td>
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<tr>
<td><strong>8. MATERIALS CHARACTERIZATION TECHNIQUES: PRINCIPLE, INSTRUMENTATION AND APPLICATIONS</strong></td>
<td>15 hrs</td>
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<tr>
<td>Electron microscopes, transmission electron microscopy (TEM), scanning electron microscopy (SEM), atomic force microscopy (AFM), photoelectron microscopy (PES)-</td>
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</tr>
</tbody>
</table>
XPS and Auger spectroscopy; particle induced X-ray emission technique (PIXE), adsorption isotherms and porosity determination; BET technique for surface area determination.

References:

3. The biomolecule-nanoparticle interface, Vincent M Rotello, Nanotoday, Vol 2, Number 3, June 2007
5. Recent advances in the liquid phase synthesis of inorganic nanoparticles, Chem. Review 2004, 104, 3893
10. Chemistry of nanomaterials: C.N.R Rao, Wiley VCH
1. ESSENTIAL AND TRACE ELEMENTS IN BIOLOGICAL SYSTEMS 3 hrs

2. METAL ION STORAGE AND TRANSPORT 6 hrs
Ferritin, transferrin, ceruloplasmin, siderophores. Transport and storage of dioxygen: hemoglobin, myoglobin, phenomenon of cooperativity, model systems (picket fence porphyrins), hemocyanin and hemerythrin.

3. TRANSPORT OF IONS ACROSS MEMBRANES 6 hrs
Thermodynamic treatment, active and passive transport, ionophores, Na⁺/K⁺ pump. Chemistry of vision and nerve conduction

4. ELECTRON TRANSPORT PROTEINS 6 hrs

5. ENZYMES 7 hrs
Mechanism of enzyme action. Examples of some typical enzyme mechanisms - chymotrypsin, lysozyme, Michaelis-Menten kinetics and derivation of the equation, modifications and extensions of Michaelis-Menten equation, significance of Michaelis-Menten parameters, graphical representation of data - Lineweaver-Burke and Eddie Hofstee plots, enzyme inhibition kinetics (competitive, non-competitive, uncompetitive and mixed) Non-productive binding, Competing substrates, Reversibility – Haldane Equation, Breakdown of Michaelis-Menten equation. Multisubstrate systems – brief description of different mechanisms (ordered, sequential and random

6. METALLOENZYMES 9 hrs
Non-reoxid enzymes – Carboxypeptidase A and Carbonic anhydrase, Redox enzymes- Superoxide dismutase (mono and binuclear) Peroxidase, Catalase, Cytochrome Oxidase, Cyt P₄₅₀, ascorbic acid oxidase, cobalamine, alcohol dehydrogenase.(Coordination environment around the metal and mechanism of action of each enzyme to be discussed)
7. COENZYMES
Structure and biological function of Coenzyme A, Thiamine pyrophosphate, Pyridoxal phosphate, NAD+, NADP+, FMN, FAD, Lipoic acid. Mechanism of reactions involving the above coenzymes (one representative mechanism for each).

8. BIOSYNTHESIS OF MACROMOLECULES

9. BIOENERGETICS

10. BIOPOLYMER INTERACTIONS
Electrostatic charges, Hydrophobic forces, Dispersion force interactions, various types of binding processes in biological systems.

References:
7. Organic Chemistry, Paula Bruice (Pearson)


CH 9P1: Practical V – Analysis of Inorganic and Biochemical Materials

**Experiments in Inorganic Chemistry**  
11 sessions

1. Estimation of metal acetates using perchloric acid in glacial acetic acid medium.
2. Analysis of steel (2 sessions)
3. Analysis of dolomite (2 sessions)
4. Analysis of Soil. (2 sessions)
5. Separation and estimation of mixture of metal ions by ion exchange chromatography. (2 sessions)
6. Determination of metal to ligand ratio by Job’s method.
7. Separation of Fe(III) ion by solvent extraction and titration.

**Experiments in Biochemistry**  
14 sessions

1. Estimation of rancidity in a sample of butter.
2. Estimation of BOD and COD of a sample.
3. Extraction of caffeine from tea leaves and characterization using IR, NMR and Mass spectrometer.
5. Estimation of sulphur drug using spectrophotometer.
8. Gel electrophoresis - separation of proteins. (2 sessions)
9. Agarose gel electrophoresis-separation of RNA/DNA
10. Separation, purification and characterization of protein from plant sample. (3 sessions)
11. Any other suitable experiments.

