DEPARTMENT OF CHEMISTRY

M.Sc. - Chemistry

SYLLABUS

Effective from the Academic Year 2016-2017

LOYOLA COLLEGE (Autonomous)

Ranked 2 in INDIA RANKING 2017 - NIRF
'College of Excellence' Status Conferred by UGC in 2014
Re-accredited with 'A' Grade (3.70 CGPA) by NAAC in 2013
Chennai - 600 034
# RESTRUCTURING-2016 (2016-17 batch ONWARDS)

## PG - Arts / Science / Commerce / Social Work

<table>
<thead>
<tr>
<th>Part</th>
<th>Semester 1</th>
<th>Semester 2</th>
<th>Summer Vacation</th>
<th>Semester 3</th>
<th>Semester 4</th>
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<td>120+2# (90+6+2*) C</td>
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Note: A theory paper shall have 5 to 6 contact hours and a practical session shall have 3 to 5 contact hours.
New format of the subject codes from the 2016 regulation

Subject codes are 10 characters long:

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<th>1st</th>
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- 1st & 2nd digits – last two digits of regulation year in YY format (If 2016, it will be 16).
- 3rd alphabet: U – UG / P – PG / M – M.Phil. / D – Ph.D.
- 4th & 5th alphabets: department wise program code (example – MT / CO / HT…..)
- 6th digit: Semester for UG / PG / M.Phil. and year for Ph.D.
- 7th & 8th alphabet: Category of paper or group of category of papers (GE/RL/OL/HE/OR/AL/ES/SK/MS/CM/CC/ ……)
- 8th & 9th digits: subject number range (01 to 99).

For example,

**Example 1:16UCH1MC01**
16 – Admitted in 2016
U – UG student
CH – Chemistry Student
1 – 1st Semester subject
MC01 – Major paper

**Example 2:16PCO2ID01**
16 – Admitted in 2016
P – PG student
CO – Commerce Student
2 – 2nd Semester subject
ID01 – Inter disciplinary paper

- For subjects which are carried forward from one regulation to the next, the first two digits representing the regulation alone will change.
- Subjects which are not carried forward from one regulation to the next, will not appear in the new regulation.
- For new subjects which need to be added to a regulation, a new subject code must be created in continuation of the last created code under that type/category.
- Subject codes which are identical (except for the first two digits which represent the regulation year) are treated as equivalent for the purpose of syllabus / question paper setting / conducting examination / etc.
# M.Sc. Chemistry (Shift - I )

(WITH EFFECT FROM 2016-2017 BATCH)

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<tr>
<th>Sl. No</th>
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<td>16PCH1MC01</td>
<td>Organic Reaction Mechanism and Stereochemistry</td>
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<td>2</td>
<td>16PCH1MC02</td>
<td>Concepts in Inorganic Chemistry</td>
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<td>3</td>
<td>16PCH1MC03</td>
<td>Quantum Chemistry and Group Theory</td>
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<td>Organic laboratory techniques-I</td>
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<td>Inorganic quantitative analysis and preparations</td>
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<td>Organic Reaction Mechanism and Heterocyclic compounds</td>
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<td>Biomolecules and Natural Products</td>
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<td>16PCH4PJ01</td>
<td>Project</td>
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Objectives

1. To understand the path, feasibility and mechanism of a reaction.
2. To understand the techniques involved in the determination of mechanism of reactions and to propose methods to determine the mechanism of reaction.
3. To understand the concept of stereochemistry and reaction mechanism.
4. To suggest synthetic route for simple organic compounds based on stereochemistry.

Unit-1: Mechanisms and Methods (1+15+1 h)

1.1 Types of mechanism, reagents and reactions. Electronic effects, Thermodynamic and kinetic requirements of reactions; Hammond postulate; microscopic reversibility. Potential energy diagrams, transition states and intermediates.

1.2 Methods of determining mechanism: Non-kinetic methods- Product analysis; Determination of the presence of intermediates-isolation, detection, trapping; cross-over experiments isotopic labeling and isotope effects; stereo chemical evidence. Kinetic methods - relation of rate with the mechanism of reaction.

1.3 Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes. Effect of structure on reactivity. The Hammett and Taft equation and linear free energy relationship, partial rate factor, substituent and reaction constants.

Unit-2: Rearrangement Reactions (1+15+1 h)

2.1 Types of rearrangements: Nucleophilic, free radical and electrophilic reactions.
2.2 Mechanisms: Nature of migration; migratory ability and memory effects, Wagner-Meerwin reactions, rearrangement of 1,2-Glycols, Demjanov, Wolff, Benzil-benzilic acid, Favorstii, Hoffmann, Curtius, Lossen, Schmidt, Beckmann, Neber, Baeyer-Villiger, Stevens, Claisen, Fries and photo Fries, Benzidine, Cope and oxy-cope, Dakin rearrangements, boron-carbon migration, non-1,2-rearrangements, Fischer-indole synthesis, Arndt-Eistert synthesis.

Unit-3: Oxidation and Reduction Reactions (1+15+1 h)
3.1 Mechanisms: direct electron transfer, hydride transfer, hydrogen transfer, displacement, addition-elimination and formation of ester intermediates, Oxidative and reductive coupling reactions.
3.2 Oxidation Reactions: Dehydrogenation by quinones, selenium dioxides, ferricyanide, manganese dioxide, permanganate, mercuric acetate leadtetraacetate, and OsO₄ oxidation of saturated hydrocarbons, alkyl groups, alcohols, halides and amines; Reactions involving cleavage of C-C bonds: cleavage of double bonds; oxidative decarboxylation, allylic oxidation, Oxidation by chromium trioxide-pyridine, Dimethylsulphoxide-dicyclohexylcarbodiimide (DMSO-DCCD).
3.3 Reduction Reactions: Replacement of oxygen by hydrogen - Wolff Kishner and Clemmenson and Rosenmund reductions with mechanism; Electrochemical and photochemical reduction, Trialkyl and triphenyltin hydrides, McFadyen-Stevens reduction, Homogeneous hydrogenation, Reduction by metal hydrides and alkoxides with stereochemistry, Hydroboration with cyclic systems, Removal of Oxygen from substrate; Reduction with cleavage; MPV, Bouveault-Blanc reduction, reduction involving anionic attack.
Unit-4: Stereochemistry-I  

4.1 Introduction to molecular symmetry and chirality – axis, plane, center, alternating axis of symmetry. Optical isomerism due to asymmetric and dissymmetric molecules with C, N, S based chiral centers. Optical purity, prochirality, enantiotopic and diastereotopic atoms, groups and faces, chirality due to helical shape, methods of determining the configuration.

4.2 Racemic modifications: Racemisation by thermal, anion, cation, reversible formation; epimerisation, mutarotation.

4.3 Cram’s and Prelog’s rules; D, L, R, S-notations; proR, proS, side phase and re phase Cahn-Ingold-Prelog rules, absolute and relative configurations; Configurations of allenes, spiranes, biphenyls, cyclooctene, helicene,binaphthyls, ansa and cyclophanic compounds, exo-cyclic alkylidene-cycloalkanes, and exo-cyclic alkylidenecycloalkanes. Topicity and prostereoisomerism – NMR distinction of enantiotopic/diastereotopic compounds.

4.4 Criteria for optical purity; Resolution of racemic modifications; asymmetric transformations; asymmetric synthesis; destruction. Optical purity calculations.

4.5 Geometrical isomerism: E, Z notations, geometrical isomerism in C=C, cyclic systems and oximes.

Unit-5: Stereochemistry-II  

5.1 Conformation and reactivity of acyclic systems; intramolecular rearrangement; neighbouring group participation; chemical consequence of conformational equilibrium - Curtin-Hammett principle.

5.2 Stability of five and six-membered rings; mono and disubstitutedcyclohexanes; conformation and reactivity in cyclohexane systems.

5.3 Fused and bridged rings; bicyclic and poly cyclic systems; decalins and Brett’s rule.

~ 5 ~
5.4 Optical rotation and optical rotatory dispersion; conformational asymmetry, ORD curves; octant rule; configuration and conformation; Cotton effect; axial haloketone rule; Determination of configuration.

5.5 Stereoselective and stereospecific synthesis.

Textbooks

References

16PCH1MC02 CONCEPTS IN INORGANIC CHEMISTRY

**SEMESTER I**

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<td>MC(T)</td>
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**CREDITS** 4

**Objectives**

1. To understand the different kinds of chemical forces in molecules.
2. To identify the nature of chemical bond in a given inorganic compound.
3. To predict the nature and topology of inorganic compounds.
4. To know the existence of compounds through weak chemical forces.
5. To identify relevant inorganic compounds for specific applications.

**Unit-1: Atomic Structure and Periodic Table**

1.1 Periodicity, Structure of atom, Bohr’s theory.
1.2 Modern views on atomic structure: Wave mechanical description of electron and orbitals- radial density functions and orbital energies, angular functions and orbital shapes.
1.3 *Slater orbitals and their uses*: computation of effective nuclear charge and radii of atoms and ions.
Unit-2: Ionic Compounds
2.1 Packing of ions in crystals and crystal structures-ccp, hcp, bcc, and fcc.
2.2 Radius ratio and structure of ionic lattices: Geometrical method of computing radius ratio, radius ratio and coordination number, stoichiometry and crystal structures. Madelung constant.
2.3 Lattice energy: derivation of Born-Lande equation, modified Born-Lande equation, factors affecting lattice energy. Layer lattices, applications.
2.4 Born-Haber cycle: Thermochemical calculations, radii of nonspherical ions, solubility and thermal properties of ionic compounds as a function of $U_0$ and $\Delta H_f$.
2.5 Polarization in ionic compounds: covalency and Fajan’s rules, effects of polarization.

Unit-3: Covalent Bond
3.1 Molecular topologies: shared and lone pairs and Lewis structures, isoelectronic and isolobel relationships, hybridization and geometry, VSEPR model, and Bent’s rule.
3.2 Molecular Orbital Theory: Symmetry of molecular orbitals formed from atomic orbital overlap, Extended Huckel theory of Hartree-Fock approximation (SCF), LCAO-MO model, TASO, LUMO, and HOMO concepts in bonding.
3.3 MO energy level diagrams of homo- and heterodiatomic molecules (CO, NO, and HCl).
3.4 Bonding in metals: packing of atoms in metals, band theory of metals and metallic properties, insulators, and semiconductors.

Unit-4: Weak Chemical Forces
4.1 van der Waals forces: Inclusion compounds-layer, channel, and cage structures (gas hydrates and clathrates).
4.2 Hydrogen bonding: associated molecules, and molecular
self-assembly.

4.3 Supramolecular architectures formed by weak chemical forces.

Unit-5: Acid-base Theory and Solvent Systems

5.1 Acid-Base theories: Bronsted-Lowry, Lux-Flood, Usanovich, Lewis, and solvent system. definitions, measures of acid-base strength, acid-base interactions, hard and soft acid and bases, classification, levelling effect, symbiosis, proton sponges.

5.2 Nonaqueous solvents: Classification-protonic and aprotic solvents, super acids, molten salts as solvents, ionic liquids and their use in synthesis.

5.3 Hard soft acid base principle: theoretical basis of hardness, class A and B.

Text Books


References


**16PCH1MC03 QUANTUM CHEMISTRY AND GROUP THEORY**

**SEMESTER I**
**CREDITS 4**
**CATEGORY MC(T)**
**NO.OF HOURS/WEEK 6**

**Objectives**

1. To understand the physical and mathematical aspects of quantum mechanics and familiarize the mathematics required for solving quantum mechanical problems.
2. To understand the quantum mechanical approach to atomic and molecular electronic structure.
3. To understand the importance of symmetry and its applications.

**Unit-1: Mathematics for Quantum Mechanics and Postulates of Quantum Mechanics**

(1+12+1 h)

1.2 Introduction to Quantum Mechanics: Failure of classical mechanics: Black body radiation, photo electric effect, hydrogen atomic spectrum and Compton effect. The need for quantum mechanics. Postulates of Quantum Mechanics and Schrodinger wave equation.

**Unit-2: Some Quantum mechanical models and their applications** (1+14+1 h)
2.1 Particle in a box (1D and 3D). Degeneracy and its application to linear conjugated molecular systems, free particle. Bohr’s correspondence principle. Quantum mechanical tunneling: Tunneling in chemical reactions (electron transfer), inversion of ammonia, proton transfer reactions.
2.2 Rigid Rotor: Wave equation and solution. Calculation of rotational constants and bond length of diatomic molecules.
2.3 Harmonic Oscillator: Wave equation and solution. Anharmonicity. Force constant and its significance

**Unit 3: Application of Quantum Mechanics to Hydrogen and poly electron atoms** (1+21+1 h)
3.1 Hydrogen atom and hydrogen like ions: Hamiltonian - wave equation and solution to hydrogen and hydrogen like systems. Radial and angular functions. Quantum numbers n, l, m and s and their importance. Radial distribution functions and their representation.
3.3 Quantum mechanical treatment of angular momentum - Simultaneous measurement. Commutators: \([x, p_x],[x, p_x^2],[L_x, L_y]\) and \([L_x^2, L_x]\) and their significance.
Unit 4: Molecular Quantum Mechanics and Chemical bonding  
(1+13+1 h)  
4.2 Hydrogen molecular ion: Use of linear variation function and LCAO methods.  
4.3 Electronic structure of conjugated systems: Hückel method applied to ethylene, allyl systems, butadiene and benzene.  

Unit 5: Group theory and applications  
(1+20+1 h)  
5.1 Group and subgroup. Symmetry elements and operations. Classification of molecules into non axial, axial and dihedral point groups - $C_{nv}$, $C_{nh}$, $D_{n}$, $D_{nh}$, $D_{nd}$, $T_{d}$ and $O_{h}$.  
5.2 Matrix representations of symmetry operations. Reducible and irreducible representations. Classes of operations.  
5.3 The Great orthogonality theorem: Reduction formula, construction of character table for $C_{2v}$, $C_{2h}$ and $C_{3v}$ point groups.  
5.4 Application of group theory to molecular vibrations, electronic spectra of formaldehyde and ethylene, chemical bonding.  

Text books  

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References

**16PCH1MC04 ANALYTICAL CHEMISTRY**

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**Objectives**

1. To learn the basic analytical methods and to have a knowledge of chemistry involved in chemical analysis.
2. To know the principle and instrumentation of different analytical techniques.
Unit 1: Data Analysis (1+10+1 h)
1.1 Errors: Precision and accuracy, Classification of errors, methods of minimization and elimination of errors.
1.2 Statistical methods: Treatment of random errors, reliability of results, rounding up of results from chemical computation, confidence interval, Normal error curve and its importance. Comparison of results: students t-test, F-test and linear regression for deriving calibration plots.

Unit 2: Chromatography (1+13+1 h)
2.1 Principles of thin layer, paper and column chromatographic techniques.
2.2 Gas chromatography: carrier gas, columns, detectors-hhot-wire detector, flame ionization detector, photo ionization detector and ECD. Determination of C,H,N and S.
2.3 HPLC: Column, solvent delivery system, sample injections, Detectors. Advantages of HPLC. Applications of HPLC in the separation of cations. Principles of preparative and analytical HPLC.
2.4 Electrophoresis and capillary electrophoresis – principle, instrumentation and applications.

Unit 3: Titrimetric Methods of Analysis (1+13+1 h)
2.1 Difference between titrimetric and volumetric analysis, Principle and reactions involved in acid-base, redox, complexometric and precipitation titrations, Different methods of expressing concentration terms, calculations involving stoichiometry- acid base and redox systems.
2.2 Acid-base titrations in non-aqueous solvents: Principle, properties – acidic and basic properties, auto-protolysis constant of solvents, dielectric constant and its effect on solvent behaviour. Detection of equivalence point – titrations in ethylene diamine, glacial acetic acid, methanol and ethanol.

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2.3 Hydrolysis of salts – hydrolysis of a salt of a strong base / weak acid, weak base / strong acid and weak acid / weak base.

Unit 4: Thermal and Electroanalytical Methods (1+16+1 h)
4.1 Thermogravimetry: Principle, factors affecting thermogram, instrumentation and thermal decomposition of CaC$_2$O$_4$.H$_2$O and CuSO$_4$.5H$_2$O. Differential techniques: Instrumentation, experimental and instrumental factors of DTA. Thermal behaviour of CuSO$_4$.5H$_2$O by DTG. Principle and determination of purity of pharmaceuticals, phase transition studies by DSC.
4.2 Electrogravimetry: Principle, instrumentation, deposition and separation. Electrolysis at constant current and estimation of copper.
4.3 Coulometry: controlled potential coulometry, Principle and separation of nickel and cobalt, coulometric titration, instrumentation - Estimation of Sb(III).
4.4 Potentiometry: Potentiometric titration, equivalence point potential for (i) Fe$^{2+}$/ Fe$^{3+}$-Ce$^{3+}$/Ce$^{4+}$ (ii) Fe$^{2+}$/ Fe$^{3+}$- MnO$_4^-$, H$^+$/Mn$^{2+}$ systems. Determination of concentration of the species at the equivalence point. Ion selective electrodes, coated/modified electrodes, Biochemical electrodes. Solid state ion selective detectors.

Unit-5: Spectrometry (1+13+1 h)
5.1 Spectrophotometry: Beer-Lambert’s law, spectrophotometric titrations, determination of Fe(III) with EDTA and determination of Fe(III) in the presence of aluminium.
5.2 Atomic Absorption Spectroscopy: Principle, instrumentation - Burner, furnace, resonance line source, detectors. Spectral and chemical interferences, determination of alkali metals in blood serum,
Determination of lead in petrol. Principle of Inductively coupled plasma (ICP) spectrometry.

5.3 Flame emission spectrometry: Principle, instrumentation and interferences, determination of alkali metals, Determination of iron in non-ferrous alloys.

5.4 Turbidimetry and nephelometry: Principle, instrumentation - determination of sulphate and phosphate.

5.5 Fluorimetry: Principle, relationship between excitation spectra and fluorescence spectra, factors affecting fluorescence emission, determination of quinine in tonic water and determination of codeine and morphine in a mixture.

Books for study:

Books for reference:


**16PCH1MC05 ORGANIC LABORATORY TECHNIQUES-I**

**SEMESTER I**

**CREDITS**  2  
**CATEGORY**  MC(L)  
**NO.OF HOURS/ WEEK**  4

**Objectives**

To develop analytical skill in

(i) Separation of organic mixture

(ii) Organic qualitative analysis

(iii) Organic preparations involving two stages.

1. **Separation and analysis**: Two component mixtures.

2. **Preparations**: Two stage processes involving nitration, halogenation, diazotization, rearrangement, hydrolysis, reduction, alkylation and oxidation. Two stage preparations

   a) *p*-Bromoacetanilide from Aniline (*Acetylation-bromination*)

   b) *p*-Nitroaniline from Acetanilide (*nitration-hydrolysis*)

   c) 1,3,5-Tribromobenzene from Aniline (*bromination-deamination*)

   d) Acetyl salicylic acid from Methyl salicylate (*Esterification-Hydrolysis*)

   e) Benzilic acid from Benzoin (*oxidation - rearrangement*)

   f) *m*-Nitroaniline from Nitrobenzene (*Nitration-Reduction*)
Text books


Reference


16PCH1MC06 INORGANIC QUANTITATIVE ANALYSIS AND PREPARATIONS

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Objectives

1. To impart the skill in estimation of metal ions by colorimetric and complexometric methods.
2. To identify the methodology to estimate a metal ion in the presence of another metal ion.
3. To impart the skill in preparations of metal complexes.

1. **Colorimetry** (visual)
   1.1 Estimation of iron.
   1.2 Estimation of nickel.

2. **Complexometric Titration**
   2.1 Estimation of zinc, nickel, magnesium, and calcium.
   2.2 Estimation of mixture of metal ions-pH control, masking and demasking agents.
   2.3 Determination of calcium and lead in a mixture (pH control).
   2.4 Determination of manganese in the presence of iron.
   2.5 Determination of nickel in the presence of iron.
3. Gravimetry and Titrimetry

3.1 Determination of nickel by gravimetry and copper by titrimetry in a mixture.
3.2 Determination of barium by gravimetry and calcium by complexometry in a mixture.