**References:**

CH 9P2: Practical VI – Instrumental Methods of Analysis
(Qualitative and Quantitative Methods)

GC Analysis
1. Qualitative identification of alcohols in a given mixture using gas chromatography.
2. Estimation of alcohols in a given mixture using gas chromatography.
4. Experiment number 3 will continue.
5. Analysis of mouth washes in a commercial sample
6. Effect of molecules on retention time in GC.

Atomic Absorption Spectroscopy
7. Estimation of iron in a given sample using atomic absorption spectroscopy. (no sample preparation.)
8. Estimation of lead in soil sample using atomic absorption spectroscopy. (with sample preparation.)
9. Experiment number 7 will continue.
10. Estimation of an alloy (Cu Zn and lead) Using atomic absorption spectroscopy. (with sample preparation.)
11. Experiment number 7 will continue.
12. Estimation of sodium by flame photometer.
UV-Visible Spectrophotometer
14. Estimation of a mixture of caffeine & benzoic acid by UV spectrophotometer.
15. Fe in pharmaceutical preparation.(with sample preparation)
16. Estimation of uranyl ion by solvent extraction and visible spectrophotometer.

Infra Red Spectroscopy
17. Determination of the purity of the commercial benzoic acid using compressed discs.

Electroanalytical Method
18. Estimation of copper in an alloy containing copper and lead by Electrogravimetric method.
19. Estimation of a mixture of chloride and iodide using potentiometric method
20. Estimation of ascorbic acid by voltametry.

Liquid Chromatography
22. Estimation of some organic compounds using HPLC.

Thin Layer Chromatography
23. Identification of phenols using TLC.
24. Identification of amino acids using TLC.
25. Preparation of TLC plates, separation of analgesics, identification and estimation by UV spectrophotometer (2 sessions)

Experiments Involving Kits
26. Affinity chromatography
27. Gel filtration chromatography.
28. Any other suitable experiments.

References:
IV SEMESTER

CH 0112: APPLIED ANALYSIS 60 Hours

1. BIOPOLYMERS 3 hrs
Determination of size, shape, molecular weight, hydrodynamic methods, sedimentation, diffusion, viscosity.

2. PROTEIN ANALYSIS 15 hrs
Protein Purification: Protein isolation, solubilities of proteins, chromatographic separations, electrophoresis and ultracentrifugation. Analysis and Determination of Protein Structure: Primary structure, protein modification, secondary structure, globular and fibrous proteins, tertiary structure, quaternary structure and prediction of protein structure; Techniques for study of biomolecules: MS (Maldi / Seldi ), Confocal microscopy, Microarrays, Flow Cytometry, Microcalorimetry, ELISA, RIA, FACS, Northern, Southern, Western blots, NMR, Electrophoresis, CD, ORD, X-Ray crystallography, DSC, TGA and DTA.

3. NUCLEIC ACID ANALYSIS 5 hrs

4. LIPID ANALYSIS 4 hrs
General composition of edible oils, qualitative tests for purity, estimation of rancidity, tests for common adulterants.

5. FOOD ANALYSIS 5 hrs
6. ANALYSIS OF DRUGS AND POISONS  5 hrs
Classification of drugs, Characterisation of common drugs: Analgesics-aspirin; Expectorants – Benadryl; Vitamins - vitamin C; Sedatives- diazepam; Antibiotics - penicillin, chloramphenicol; Cardiovascular – sorbitrate. Drugs of abuse - Analysis of narcotics (nicotine, morphine, heroin); Estimation of drug residues in biological samples. General discussion of poisons with special reference to mode of action of snake venom, cyanide, carbon monoxide. Estimation of cyanide, carbon monoxide and barbiturates.

7. CLINICAL CHEMISTRY  5 hrs
Blood analysis: serum electrolytes, serum proteins, blood glucose, blood urea nitrogen, uric acid, and blood gas analysis.
Enzyme analysis: Assay of alkaline phosphatases, isoenzymes of lactate dehydrogenase, aldolase,. Metal deficiency and disease; Estimation of calcium, iron, and copper.

8. POLLUTION ANALYSIS  10 hrs
Water Pollution: Objectives of analysis; Parameters of analysis: colour, turbidity, total solids, conductivity, acidity, alkalinity, hardness, chloride, sulphate, fluoride, silica, phosphates and different forms of nitrogen; Heavy metal pollution: public health significance of cadmium, chromium, copper, lead, zinc, manganese, mercury and arsenic, general survey of instrumental techniques for the analysis of heavy metals in aqueous systems.