4. Preparations and estimation of one metal ion in one experiment

4.1 Potassium tris(oxalato)ferrate(III)
4.2 Hexaamminenickel(II) tetrafluoroborate
4.3 Potassium tetrachlorocuprate(II)
4.4 Tris(thiourea)(sulfato)zinc(II)

5. Determination of iron by colorimetry and calculation of percentage of Fe in $\text{K}_3[\text{Fe(C}_2\text{O}_4)_3]$.

Text books


References


16PCH2MC01 ORGANIC REACTION MECHANISM AND HETEROCYCLIC COMPOUNDS

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Objectives

1. To understand the mechanism of organic chemical reactions.
2. To appreciate the concept of substitution, addition and elimination reactions and their reaction mechanisms.
3. To comprehend the importance of heterocyclic compounds.

Unit-1: Aromatic and Aliphatic Electrophilic Substitution  
(1+18+1 h)

1.1 Aromaticity: Aromaticity in benzenoid, non-benzenoid, heterocyclic compounds and annulenes; alternant and non-alternant hydrocarbons, Huckel’s rule, energy level of $\pi$-molecular orbitals, antiaromaticity, homoaromaticity, PMO approach. Bonds weaker than covalent, addition compounds, crown ether complexes and cryptands, inclusion compounds, cyclodextrins, catenanes and rotaxanes; NMR as a tool for aromaticity - anti- and homo-aromatic systems.

1.2 Aromatic electrophilic substitution: Mechanism, orientation and reactivity - Quantitative treatment of reactivity in the substrates and reactivity of the electrophiles.

1.3 Reactions involving nitrogen electrophiles: nitration, nitrosation and diazoniumcoupling; Sulphur electrophiles: sulphonation; Halogen electrophiles: chlorination and bromination; Carbon electrophiles: Friedel-Crafts alkylation, acylation and arylation reactions.

1.4 Aliphatic substitution Mechanisms: SE2 and SEi, SE1; Substitution by double bond shifts; other mechanism: addition-elimination and cyclic mechanism.

1.5 Hydrogen as electrophile: (a) Hydrogen exchange; hydro dehydrogenation; ketoenoltautomerism. b) Halogen electrophiles: Halogenation of aldehydes, ketones and carboxylic acids c) Nitrogen electrophiles: aliphatic diazonium coupling; direct formation of diazo compounds; direct amination; insertion by nitrenes. d) Sulphur electrophiles: sulphonation, sulphenylation. e) Carbon electrophiles: acylation; alkoxy carbonyl alkylation; alkylation; Stork-enamine reaction; insertion by carbene.
Unit-2: Aromatic and Aliphatic Nucleophilic Substitution (1+13+1 h)

2.1 Mechanisms: $S_{N}Ar$, $S_N1$ and Benzyne mechanisms. Reactivity, Effect of structure, leaving group and attacking nucleophile.


Unit-3: Elimination and Free Radical Reactions (1+13+1 h)


3.2 Long lived and short lived radicals – Production of radicals by thermal and photochemical reactions, Detection and stability of radicals, characteristics of free radical reactions and free radical, reactions of radicals; polymerization, addition, halogenations, aromatic substitutions, rearrangements. Reactivity: Reactivity on aliphatic, aromatic substrates, reactivity in the attacking radical, effect of solvent.

~ 21 ~
Unit-4: Addition to Carbon Multiple Bonds (1+10+1 h)

4.1 Mechanisms: (a) Addition to carbon-carbon multiple bonds- Addition reactions involving electrophiles, nucleophiles, free radicals, carbenes and cyclic mechanisms-Orientation and reactivity, hydrogenation of double and triple bonds, hydroboration, Birch reduction, Michael reaction, addition of oxygen and Nitrogen; (b) Addition to carbon-hetero atom multiple bonds: Mannich reaction, LAH reduction of Carbonyl compounds, acids, esters, nitrites, addition of Grignard reagents, Reformatsky reaction, Tollens reaction, Wittig reaction, Prins reaction.


Unit-5: Heterocyclic Chemistry (1+11+1 h)

5.1 Nomenclature, reactivity, aromaticity, spectral properties.

5.2 Synthesis and reactions of indole, isoindole, oxazole, imidazole, thiazole, pyridine, pyrimidine, pyridazine, pyrazine, chromans, chromons, coumarins, carbazoles, uracil, uric acid and xanthines.

5.3 Oxygen Heterocyclic Compounds: Classification, color reactions of various classes of flavonoids – chemistry and synthesis of flavones (luteolin), isoflavones (daidzein), flavonols (kaempferol) and anthocyanidins (cyanidin).
Text books

References
Objectives
1. To know the nature of metal-ligand bonding in coordination compounds and bonding parameters.
2. To know the chemical and photochemical behaviour of coordination compounds.
3. To know the mechanisms of reactions of coordination compounds.
4. To understand the importance of coordination compounds in the emerging field of supramolecular chemistry and nanotechnology.
5. To know the application of coordination compounds in catalysis and biology.

Unit-1: Theories of Coordination Compounds
1.1 Structural features of complexes of coordination numbers 2 to 6 and higher coordination numbers.
1.2 Crystal Field Theory: inadequacy of valence bond theory, crystal field splitting in $Td$ and $Oh$ fields, high spin vs low spin complexes, spin crossover. Computation of CFSE in tetrahedral geometry and LS and HS octahedral geometries, factors which determine $10Dq$ values, spectrochemical series. Evidences of crystal field splitting.
1.3 Jahn-Teller theorem: Jahn-Teller effect-consequences, static and dynamic Jahn-Teller effect. Tetragonal distortions from $Oh$ symmetry and crystal field splitting in tetragonally distorted octahedral and square planar geometries.
1.4 Molecular Orbital Theory: Evidences of metal-ligand covalency, TASO-MO concepts of $Oh$ and $Td$ complexes, MO energy level diagrams of $\sigma$- and $\pi$-
bonding in $O_h$ complexes, nature of metal-ligand $\pi$-bonds, evidences for $\pi$-back bonding, spectrochemical series, and $\pi$- acceptor series, evidences for back bonding from vibrational spectroscopies.

1.5 Angular Overlap Model: Principles, quantification of metal-ligand orbital interactions ($e_{\sigma}$- and $e_{\pi}$-parameters), angular overlap and geometry, angular scaling factors for $e_{\sigma}$- and $e_{\pi}$- parameters, computation of $\Delta_{\sigma}$ and $\Delta_{\tau}$ and their relationship.

Unit-2: Electronic Structure and Geometry of Coordination Compounds

2.1 Molecular magnetism: diamagnetic and paramagnetic susceptibilities, temperature dependent paramagnetism, the Curie law, ferromagnetic and antiferromagnetic interactions. Methods of determining magnetic susceptibility: Gouy and Faraday balances, vibrating sample magnetometer (VSM) and SQUID. Van Vleck equation and magnetic moments of free metal ions.

2.2 IR spectroscopy: differentiation of linkage isomers-cyano- and isocyano-, nitro- and nitrito-, thiocyanato- and isothiocyanato complexes, IR spectra of terminal and bridging carbonyls.

2.3 Electronic absorption spectroscopy: derivation of term symbols, electronic states and spectra of $O_h$ and $T_d$ complexes of $d^n$ metal ions, Orgel and Tanabe-Sugano diagrams.

Unit-3: Organometallic Compounds and Reaction Mechanisms

3.1 Classification of reaction types: reactions involving (a) change in the composition and (b) change in the position of ligand in the coordination sphere, (c) electron transfer reactions.

3.2 $Trans$-effect and synthesis of square planar complexes; mechanism of replacement of coordinated water in $O_h$
complexes: $D$, $A$, $I_a$ and $I_d$ mechanisms; hydrolysis of $O_h$ complexes.

3.3 Electron transfer reactions: mechanisms of inner- and outer-sphere and long range electron transfers.

3.4 Nomenclature of chiral complexes, study of absolute configurations of chiral complexes-ORD and CD, the hapto nomenclature in organometallic chemistry.

3.5 Structure and bonding in metal alkenes, metal-alkynes, and organometallic compounds of cyclic- and open chain $\pi$-donors, metallocenes, metal-aryls, double- and triple decker sandwich complexes.

3.6 Catalysis involving organometallic compounds: alkene isomerization and metathesis; Ziegler-Natta catalyst and alkene polymerization; Wilkinson catalyst and alkene hydrogenation; carbonylation, hydroformylation, hydrocarboxylation, Fischer-Tropsch synthesis, Wacker process.

Unit-4: Supramolecular Chemistry and Photochemistry
4.1 Crystal field and charge transfer (MLCT, CTMM) photochemistry: photosubstitution and photoisomerization reactions.

4.2 Molecular recognition: molecular receptors, recognition of neutral molecules anions and cations.

4.3 Macrocyclic complexes. Supramolecular assemblies and architectures: nature of supramolecular interactions, supramolecular assemblies formed by templates and self-assembly.

Unit-5: Bioinorganic Chemistry
5.1 Metalloproteins and enzymes-general introduction and properties.

5.2 Heme proteins: haemoglobin and myoglobin-structure, mechanism of oxygen transport; cytochromes-biological roles and structural features.

5.3 Copper proteins: structure and functions of type-I, type-II and type-III.
5.4 Photosynthesis: chlorophyll, photosystem-I and photosystem-II, photosynthetic reaction center and Z-scheme.

5.5 Enzymes: superoxide dismutase, carboxy peptidase A-structure and functions.

Text Books

References
Objectives

1. To understand the quantization of energy and interaction of electromagnetic radiation with matter.
2. To understand the fundamentals of different branches of spectroscopy.
3. To elucidate the structures of molecules using different spectral techniques.

Unit 1: Rotational and Vibrational Spectroscopy

(1+23+1 h)

1.1 Diatomic molecules as rigid rotors - intensity of spectral lines, selection rules, effect of isotopic substitution. Diatomic molecules as non-rigid rotors - rotational spectra of linear and symmetric top polyatomic molecules.


1.3 Vibrations of polyatomic molecules - Symmetry and fundamental vibrations, overtones, combination, difference bands. Influence of rotations on the spectra of polyatomic molecules - parallel and perpendicular vibrations in linear and symmetric top molecules.

1.4 Interpretation of IR spectra of organic and inorganic compounds - Frequencies of various functional groups containing oxygen, nitrogen and hydrocarbons. Factors affecting the fundamental vibrational frequencies. Linkage, geometrical isomers, coordinated and lattice water. NO$_2$, CO$_3$, ClO$_4^-$, and SO$_4^{2-}$. 
1.5 Raman Effect - Rayleigh and Raman scattering, Stokes and anti-Stokes radiation, molecular polarizability, selection rules.

1.6 Raman spectra: Rotational Raman spectra - linear molecules, symmetric top and spherical top molecules. Vibrational Raman spectra - symmetry and Raman active vibrations, rule of mutual exclusion. Rotational fine structure. Structure determination from Raman and Infrared.

**Unit 2: Electronic spectroscopy** (1+13+1h)


2.2 Characterization of organic compounds: application of Woodward-Fieser rules to conjugated dienes, α, β-unsaturated carbonyl compounds, benzene and its substituted derivatives, polycyclic aromatic hydrocarbons, polyenes, polyynes, and heterocyclic compounds.

2.3 Charge transfer transitions: Intensity, electronic spectra of charge transfer complexes of organic compounds, charge transfer transitions in inorganic and coordination compounds.

**Unit 3: Mass spectroscopy** (1+10+1h)

3.1 Determination of molecular formula - molecular ion, nitrogen rule, isotope peaks, metastable ions, Mc Lafferty rearrangement, Retro Diels Alder reaction.

3.2 Fragmentation - Basic fragmentation types and rules, Fragmentation patterns of hydrocarbons, oxygen and nitrogen containing organic compounds and carbonyl compounds.

3.3 Ionisation techniques - Principle of Electrospray ionisation (ESI)-MS, Matrix-assisted laser
desorption/ionisation (MALDI)-MS and Fast atom bombardment (FAB)-MS.

**Unit 4: NMR and EPR spectroscopy** (1+24+1h)

4.1 Theory of Nuclear magnetic resonance (NMR) spectroscopy - nuclear spin, magnetic nuclei, nuclear magnetic moment, NMR transition, Bloch equations, relaxation mechanisms.

4.2 Parameters of NMR - chemical shift, shielding and deshielding, factors affecting chemical shift-inductive effect, anisotropy, hydrogen bond. Region of proton chemical shift in inorganic molecules, chemical shift equivalence and magnetic equivalence. NMR of paramagnetic compounds: Shift reagents in NMR.

4.3 Spin-spin splitting - mechanism and application to structure determination. Coupling constants: mechanism of coupling, first order patterns, second order effects, examples of AB, AX, ABX systems, geminal coupling, vicinal coupling, variation of coupling constants with bond angle, dihedral angle. Long-range coupling, aromatic coupling, virtual coupling.

4.4 Fourier Transform (FT) and 2D NMR spectroscopy: Principle of FT-NMR, Free induction decay (FID). Introduction of 2D techniques: Correlation spectroscopy (COSY), Nuclear overhauser effect spectroscopy (NOESY) and Hetero-COSY. $^{13}$C, $^{19}$F and $^{31}$P NMR spectra of typical examples. Principle of solid state NMR.

4.5 Electron paramagnetic resonance (EPR) spectroscopy - theory of EPR, presentation of the spectrum, nuclear hyperfine splitting in isotropic systems.

4.6 EPR spectra of anisotropic systems - anisotropy in g-value, causes of anisotropy, anisotropy in hyperfine coupling, hyperfine splitting caused by quadrupole nuclei. EPR spectra of systems with more than one unpaired electrons: Zero-field splitting (ZFS), causes of ZFS, ZFS and EPR transitions. EPR of triplet
naphthalene, copper salen complex and high-spin Mn(II) complexes.

4.7 Structural elucidation of organic compounds by combined spectral techniques.

Unit-5: NQR and Mossbauer Spectroscopy (1+10+1h)

5.1 Principle of Nuclear quadrupole resonance (NQR) spectroscopy - nuclear charge distribution and quadrupole moment, quadrupole nucleus and its interaction with electric field gradient, nuclear orientations, asymmetry parameter, quadrupole energy levels, transitions in spherical and axially symmetric fields, effect of magnetic field.

5.2 Applications of NQR spectroscopy: quadrupole coupling constant and its interpretation, structural information from NQR spectra of haloorganic compounds, point group symmetry, phase transitions, chemical bonding and hydrogen bonding.

5.3 Principle of Mossbauer spectroscopy: Doppler shift, recoil energy. Isomer shift, quadrupole splitting, magnetic interactions. Applications: Mossbauer spectra of high and low-spin Fe and Sn compounds.

Text books


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References
Objectives
1. To develop analytical skill in organic quantitative analysis.
2. To understand the techniques involved in estimations of organic compounds.

1. Estimations
   a) Phenol (bromination)
   b) Aniline (bromination)
   c) Ethyl methyl ketone (iodimetry)
   d) Glucose (redox)
   e) Ascorbic acid (iodimetry)
   f) Aromatic nitro groups (reduction)
   g) Glycine (acidimetry)

2. Extraction
   a) Caffeine from tea leaves
   b) Nicotine from tobacco leaves
   c) Citric acid from citrus fruits
   d) Lycopene from tomatoes.

3. Separation of components of a mixture (Demonstration)
   a) Thin layer chromatography
   b) Column chromatography
   c) Paper chromatography.

Text books
Objective
1. To study the principle of distribution of common and rare metal ions in different groups.
2. To know inter- and intra-group precipitation and separation of metal ions.
3. To improve the skill in the qualitative analysis of rare metal ions in different groups.
4. To identify the methodology to analyse a metal ion in the presence of another metal ion.

1. Theoretical Principles

1.1 Classification of cations into groups, group reagents.
1.2 Inter group and intragroup separations.
1.3 Confirmatory test for cations-the reaction and the product.

2. Analysis of mixture of cations

Analysis of a mixture of four cations containing two common and two rare.

Cations to be tested.

- **Group-I**: W, Tl and Pb.
- **Group-II**: Se, Te, Mo, Cu, Bi and Cd.
- **Group-III**: Tl, Ce, Th, Zr, V, Cr, Fe, Ti and U.
- **Group-IV**: Zn, Ni, Co and Mn.
- **Group-V**: Ca, Ba and Sr.
- **Group-VI**: Li and Mg.
Text Books

16PCH2ES01 BIOMOLECULES AND NATURAL PRODUCTS

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Objective
1. To enable the student to understand and appreciate the importance of biomolecules.
2. To understand the techniques involved in the extraction and methods of determination of structure of natural products.

Unit-1: Carbohydrates and Lipids (1+10+1 h)
1.1 Carbohydrates: Synthesis of glycosides, amino sugars, sucrose and maltose.
1.2 Biological importance of glycosides, amino sugars, sucrose, maltose cellulose, starch, glycogen, dextran, hemicellulose, pectin, agar-agar, chitosan, and chrysin.
1.3 Carbohydrate metabolism: glycolysis and gluconeogenesis, pentose phosphate pathway, Carbohydrate in plants and bacteria, tricarboxylic acid (TCA) cycle. Relation between glycolysis and respiration.
1.4 Lipids: synthesis and degradation of neutral lipids, Phospho lipids (lecithines, cephalins, plasmalogens) and glycolipids.
1.5 Lipid Metabolism: Oxidation of glycerol – β-oxidation of fatty acids; Fatty acid metabolism: Regulation of fatty acid metabolism; Allosteric regulation.

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Unit-2: Proteins and nucleic acids (1+10+1 h)
2.1 Separation and purification of proteins – dialysis; gel filtration - electrophoresis. Catabolism of amino acids: transamination, oxidative deamination and decarboxylation. Biosynthesis of proteins: Role of nucleic acids. Amino acid metabolism; the urea cycle.
2.2 Structure and synthesis of nucleosides and nucleotides; Structure of RNA and DNA, Watson-Crick model; Solid phase synthesis of oligonucleotides.
2.3 DNA intercalators; Chemical synthesis of DNA; Catalytic RNA, siRNA; micro RNA; Synthesis and Application of Unnatural Nucleosides; Fluorescently Labeled Nucleosides and oligonucleotide probes; Single Nucleotide Polymorphism (SNPs).

Unit-3: Vitamins, Hormones and antioxidants (1+12+1 h)
3.1 Vitamins: Types, structure discussion, properties and biological importance of Vitamin A, Vitamin B complex: B$_1$, B$_{12}$, Folic acid, Vitamins C, D and E.
3.3 Antioxidants: Nutrients with an antioxidant role, the need for biological antioxidants, pro-oxidant activity of biological antioxidants, Nutrients associated with endogenous antioxidant mechanisms, Nutrients with radical-quenching properties, β-Carotene and other carotenoids, requirement for antioxidant nutrients.
3.4 Free radicals induced damages, lipid peroxidation, measurement of free radicals, disease caused by radicals, reactive oxygen species, antioxidant defence system, enzymic and non-enzymic antioxidants, role of antioxidants in prevention of diseases, phytochemicals as antioxidants.
Unit-4: Alkaloids (1+9+1 h)
4.1 Classification and isolation. General methods of structural elucidation of alkaloids.

Unit-5: Terpenoids and carotenoids (1+9+1 h)
5.1 Classification and isolation. General methods of determination of structure.
5.2 Structural elucidation of Cadinene, Vitamin A, β-carotene, Abietic acid, Gibberelic acid, Zinziberine and Squalene.

Text books

References


16PCH2ES02 SURFACE CHEMISTRY AND CATALYSIS

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Objectives

1. To understand the basic concepts of surface chemistry and colloids.
2. To know the different methods of catalysis
3. To learn the various techniques and mechanisms involved in catalysis.

Unit 1: Adsorption (1+8+1 h)


1.3 Adsorption from solution- Gibbs adsorption isotherm, surface films.


Unit 2: Colloids (1+8+1 h)

2.1 Surfactants – anionic, cationic and amphoteric, hydrophile-lipophile balance.
2.2 Micelles – formation, critical micellar concentration (CMC), factors affecting CMC in aqueous media, micellar catalysis.