9. SOIL ANALYSIS  4 hrs
Chemical properties of soil-types of soil colloids, types of clays and their swelling and adsorption properties, cation exchange capacity and its determination, acid soils-types of soil acidity, liming, measurement of pH and conductivity of soil- saline and alkaline soils, analysis of major constituents of soil-organic matter, nitrogen, sulphur, sodium, potassium and calcium.

10. RADIOACTIVE POLLUTION  4 hrs
Detection and monitoring of radioactive pollutants; Methods of safe disposal of radioactive wastes, dosimetry, analysis of data, advantages and restrictions of radiotracer experiments, safety aspects.
References:

10. Analysis of Food and Food Products, Morris Jacobs
CH 0212: ORGANOMETALLIC CHEMISTRY AND INORGANIC REACTION MECHANISMS

1. ORGANOMETALLIC COMPOUNDS
Classification based on the hapticity of ligands and the polarity of C-M bond, nomenclature of organometallic compounds, 16- and 18-electron rules, electron counting – covalent and ionic models, stability and decomposition pathways.

2. ORGANOMETALLIC COMPOUNDS OF MAIN GROUP ELEMENTS
Group trends; Synthesis, Structure and bonding in Li, Be, Mg and Al alkyls.

3. ORGANOMETALLIC COMPOUNDS OF TRANSITION METALS
Classification, structure, bonding, general methods of preparation and important classes of reactions of transition metal alkyls, carbenes and carbynes
Structure and bonding in transition metal complexes with dihapto to octahapto \( \pi \)-donor ligands-alkene, allyl, 1,3-butadiene, cyclopentadienyl, arene, cycloheptatrienyl and cyclooctatetraenyl complexes, metallocenes with special reference to ferrocene, cyclometallation and ring slippage reactions, activation of small molecules (CO and methane), Isolobal analogy and its applications.

4. ORGANOMETALLIC COMPOUNDS IN ORGANIC SYNTHESIS
General introduction. Greens rules. Use of iron and chromium carbonyls in the synthesis of aromatic compounds, rhodium complexes in hydrogenation, hydroformylation, decarbonylation reactions and Monsanto Acetic acid process. Palladium complexes in the synthesis of carbonyl compounds. Heck reaction, Wacker process. Use of zinc dialkyls, Grignard reagents, lithium alkyls, Gilman reagents (lithium dialkyl cuprates), (comparison with respect to reactivity) organoselenium, organoaluminium (including Zeigler Natta catalysis), organosilicon, organotin and organomercurials in organic synthesis.

5. INORGANIC REACTION MECHANISMS
Kinetic lability and inertness, classification of metal ions based on lability, types of nucleophilic substitution reactions, kinetics and mechanism of nucleophilic substitution in square planar and octahedral complexes- trans effect, ligand field effects and reaction rates, reaction rates influenced by acids and bases, \( S_n1CB \) mechanism; racemization and isomerization, mechanisms of redox reactions- outer sphere mechanism, Marcus equation for outer sphere cross reactions, excited state outer sphere electron transfer reactions, photochemical reactions of ruthenium complexes, inner sphere mechanism; oxidative addition and reductive elimination, migratory insertion, nucleophilic and electrophilic attack on coordinated ligands, template reactions.
References

Recall: aldol, knoevenagel, claisen condensations; wittig reaction, Diels-Alder reaction, Friedel-Crafts reaction, Michael addition, Chichibabin reaction and Alkylation of acetylides.

1. C-C & C-N BOND FORMING REACTIONS 13 hrs
Chemistry of enolates – E,Z geometry of enolates, kinetic vs thermodynamic control of enolates, stereoselective enolate reactions, alkylation of aldehydes, esters, nitriles; Enamines and Metalloenamines.
Mannich, Benzoin, Stobbe, Dieckmann, Darzen’s reaction, Henry reaction, Horner-Wordwoth-Emmons reaction and their selectivities; Mukaiyama reaction, Nazarov cyclization, Prins reaction, Noyori reaction.

2. SELECTIVE ORGANIC NAME REACTIONS 12hrs
Oppenauer oxidation, Meerwein-Ponndorf-Verley, Wolff-Kishner and Clemmensen reductions, Birch reduction; Robinson annulation, Stork-enamine synthesis, Barton reaction, Hofmann-Loffler-Freytag reaction, Shapiro reaction, Passerini reaction, Ugi reaction, McMurry olefination, Suzuki coupling, Mitsonobu reaction, Nef reaction, Sharpless asymmetric epoxidation and asymmetric dihydroxylation.