2.3 Uses of CMC for the synthesis of zeolites, mesoporous and metal organic framework materials.

2.4 Emulsions – micro and macro, selection of surfactants as emulsifiers, preparation; elastic and non-elastic gels.

**Unit 3: Homogeneous and Heterogeneous catalysis**  
(1+13+1 h)

3.1 Introduction to catalysis - activity, selectivity, promoters, stabilisers and poisons, catalysts deactivation, auto catalysts, turnover number and inhibitors.

3.2 Homogeneous catalysed reactions – general mechanism, activation energy for the process, acid-base catalysis – catalytic activity, acid-base strength, acidity functions. Homogeneous catalysts for the polymerization of olefins, oxidative dehydrogenation, ethyl benzene to styrene.

3.3 Steps involved in heterogeneous catalysis, thermodynamic considerations. Preparation of catalysts – precipitation and impregnation methods. Role and load of supports. Heterogeneous catalysts for catalytic cracking and Fischer-Tropsch synthesis.

**Unit 4: Photo and Bio Catalysis**  
(1+12+1 h)

4.1 Photocatalysis: n- and p-type and metallised semiconductors as photocatalysts (TiO_2 and ZnO) – application for the degradation of dyes, solar energy conversion, electrochemical cells, photoelectrolysis of water. Photocatalysis for organic reactions-oxidation, reduction, polymerization, substitution and isomerization reaction using TiO_2.

4.2 Biocatalysis – Mechanisms - covalent catalysis, acid-base and metal-ion catalysis, entropy and geometric effects, structural complementary of the active site to the transition state, prevention of the side reactions, the size of the enzymes. Application of enzymes in organic
synthesis - Oxidoreductase: Oxidation - alcohols, epoxides, sulfoxides, amino acids, lactones; Reduction: \(\alpha\)-hydroxyl aminoacid; Transferase-amino acids, amines.

**Unit 5: Surface Characterisation Techniques** (1+9+1 h)

5.1 Surface area determination – BET, pore volume, and pore size distribution-BJH and t-plot methods.

5.2 Thermal methods – temperature programmed desorption and reduction.

5.3 Spectroscopic techniques: X-ray photoelectron spectroscopy, Auger electron spectroscopy, surface plasmon resonance, X-ray fluorescence spectroscopy – Principle and applications in surface analysis.

**Text Books**


**Reference Books**


16PHE2FC01 LIFE SKILLS TRAINING

SEMESTER II
CATEGORY FC(T)
CREDITS 2
NO.OF HOURS/ WEEK 2+2

OBJECTIVES OF PG SYLLUBUS

1. To improve and sustain the primal level of competence and performance of PG students through an advanced training of holistic development of oneself.

2. To empower through various skills and strengthen them to face the future life issues and challenges.

3. To equip them with practical and value based learning of soft skills for a better life in future.

INSIDE CLASS HOURS (2 hrs)

Unit – I: Constructing Identity


Unit – II: Capacity Building

Motivation – Definition, types (Intrinsic and Extrinsic), Theories (Maslow’s hierarchical needs, etc), Factors that affect motivation, Challenges to motivation, Strategies to keep motivated, motivational plan. Time Management Skills– steps to improve time management, overcoming procrastination, assessing and planning
weekly schedule, challenges, goal settings, components of goal settings, consequences of poor time management, control of interruption and distractions. Communication, public speaking, talents, creativity, learning,

Unit – III: Professional Skills


Unit – IV: Life Coping Skills

Life skills – Personal and reproductive Health, love, sex, marriage and family – family life education – Gender Equity - child bearing and Childrearing practices, Geriatric Care - adjustability Human Relationship – formal and informal - peer group – friends – same and other gender - family – Colleagues – community – emotional intelligence - Stress Coping skills – Definition of stress, strategies to alleviate stress, problem and emotion focused coping, techniques to reduce stress, stress reaction phases, crisis intervention steps, creating positive affirmations, Signs, Symptoms and Reactions of Stress.

Unit – V: Social Skills

Human Rights Education, Understanding Human Rights, International and national mechanisms, protection and preservation
of HRs, Human Rights in the context of new, technological and
electronic society, **Peace Education**, Social Harmony in the context
of religious fundamentalism and fanaticism, Understanding Peace
and Justice, Conflict Resolution Strategies

**Reference books**

1. Healing Your Emotional Self: A Powerful Program to Help You Raise Your Self-Esteem, Quiet Your Inner Critic, and Overcome Your Shame by Beverly Engel
2. Self-knowledge and self-discipline by B. W. Maturin
3. Motivation: Biological, Psychological, and Environmental (3rd Edition) by Lambert Deckers
4. Getting Things Done: The Art of Stress-Free Productivity by David Allen
5. Managerial Skills in Organizations by Chad T. Lewis

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**OUTSIDE THE CLASS HOURS (2 hrs)**

- Each student will choose either of the above-mentioned modules and is expected to undergo a training/workshop in that module.
- She/he will have to accomplish ten hrs outside the class hours to fulfill the 2 credits.
Methodology
Inputs, ABL model, Documentaries, group activities and Interaction, Special workshop by professionals.

Evaluation
There will be end test and a Project for ‘inside the class hours’. Viva Voce will be conducted for the ‘Outside the class hours’.

16PCH3MC01 MAIN GROUP ELEMENTS AND NUCLEAR CHEMISTRY

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Objectives
1. To know the structure and bonding in inorganic chains, rings, and cages.
2. To identify ligands of main group elements and complexing agents for main group metals.
3. To identify specific reagents of main-group elements used in synthesis.
4. To understand theory of radioactivity and applications of radioisotopes.
5. To know the working principle and safety features of nuclear reactors.

Unit-1: Inorganic Chains, Rings, and Cages
1.1 Catenation and hetero catenation: allotropes of carbon, graphite, diamond, fullerenes, carbon nanotubes and graphenes. Hetero catenation-by coupling cyclic silicon and phosphorous compounds.
1.2 Alkali and alkaline earth metal complexes: complexes of β-diketones, crown ethers, cryptands, and calixarenes; biological roles of alkali and alkaline earth metal ions and ionophores.
1.3 Electron deficient, electron precise, and electron rich compounds: boranes and carboranes: synthesis of neutral boron hydrides, polyhedral borane anions and dianions, structure of polyhedral boranes- nido-, arachno-, and closo-frameworks, general formula, PSEPT (Wade’s rules) and polyhedral geometries; carboranes-synthesis and polyhedral geometries, metalloboranes, and metallocarboranes. Silanes and cyclopoly silanes, hydrometallation-hydroboration and hydrosilylation. Hydroboration reaction as precursor for metalloborane and heteroborane clusters. Styx number. Synthetic importance of diborane, boranes.

Unit-2 Nitrogen and Sulphur Compounds
2.1 Boron-nitrogen compounds: azaboranes, pyrazaboles, borazines, and B-N clusters.
2.2 Silicates: classification-orthosilicates, noncyclic silicate anions, cyclic silicate anions, infinite chain anions, infinite sheet anions, framework minerals, and zeolites-typical examples and structure, cyclic siloxanes
2.3 Poly acids: structure of isopoly and heteropoly anions and polycations of W and Mo.
2.4 P-N and P-S compounds: polyphosphazene, cyclophosphazenes, and cyclic aminophosphanes, phosphorus-oxide and phosphorus-sulfide cages.
2.5 Cyclic sulfur-nitrogen compounds: tetrathirane, polythiazyl, and SxNy compounds.

Unit-3: Main Group Organometallics and Reagents
3.1 Organometallic compounds of Li, Be, and Mg: synthesis and applications. Organometallic reagents-structure and bonding.
3.2 Organometallic compounds of Si and Al: silsesquioxanes, aryl- and alkyl silicon halides, aluminium alkyls.
3.3 Specific reagents of main-group elements: fluorinating
agents-ClF, ClF₃, and BrF₃ (harsh); SF₄, SbF₃, and SbF₅ (moderate)

3.4 Special techniques for the synthesis of air sensitive compounds: the vacuum line, plasmas, photochemical apparatus, and electrolysis. Synthetic importance of PCl₃, and silylating agents. Drying of solvents.

**Unit-4: Halogen and Noble Gas Chemistry**

4.1 Halogen oxides and oxo compounds: Dichlorine monoxide, chlorine dioxide, dibromine monoxide, and iodine pentoxide-preparation and properties; halogen oxyfluorides trioxohalo fluorides) and ionic oxyhalogen species.

4.2 Xenon oxides and fluorides: xenon trioxide, difluoride, tetrafluoride, xenon oxofluoride.

4.3 Halogen compounds of nitrogen: nitrogen trifluoride, tetrafluoro hydrazine, dinitrogen difluoride, haloamines, oxohalides, and nitrogen trifluoride oxide.

4.4 Sulfur fluorides: Synthesis and reactivity of disulfur difluoride, sulfur tetrafluoride, substituted sulfur fluorides.

4.5 Structure of halogen oxides and halogen oxo compounds with the aid of VSEPR model. Reactivity of the halides of N, S, and Xe and applications.

**Unit-5: Radiochemistry and Nuclear Reactions**

5.1 Introduction. Types of nuclear reactions: Spallation, fusion-hydrogen bomb, stellar energy, nuclear fission-theory of nuclear fission; chain reaction, nuclear cross section, critical mass; atom bombs, nuclear fission reactors, breeder reactors-fuels used in nuclear reactors, moderators, coolants; nuclear fusion; separation of isotopes, nuclear reactors in India.

5.2 Measurement of radioactivity: ionization chamber, GM counters, scintillation counters.

5.3 Reprocessing of spent fuels: Nuclear waste streams from nuclear reactors, sequestering agents for radioisotopes,
solvent extraction and ionic liquid technology.

5.4 Applications: Dating of objects-principles, $^{14}$C dating (specific examples) and applications, neutron activation analysis, isotopic dilution and labeling studies, nuclear medicine-$^{99m}$Tc radiopharmaceuticals.

5.5 Isotopes used in nuclear fission reactions. Use of radioisotopes in noninvasive imaging techniques and in nuclear medicine.

Text books

References
Objectives
1. To know the limitations of quantum chemistry and classical thermodynamics in the evaluation of macroscopic properties.
2. To understand the interlinking of quantum chemistry and statistical thermodynamics that leads to classical thermodynamics.
3. To apply the concepts of statistical thermodynamics for the study of equilibrium reactions and reaction rates

Unit 1: Classical Thermodynamics (1+16+1 h)
1.3 Ternary systems involving three liquids. Solubility of ionic solids in water-Solubility curves. Ternary system involving water and two soluble ionic solids. Formation of double salts.

Unit 2: Irreversible Thermodynamics (1+10+1 h)
2.1 Near equilibrium process: General theory- Conservation of mass and energy- Entropy production in open system by heat, matter and current flow; Force and flux.
2.2 Onsager theory: Validity and verification – Principle of microscopic reversibility, Onsager reciprocal relations.
2.3 Thermoelectricity-Electro kinetic and thermo mechanical effects
2.4 Application of irreversible thermodynamics to biological and non-linear systems.

**Unit 3: Statistical Concepts of Thermodynamics** (1+13+1 h)

3.1 Macro and micro states: Distribution of particles in different energy levels. Maxwell- Boltzmann statistics. Distribution of molecular velocities.

3.2 Partition functions: Canonical and molecular partition functions. Separation of partition functions. Translational, rotational, vibrational and electronic partition functions. Interpretation of partition function.

3.3 Statistical approach to Thermodynamic properties: Internal energy, entropy, enthalpy, Helmholtz function, pressure, Gibbs function, residual entropy, equilibrium constant, average energies and equipartition principle. Heat capacity of mono and diatomic gases. Ortho- and para hydrogen, heat capacity of solids- Einstein and Debye models.


3.5 Statistical approach to equilibrium constants – Free energy function

**Unit 4: Kinetics of reactions in gas phase and in solutions and catalysis** (1+23+1 h)

4.1 Theories of reaction rates - Kinetic theory of collisions – bimolecular, unimolecular - Lindemann - Christiansen hypothesis, Hinshelwood treatment, bimolecular reactions in gas phase (involving atoms and free radicals) potential energy surface. Conventional transition state theory -Evaluation of thermodynamic parameters of activation, application of ARRT to reactions between atoms, molecules and atoms & molecules- time and true order.
4.2 Factors determining reaction rates in solution - ionic strength - primary and secondary salt effects, dielectric constant – concept of electrostriction, hydrostatic pressure - volume of activation.


**Unit 5: Kinetics of Complex and fast Reactions** (1+18+1 h)

5.1 Rate expressions for opposing, parallel and consecutive reactions; Chain reactions – chain length, Rice-Herzfeld pyrolysis of acetaldehyde, hydrogen-halogen (thermal and photochemical) reaction, Gas phase auto oxidation; explosion and explosion limits.


5.3 Flow techniques - relaxation theory and relaxation techniques - Temperature, Pressure, electric field and magnetic field jump methods; Flash photolysis and pulse radiolysis.

**Text Books**


References

16PCH3MC03 SCIENTIFIC RESEARCH METHODOLOGY AND COMMUNICATIONS

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Objectives
1. To introduce the purpose and importance of research for future development.
2. To know the various indexes and abstracts in science and technology.
3. To learn literature search for current awareness and for retrospective survey.
4. To know the methodology of writing thesis and journal articles.
Unit-1: Meaning of Research (1+9+1 h)
1.1 The search for knowledge, purpose of research, nature of scientific knowledge, scientific method, role of theory, characteristics of research. Types of research: fundamental or pure research, applied research, action research, historical research, experimental research.
1.2 Assessment and evaluation-purpose and general methodology.

Unit-2: The Chemical Literature (1+11+1 h)
2.1 Sources of chemical information: primary, secondary and tertiary sources. Indexes and abstracts in science and technology.

Unit-3: The Chemical abstract services (1+8+1 h)
3.1 The Chemical Abstracts: Current awareness searching: CA weekly issues, CA issue indexes. Retrospective and forward searching. CA Collective indexes: Collective index (CI), decennial index (DI).
3.2 Access points for searching CA indexes: index guide, general subject terms, chemical substance names, molecular formula, ring systems, author names, patent numbers. Locating the reference: finding the abstract, finding the original document, chemical abstract service source index.
3.4 Journal home pages.

Unit-4: The Scientific Writing (1+13+1 h)
4.1 Scientific writings: research reports, thesis, and journal articles. Requirement of technical communications:
eliminating wordiness and jargon-tautology, redundancy, imprecise words, superfluous phrases. Lab notebook maintenance.

4.2 Steps to publishing scientific articles in journals: types of publications-communications, articles, reviews; where to publish, specific format required for submission, organization of the material.

4.3 Documenting: abstracts-indicative or descriptive abstract, informative abstract, footnotes, end notes, referencing styles, bibliography-journal abbreviations (CASSI), abbreviations used in scientific writing.

Unit-5: Seminar-Scientific Communication (1+9+1 h)

5.1 Recent Advancements in Chemistry: Supramolecular Chemistry, Green Chemistry, Material Chemistry, Organic Synthesis, Nano materials, chemistry,

Text Books

References
Objectives
The students will be able to
1. apply the concepts of equilibrium, thermodynamics, phase rule and colligative properties to various experiments.
2. acquire analytical skills for quantitative analysis.

Experiments
1. Verification of Freundlich adsorption isotherm – Study of adsorption acetic acid or oxalic acid on charcoal and determination of concentration of the given acid.
2. Construction of Phase diagram for two components – Compound forming systems: Diphenylamine – Benzophenone.
3. Determination of equilibrium constant for the formation of potassium triiodide from iodine and KI and the concentration of unknown potassium iodide solution.
4. Comparison of acid strengths using acid catalysed hydrolysis of methyl acetate.
5. Determination of rate constant and order for the reaction between potassium persulphate and potassium iodide and determine the temperature coefficient and energy of activation.
6. Kinetic study of acetone and iodine in acidic medium and the determination of order with respect to acetone and iodine.
7. Determination of order of saponification of ethyl acetate by sodium hydroxide.
8. Study the primary salt effect on the kinetics of ionic reactions and test the Bronsted relationship (iodide ion is oxidized by persulphate ion).
9. Determination of energy of activation for the acid catalysed hydrolysis of methyl acetate.
12. Determination of heat of solution of oxalic acid from solubility and thermometric measurements.

Text Books
2. Sundaram, Krishnan, Raghavan, Practical Chemistry (Part II), S. Viswanathan Co. Pvt., 1996.

References

16PCH3ES01 APPLIED ORGANIC CHEMISTRY

SEMMESTER  III  
CATEGORY  ES(T)  
CREDITS  3  
NO.OF HOURS/ WEEK  4

Objectives
1. To understand the elements of chemical engineering in organic synthesis
2. To appreciate the techniques involved in environment friendly organic synthesis

~ 55 ~
Unit -1: Organic Chemical Technology (1+13+1 h)
1.1 Unit operations in chemical engineering: Fluid flow: Reynold’s number; Bernoullis’ equation, Turbulent flow. Mass transfer: Distillation - two and three component systems. Leaching and extraction; stirrers and driers.
1.2 Energy balance over a flow system, heat of reaction, Chemical equilibrium, entropy changes, vapour phase and liquid phase catalytic reactions.
1.3 Factors affecting chemical process kinetics, scaling up of reactions from laboratory to pilot plant to main plant; Materials of construction; Study of industrial scale nitrations, sulphonation and halogenations reactions.
1.4 Quality control, R & D, standardization.

Unit-2: Organometallic Compounds (1+8+1 h)
2.1 Synthesis and reactions involving organolithium (n-BuLi, PhLi), organocadmium, organomagnesium, organopalladium, organoselenium, organocobalt, organoaluminium, and organocopper.
2.2 Reactions promoted by samarium diiodide and dicyclopentadienyl samarium – Barbier type reaction, ketyl-alkene coupling reactions, pinacolic coupling reactions, acyl anion reactions and McMurray olefination.

Unit-3: Polymer supported Reagents in Organic Synthesis (1+8+1 h)
3.1 Introduction, choice of polymers, properties and advantages of polymer support and reagents.
3.2 Intramolecular cyclization reactions, bromination by using poly-N-bromosuccinimide, use of polystyrene carbodiimide.
3.3 Acylation with polystyrene anhydride, diazotransfer reaction, Wittig reactions, alkylation, oxidation with peracid and chromic acid, use of polymer supported photosensitizers.

~ 56 ~
Unit-4: Green Chemistry, (1+8+1 h)
4.1 Green methods, green products, recycling waste. Twelve principles of green chemistry.
4.2 Designing green synthesis-Green reagents: dimethyl carbonate, polymer supported reagents. Green solvents: water, ionic liquids, deep eutectic solvents, supercritical carbon dioxide. Solid state reactions: solid phase synthesis, solid supported synthesis.

Unit-5: Microwave Synthesis, Sonochemistry and Phase Transfer reactions (1+13+1 h)
5.1 Microwave assisted synthesis: Principle, instrumentation, types, limitations and precautions. Applications: Esterification, deprotection of esters and ethers, C- and N-alkylation and condensation of active methylene compounds, rearrangement reactions, synthesis of enamino-ketones and electrophilic alkenes.
5.2 Sonochemistry: Principle, instrumentation, types and precautions. Applications: Esterification, hydrolysis, substitution and addition reactions, oxidation and reduction reactions, coupling reactions.
5.3 Types of phase transfer catalysts, Mechanism and advantages, Preparation of quaternary ammonium salts and crown ethers. Application: Substitution, esterification, addition, condensation and polymerization reactions.

Text books

References

16PCH3ES02 PHYSICAL CONCEPTS IN INORGANIC CHEMISTRY

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Objectives:
1. To quantify bonding parameters in cubic and distorted geometries from absorption spectra.
2. To identify coordination compounds with noble electrochemical and photochemical properties suitable for the construction of supramolecular assemblies and nanostructures.
3. To understand the importance of inorganic
photosensitizers for solar energy conversion.

4. To familiarize the applications of photochemistry in metal complexes

UNIT-1: Electronic Structure and Geometry of Coordination Compounds (1+12+1 h)

1.1 Electronic spectroscopy of metal complexes: principles, classification of electronic spectra, factors influencing band shape–crystal field spectra of $O_h$ and $T_d$ complexes, Jahn-Teller effect. Spectrochemical series, structural evidence from electronic spectra, evaluation of $D_o$ and $D_t$ values in $O_h$ and $T_d$ complexes of Co(III) and Ni(II), quantification of covalency nephelauxetic ratio.