3. REAGENTS IN ORGANIC SYNTHESIS 10 hrs
Use of the following reagents in organic synthesis and functional group transformations: lithium diisopropylamide (LDA), dicyclohexylcarbodiimide (DCC), trimethylsilyl iodide, Woodward and Prevost reagents, osmium tetroxide, HIO₄, Pb(OAc)₄, O₃, DDQ, Selenium dioxide, 4-dimethylaminopyridine (DMAP), Ceric ammonium nitrate, phase transfer catalysts, crown ethers and Merrifield resin, Peterson’s synthesis, Baker yeast.

4. RETROSYNTHETIC ANALYSIS 22 hrs
The disconnection approach: Basic principles; introduction to synthons and synthetic equivalents; chemo selectivity; one-group C-X and two-group C-X disconnections; synthesis of aromatic compounds; reversal of polarity, cyclisation reactions; amine synthesis.
Protecting groups: protection of alcohols, carbonyl compounds, amines and carboxylic acids.
One group C-C and two group C-C disconnections: carbonyl compounds, alkene synthesis, use of acetylides and aliphatic nitro compounds in synthesis, 1,3-difunctionalised compounds, α,β-unsaturated carbonyl compounds, carbonyl condensations, 1,5-difunctionalised compounds, Michael addition and Robinson annulation.
Introduction to Ring synthesis: synthesis of 3,4,5,6 membered rings and saturated heterocycles.

5. GREEN CHEMISTRY

Principles of green chemistry

References

1. ELECTRICAL AND MAGNETIC PROPERTIES OF SOLIDS  

2. DEFECTS IN SOLIDS  
Point defects – Schotky and Frenkel defects, Colour centers and non-stoichiometry, Line defects – edge dislocation and screw dislocation, Plane defects – grain boundary and stacking faults.

3. PHASE TRANSITIONS IN SOLIDS  
Definition and classification – first and second order phase transitions with examples.

4. SUPERCONDUCTIVITY  
Definition, Meissner effect, type I and type II superconductors, features of superconductors, Frolich diagram, Cooper pairs, theory of low temperature superconductivity, high $T_c$ superconductors.

5. GEOMETRIC CRYSTALLOGRAPHY  
Crystalline and amorphous states of matter, crystallites, periodicity in crystals. Symmetry elements – symmetry operation, axis of symmetry, plane of symmetry, Centre of symmetry; derivation of nonoccurrence of five fold rotation axis, pure rotation, roto- inversion, roto-reflection axes, screw axes, glide planes; Combination of symmetry classes- Euler’s construction (interfacial angles) and its application to the general Formula of the type- $A.B = C$. Symmetry groups- plane groups, point groups, space groups, Bravais lattices, seven crystal systems and number of point groups in each crystal system, crystal classes; Stereographic projections of the following point groups: 222, 32, 422, 622, 23, 432 (Supporting the interfacial angles Euler’s Construction); Space group representation- Hermann – Maugin symbols.
6. X-RAY DIFFRACTION  
X-rays, Bragg’s equation and Bragg’s method, Miller indices, unit cell parameters and (Mentioning of crystal systems whenever required). X-ray structural analysis of solid substances: powder diffraction pattern of primitive, face-centered and body centered cubic lattices, indexing of reflections, identification of space groups from systematic absences (space group extinctions). The concept of reciprocal lattice and construction of Ewald’s sphere, derivation of Bragg’s law from reciprocal lattice, structure factor(s) and its relation to intensity, intensities from atomic positions for BCC and FCC lattices. Phase problem—heavy atom (Patterson’s) method and introduction to the principle of direct methods of phase determination. Electron density function and Fourier synthesis, electron density map(s).

7. ELECTRON AND NEUTRON DIFFRACTION  
Principle and applications

8. DYNAMICS OF ATOMS IN SOLIDS  
Dispersion Curves of an elastic structureless medium, Longitudinal and Transverse Modes, Optical and Acoustic Modes of Crystals, Total Vibrational Energy of Crystals. Case study of calcite

References:


CH 10PJ: RESEARCH PROJECT

The student is expected to carry out independent research putting in 18 hours of work per week and submit a project report, which will be evaluated.