1.2 Tetragonal distortion in octahedral complexes and evaluation of $D_{q_{xy}}$ and $D_{q_z}$ in tetragonally distorted octahedral Co(III) complexes. Causes of tetragonal distortion in transition metal complexes and effect on their electronic spectra.

1.3 Infrared and Raman Spectroscopy-functional group interpretation. Determination of coordination sites and linkage isomers ($\text{NO}_2^-$, $\text{SCN}^-$, $\text{ClO}_4^-$), Assigning denticity of ligands ($\text{SO}_4^{2-}$ and $\text{CO}_3^{2-}$), Effect of coordination on ligand vibrations-$\text{NH}_3$, $\text{H}_2\text{O}$, glycine, $\text{PPh}_3$, 2,2'-bipyridine, 1,10-phenanthroline.

1.4 Raman effect and molecular structure-CO, HCN, CO$_2$, N$_2$O and H$_2$O. Applications of resonance Raman spectroscopy to structural elucidation of the active sites in heme and non-heme oxygen carriers.

UNIT-2: Spin Resonance Spectroscopy and Characterization of Coordination Compounds (1+11+1 h)

2.1 Nuclear magnetic resonance spectroscopy: NMR spectra of quadrupole nuclei, effect of quadrupole nuclei on spin-spin splitting and hyperfine splitting. NMR of paramagnetic transition metal complexes: scalar shift, pseudo contact shift and covalency. Fluxional
isomerism.

2.2 Electron spin resonance spectroscopy: principle-hyperfine and zero field effects, nuclear quadrupole interaction. Interpretation of g in cubic, axial rhombohedral geometry, factors affecting ‘g’ values. Calculation of $g_{\perp}$ and $g_{\parallel}$ (Cobalt complexes)–metal-ligand covalency. Huxional behaviour in coordination compounds.

2.3 EPR spectra of bis(salicylaldimine)copper(II), [(NH$_3$)$_5$–Co–O$_2$–Co(NH$_3$)$_5$]$^{5+}$, diethylidithiophosphinato copper(II), Co(II)-phthalocyanin complex, K$_2$[IrCl$_6$]. Interpretation of ‘g’ and ‘A’ values from ESR spectral data in MnF$_6^{4+}$, CoF$_6^{4+}$ and CrF$_6^{3-}$. ESR spectra of dinuclear Cu(II) complexes. Nuclear quadrupolar interaction–CuK$_2$(SO$_4$)$_2$.6H$_2$O

2.4 Mossbauer spectroscopy: principle, isomer shift and site symmetry of metal ions in coordination compounds. Applications-low and high spin Fe(II) and Fe(III) complexes, π-bonding effects in iron complexes, spin crossover in Fe(II) complexes. Identification of diamagnetic and covalent compounds - Structural aspects of Iron carbonyls, Fe[Fe(CN)$_6$], [Fe$_3$(CO)$_{12}$], FeSO$_4$.7H$_2$O, FeCl$_3$, K$_4$[Fe(CN)$_6$], K$_3$[Fe(CN)$_6$] and Iron-sulphur Proteins. Tin compounds-tin halides and organotin compounds. Iodine compounds-isomer shifts of $^{127}$I and $^{129}$I-applications to alkali metal iodides and molecular iodine.

UNIT- 3: Electrochemical Studies and Photochemistry

(1+8+1 h)


3.2 Solar and renewable energy: light-to-chemical energy

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conversion in lamellar solids and thin films, solar energy conversion by dye-sensitized photovoltaic cells and by coordination compounds anchored onto semiconductor surfaces. Photochemical activation and splitting of water, CO₂ and N₂.

3.3 Photochemistry of lanthanide complexes: A-E-T-E processes, NIR-to-visible photon up conversion, nonlinear optical behavior, exciton multiplication and relaxation dynamics in quantum dots and applications. Ru(II) and Os(II) polypyridyl complexes employed in solar energy conversion.

Unit-4 Photochemistry of transition metal complexes

(1+9+1 h)

4.1 Adamson’s Model, Photoreactions-photoaquation, substitution reactions, photoracemisation reaction of Cr(III), Co(III) and Cu(II) complexes

4.2 Manganese based photo systems for water-splitting.

4.3 Complexes of Rh, Ru, Pd and Pt-photochemical generation of hydrogen from alcohol, photocarbonylation of hydrocarbon, photocatalytic hydrogenation of alkene, photochemical reaction of water.

Unit-5 Photoinduced electron transfer

(1+10+1 h)

5.1 Electron transfer (ET)–photoinduced ET in chromophore–quencher, MLCT-ET schemes for type-1 and type-2 metal organic dyads.

5.2 Thermodynamics of photoinduced electron transfer: electron transfer theory, experimental determination of rates of photo induced intramolecular electron transfer, [Ru(bpy)_3]^{2+}, Marcus free energy relationship.

5.3 Electrochemistry and photophysics of monoquat(N-methyl-4,4'-bipyridine) to [Ru(bpy)_3]^{2+} chromophore. Inner sphere acceptors and donors of bpy ligands, aromatic amine, electro donors, driving force dependence for ET, phenothiazine electron donor,
pyrazole and polypyridine.

Text Books

References
2. D. C. Neckers, G. V. Bunav, W. S. Jenks, Advances in


16PCH3TP01 SUMMER TRAINING PROGRAMME

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Objectives:

1. A staff member of a department (GUIDE) will be monitoring the performance of the candidate.

2. The summer training program falls between Semester II and III. Students are expected to undergo this training soon after the second semester examinations.

3. The training will commence not later than one week after the completion of the semester examination.

4. Organizations for the summer placement must be confirmed before the commencement of the second continuous internal tests.

5. Students must submit letter of induction to the respective guide within the first week of the internship.

6. The student has to spend a total of 20 working days in the respective field.

7. Students are expected to submit weekly reports along with daily time sheets to the respective supervisors.

8. The reports will be used to evaluate the student’s performance.

9. Students should submit a letter of completion from the organization duly signed by the authorities.

10. If the staff is satisfied with the performance of student, he/she will be marked “COMPLETED” at the end of the semester and the details will be submitted to COE office through the HOD.
Objectives:

1. To introduce and give an insight into the fascinating area of solid state physics, solid state chemistry and material science.
2. This will enable the students in pursuing higher studies and go for research.

Unit 1: Crystallography (1+23+1 h)

1.1 Introduction - Crystal planes and directions – Unit cells, Miller indices, Two and three dimensional space lattices, crystal systems, reciprocal lattices, symmetry elements (2D &3D), matrix representation of symmetry operations, point groups (2D & 3D) operators - proper and improper axis, mirror planes, Glide planes, screw axis, derivation of space groups (2D and 3D).

1.2 Crystal structure – Analysis by powder X-ray diffraction and single crystal analysis, single crystal analysis and its applications. Electron charge density maps, neutron diffraction – method and applications.


1.4 Characterization techniques – TG, DTA and DSC methods, SEM and TEM Analysis -working principle and instrumentation. Determination of hardness, elastic behavior - Atomic model of elastic behavior. Modulus as parameter in design rubber like elasticity. Plastic deformation–tensile stress – strain curve. Deformation...
by slip. Work hardening and dynamic recovery - Effect of grain size and dislocation motion.

**Unit 2: Properties of crystals - Optical, dielectric and diffusion studies** (1+18+1 h)

2.1 Optical studies - Electromagnetic spectrum (qualitative) – refractive index – reflectance – transparency, translucency and opacity. Types of luminescence – photoluminescence, cathodoluminescence and electroluminescence.

2.2 Dielectric studies- Polarisation - electronic, ionic, orientation, and space charge polarisation. Effect of temperature on dielectric constant. Dielectric loss. Types of dielectric breakdown – intrinsic, thermal, discharge, electrochemical and defect breakdown.


**Unit 3: Special Materials** (1+13+1 h)

3.1 Semiconductors - Types of semiconductors - intrinsic and extrinsic, direct and indirect band gap, Elemental and compound semiconductors. Defect semiconductors- stoichiometric and non-stoichiometric defects. Applications: p-n junction as transistors and rectifiers, photovoltaic and photogalvanic cell, photoelectrocatalytic splitting of water using TiO₂, SrTiO₃, ZnO, TiO₂₋ₓFₓ and WO₃₋ₓFₓ.

3.2 Superconductivity: Meissner effect, Critical temperature and critical magnetic Field, Type I and Type II superconductors, BCS theory of superconductivity - Cooper pair of electrons, Applications of superconductors.

3.3 Soft and hard magnets - Domain theory - Hysteresis Loop - Applications. Magneto resistance and giant
magneto resistance (GMR) materials. Ferro, ferri and antiferromagnetic materials - examples and applications, magnetic parameters for recording applications.

3.4 Ferroelectric, Piezoelectric, and pyroelectric materials – properties and applications. Shape memory Alloys - characteristics and applications, Non- linear optics - Second Harmonic Generators (SHG), mixing of Laser wave lengths by quartz, ruby and LiNbO₃.

Unit 4: Polymers (1+13+1 h)
4.1 Introduction - Monomers, Oligomers, Polymers and their characteristics. Plastics, elastomers, fibres, homopolymers and co-polymers. Bonding in polymers: Primary and secondary bond forces in polymers; cohesive energy. Determination of Molecular mass of polymers: Number Average molecular mass (Mₙ) and Weight average molecular mass (Mₔ) of polymers.


4.3 Reactions of polymers – Hydrolysis, acidolysis, aminolysis, addition and substitution reactions.

4.4 Conducting Polymers: Polyphenylene, polypyrrole and polyacetylene.

4.5 Polymer Processing Techniques - Calendaring, die casting, compression moulding, injection moulding, blow moulding and reinforcing.

Unit 5: Nanomaterials (1+13+1 h)
5.1 Synthesis - Physical and chemical methods - inert gas condensation, arc discharge, laser ablation, sol-gel method, solvothermal and hydrothermal method, chemical vapor deposition (CVD) - reaction types,
different kinds of CVD techniques - metallo organic CVD (MOCVD), plasma enhanced CVD (PECVD), and low pressure CVD (LPCVD).


5.3 Surface characterization - AFM and STM (principle, instrumentation and applications).

5.4 Applications – Nanomaterials for environmental remediation – nanomaterials as sorbents, nanofiltration, and nanoscale biopolymers and nanoreactors for remediation.

Books for study
Books for reference:

16PCH4MC01 ORGANIC SYNTHESIS AND PHOTOCHEMISTRY

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Objectives
1. To understand the molecular complexity of carbon skeletons and the presence of functional groups and their relative positions.
2. To apply disconnection approach and identifying suitable synthon to effect successful organic synthesis.
3. To study various synthetically important reagents for any successful organic synthesis
4. To learn the concepts of pericyclic reaction mechanisms.
5. To gain the knowledge of photochemical organic reactions.

Unit 1: Reagents for Organic Synthesis (1+16+1 h)
1.1 Reagents for functional group transformations: Lithium diisopropylamide (LDA), Gilmann reagent, dicyclohexylcarbodimide (DCC), dichlorodicyanoquinone (DDQ), Silane reagents-trialkylsilyl halides, trimethylsilyl cyanide, trimethylsilane, t-butyldimethylsilane.
1.2 Crown ethers, cyclodextrins, Ziegler-Natta catalyst, diazomethane, Stark enamine reaction, phosphorous ylides- Wittig and related reactions, sulphur ylides– reactions with aldehydes and ketones, 1,3-dithiane anions, Peterson reaction.

Unit 2: Modern Synthetic Reactions (1+21+1 h)
2.1 Chromium and manganese reagents (PCC, PDC, Jones reagent, MnO₂), Oxygen (singlet and triplet), ozone, peroxides and peracids, lead tetraacetate, periodic acid, NBS, chloramine-T, Sommelet oxidation, Oppenauer oxidation, Fenton’s reagent, Sharpless asymmetric epoxidation.
2.2 Catalytic hydrogenation (homogeneous and heterogeneous) – catalysts (Pt, Pd, Rh-C, Ni, Ru), Wilkinson catalyst, LiAlH₄ and derivatives of LAH, NaBH₄, DIBAL-H, Sodium cyanoborohydride, dissolving metal reactions (Birch reduction). Leukart reaction (reductive amination) Diborane as reducing agent, Meerwein-Ponndorf-Verley reduction, tributyltin hydride, stannous chloride, and Baker’s yeast reduction.
2.3 Named Reactions: Suzuki coupling, Heck reaction, Negishi reaction, Baylis-Hillman reaction, Henry reaction Nef reaction, Kulikovich reaction, Ritter

2.4 Electroorganic synthesis: Electro-oxidation and -reduction reactions.

**Unit 3: Organic Synthetic Methodology** (1+16+1 h)

3.1 Retrosynthetic analysis; Alternate synthetic routes. Synthesis of organic mono and bifunctional compounds via disconnection approach. Key intermediates, available starting materials and resulting yields of alternative methods.

3.2 Convergent and divergent synthesis, Synthesis based on umpolung concepts of seebach. Protection of hydroxyl, carboxyl, carbonyl, thiol and amino groups. Illustration of protection and deprotection in synthesis.

3.3 Control elements: Regiospecific control elements. Use of protective groups, activating groups, and bridging elements. Stereospecific control elements. Functional group alterations and transposition.

**Unit 4: Pericyclic Reactions** (1+12+1 h)

4.1 Woodward Hoffmann rules; The Mobius and Huckel concept, FMO method and correlation diagrams.

4.2 Cycloaddition and Cheletropic reactions; [2+2], [2+4], [6+4] and 1,3-dipolar cycloadditions; Electrocyclization reactions of conjugated dienes and trienes. Sigmatropic rearrangements: (1,3), (1,5), (3,3) and (5,5)-carbon migrations, degenerate rearrangements. Group transfer reactions.

**Unit 5: Organic Photochemistry** (1+15+1 h)

5.1 Photochemical excitation: Experimental techniques; electronic transitions; Jablonskii diagrams; intersystem
crossings; energy transfer processes; Stern Volmer equation.

5.2 Reactions of electronically excited ketones; $\pi \rightarrow \pi^*$ triplets; Norrish type-I and type-II cleavage reactions; photo reductions; Paterno-Buchi reactions; photochemistry of $\alpha,\beta$-unsaturated ketones; cis-trans isomerisation.

5.3 Photon energy transfer reactions, Photocycloadditions, Photochemistry of aromatic compounds; photochemical rearrangements; photostationary state; di-$\pi$-methane rearrangement; Reaction of conjugated cyclohexadienone to 3,4-diphenyl phenols; Barton’s reactions; Low temperature photochemistry, Flash photolysis.

Text Books

References

**16PCH4MC02 ELECTROCHEMISTRY**

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**Objectives:**

1. To understand the behavior of electrolytes in solution.
2. To know the structure of the electrode surface.
3. To understand the importance of electrode kinetics and to know the applications of electrode process.

**Unit 1: Ionics**

(1+21+1 h)


1.3 Evaluation of thermodynamic quantities – ΔG, ΔH and ΔS. Calculation of \( K_a \), \( K_b \), \( K_{sp} \), \( K_w \), \( K_h \) and pH using emf data.
Unit 2: Electrical Double Layer (1+10+1 h)

2.1 Interfacial phenomena - Evidences for electrical double layer, polarisable and non-polarisable interfaces. Electrocapillarity - Lipmann’s equation, electro capillary curves. Electro-kinetic phenomena electro-osmosis, electrophoresis, streaming and sedimentation potentials, mention of colloidal and poly electrolytes.

2.2 Structure of electrical double layer: Helmholtz-Perrin, Guoy-Chapmann and Stern models of electrical double layer- Applications and limitations.

Unit 3: Electrodics of Elementary Electrode Reactions (1+15+1 h)

3.1 Behavior of electrodes: Standard electrodes and electrodes at equilibrium. Ohmic and non-Ohmic behaviors. Study of electrode reaction. The model of three electrode system. Sign conventions. Rates of electro chemical reactions. Over potential and chemical & electro chemical conditions for the discharge of ions.


Unit 4: Electrodics of Multistep Multi Electron System (1+16+1 h)

4.1 Rates of multi-step electrode reactions, Butler - Volmer equation for a multi-step reaction (examples of multi
electron reactions). Rate determining step of an electrode reaction. Transfer coefficients and stoichiometric number.

4.2 Electro-chemical reaction mechanisms Proposal of electro-chemical reaction mechanisms- Electrochemical reaction order. Surface coverage - Rate expressions. Reduction of (i) $I_3^-$ and (ii) $Fe^{2+}$. Dissolution of iron to iron (II). Overvoltage and evolution of oxygen and hydrogen at different pH. Symmetry factors vs transfer coefficients. Corrosion and passivation of metals-Pourbiax and Evan’s diagrams.

**Unit 5: Concentration Polarisation and Electroanalytical Techniques** (1+18+1 h)

5.1 Transport of the electro active species to electrode- Different types of over voltages-Chemical and electro chemical over potentials. Phase, activation and concentration over potentials.

5.2 Diffusion, migration and hydrodynamic modes of transports. The role of supporting electrolytes. Polarography- principle and applications, principle of square wave polarography, cyclic voltammetry-, anodic and cathodic stripping voltammetry, differential pulse voltammetry and amperometric titrations.

5.3 Electrochemical process as source of energy – sodium and lithium ion batteries, solid oxide fuel cells, electrocatalysis – anodically and cathodically initiated processes.

**Text Books**


References

16PCH4MC03 PHYSICAL CHEMISTRY PRACTICAL – II

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Objectives
1. To understand and apply the concepts of electrochemistry.
2. To learn sample handling in different experimental techniques.
3. To learn the operations of instrumentals techniques for quantitative estimation.

Experiments
1. Determination of the equivalent conductance at different concentrations and to examine the validity of the Onsager’s theory as limiting law at high dilutions for a strong electrolyte.
2. Verification of Ostwald’s dilution Law and determination of dissociation constant of weak acid or weak base.
3. Conductometric titration of mixture of strong and weak acids with a strong base.
4. Comparing the relative strengths of acetic and monochloro acetic acid by conductance method.
5. Determination of solubility product of inorganic compounds using conductometer.
6. Determination of the strength of Fe (II) by potentiometric redox titration.
7. Determination of the amount of KCl and KI present in a mixture by potentiometric titration.
8. Determination of pK_{a1} and pK_{a2} of a weak dibasic acid by potentiometry.
9. Determination of dissociation constant of weak acid by potentiometry.
10. Calibration of a pH meter and measurement of pH of different buffer solutions.
11. Determination of pH of the given solution with the help of indicators using buffer solutions and by colorimetric method.
12. Determination of metal to ligand ratio of complexes by Job’s method using UV-visible Spectrophotometer.
14. Determination of the concentration of a given solution by studying the reversibility of a redox process by Cyclic voltammetry.
15. Estimation of iron, copper and nickel by spectrophotometric method.
16. Separation and analysis of mixtures using HPLC.

**Text Books**
2. Sundaram, Krishnan, Raghavan, Practical Chemistry (Part II), S. Viswanathan Co. Pvt., 1996.

**References**

**16PCH4PJ01 DISSERTATION/PROJECT**

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<td>NO. OF HOURS/ WEEK</td>
<td>15</td>
</tr>
</tbody>
</table>

**Objectives**
To make the student to understand and present a research finding on a topic in the subject related to Chemistry under the guidance of a department staff.

**Testing**
The student will be tested both in subject matter of the report and the mode of presentation in a review meeting to be held in

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the middle of the semester, with a panel of three senior staff of the department. This progress reporting will carry 20% marks. Upon submission of the project report to the office of the Controller of Examinations, the viva-voce examination will be conducted by the supervisor and the external expert suggested by the supervisor. The project report and the viva-voce will be evaluated for 80% marks.

**Project report:** 60 Marks

Standard of subject and plan
Preparation and mastery
Originality and logical development
Summary and references

**Viva-voce** 20 Marks

Economy of time
Communication
Blackboard use and teaching aids
Language and diction
Answer to questions