

B.Sc. Programme in CHEMISTRY

(Choice Based Credit System)

Core Papers: Chemistry (Theory & Practical)

Semester	Course Code	Name of the Course	Credits / Hours
I	CHC101	Inorganic Chemistry & Organic Chemistry	(6 credits: Theory-04, Practicals-02) Theory: 60 Hours (04 Credits) Practical: 60 Hours (02 Credits)
II	CHC102	Physical Chemistry & Organic Chemistry	
III	CHC103	Chemistry & Organic Chemistry	
IV	CHC104	Physical Chemistry & Inorganic Chemistry	

Skill Enhancement Course (SEC)

Semester	Course Code	Name of the Course	CREDITS/HOURS
III	CHS101	Natural Resources And Analysis	4 Credits: Theory -03, Practical-01 Theory: 45 Hours (03 Credits) Practical: 30 Hours (01 Credit)
IV	CHS102	Chemistry of Cosmetics and Perfumes	

F.Y.B.Sc CHEMISTRY

SEMESTER I

CHC-101: Inorganic and Organic Chemistry

Course Objectives: THEORY COURSE OBJECTIVES

Section A

- To discuss Bohr's theory, Quantum theory for structure of an atom.
- To draw the radial plots, probability distribution curves.
- To generalize the rules for electronic configuration of an atom.
- To explain the general characteristics of ionic compounds and covalent compounds.
- To discuss valence bond theory, VSEPR, and molecular orbital theory for covalent compounds.

Section B

- To understand the curved arrow notations in organic reaction mechanisms.
- To understand the concept of physical effects and electronic displacement with referenceto organic molecules.
- To understand the structure, shape and reactivity of organic molecules.
- To study the strength of organic acids and bases.
- To understand the aromaticity of compound.
- To understand the concept of isomerism, stereoisomerism, configuration, chirality andoptical rotation.
- To understand the difference between conformational and configurational isomers.
- To draw conformations with respect to ethane, butane and cyclohexane.
- To learn the interconversion of Wedge Formula, Newman, Sawhorse and Fischer representations.
- To understand rules for nomenclature and assigning configuration to configurationalisomers.

- To understand various methods of preparation and reactions of alkanes, alkenes and alkynes.

Course Structure

Section A: Inorganic Chemistry-1

(30 Lectures: 02 Credits)

Chapter 1: Atomic Structure:

(14 Lectures)

Review of: Bohr's theory and its limitations, dual behaviour of matter and radiation, de Broglie's relation, Heisenberg Uncertainty principle. Hydrogen atom spectra. Need of a new approach to Atomic structure.

What is Quantum mechanics? Time independent Schrodinger equation and meaning of various terms in it. Significance of ψ and ψ^2 , Schrödinger equation for hydrogen atom. Radial and angular parts of the hydrogenic wave functions (atomic orbitals) and their variations for 1s, 2s, 2p, 3s, 3p and 3d orbitals (Only graphical representation). Radial and angular nodes and their significance. Radial distribution functions and the concept of the most probable distance with special reference to 1s and 2s atomic orbitals. Quantum numbers and their significance, Discovery of spin, spin quantum number (s) and magnetic spin quantum number (ms). Shapes of s, p and d atomic orbitals, nodal planes.

Rules for filling electrons in various orbitals, Electronic configurations of the atoms. Stability of half-filled and completely filled orbitals, concept of exchange energy. Relative energies of atomic orbitals, Anomalous electronic configurations.

Chapter 2: Chemical Bonding and Molecular Structure

(16 Lectures)

Ionic Bonding: General characteristics of ionic bonding. Energy considerations in ionic bonding, lattice energy and solvation energy and their importance in the context of stability and

solubility of ionic compounds. Statement of Born-Landé equation for calculation of lattice energy, Born-Haber cycle and its applications, polarizing power and polarizability. Fajan's rules, ionic character in covalent compounds, bond moment, dipole moment and percentage ionic character.

Covalent bonding: VB Approach, Shapes of some inorganic molecules and ions on the basis of VSEPR and hybridization with suitable examples of linear, trigonal planar, square planar, tetrahedral, trigonal bipyramidal and octahedral arrangements.

Concept of Resonance and Resonating structures in various Inorganic and Organic compounds.

MO Approach, Rules for the LCAO method, bonding and antibonding MOs and their characteristics for s-s, s-p and p-p combinations of atomic orbitals, nonbonding combination of orbitals, MO treatment of homonuclear diatomic molecules of 1st and 2nd periods (including idea of s-p mixing) and heteronuclear diatomic molecules such as CO, NO and NO⁺. Comparison of VB and MO approaches.

Section B: Organic Chemistry – I

(30 Lectures: 02 Credits)

Chapter 1: Fundamentals of Organic Chemistry

(8 Lectures)

Curved arrow notation, drawing electron movement with arrows, half and double headed arrows, in organic reaction mechanisms.

Physical Effects, Electronic Displacements: Inductive Effect, Electromeric Effect, Resonance and Hyperconjugation. Cleavage of Bonds: Homolysis and Heterolysis.

Structure, shape and reactivity of organic molecules: Nucleophiles and electrophiles. Reactive Intermediates: Carbocations, Carbanions and free radicals.

Strength of organic acids and bases: Comparative study with emphasis on factors affecting pK values. Aromaticity: Benzenoids and Hückel's rule.

Chapter 2: Stereochemistry

(10 Lectures)

Concept of isomerism. Types of isomerism. Stereoisomerism, conformational isomerism. Conformations with respect to ethane, butane and cyclohexane. Interconversion of Wedge

Formula, Newmann, Sawhorse and Fischer representations. Concept of chirality (upto two carbon atoms). Configuration: Geometrical and Optical isomerism; Enantiomerism, Diastereomerism and Meso compounds). Threo and erythro; D and L; *cis* – *trans* nomenclature; CIP Rules: R/ S (for upto 2 chiral carbon atoms) and E / Z Nomenclature (for upto two C=C systems).

Chapter 3: Aliphatic Hydrocarbons

(12 Lectures)

Functional group approach for the following reactions (preparations & reactions) to be studied in context to their structure.

Alkanes: (Upto 5 Carbons). *Preparation:* Catalytic hydrogenation, Wurtz reaction, Kolbe's synthesis, from Grignard reagent. *Reactions:* Free radical Substitution: Halogenation.

Alkenes: (Upto 5 Carbons) *Preparation:* Elimination reactions: Dehydration of alkenes and dehydrohalogenation of alkyl halides (Saytzeff's rule); *cis* alkenes (Partial catalytic hydrogenation) and *trans* alkenes (Birch reduction). *Reactions:* *cis*-addition (alk. KMnO_4) and *trans*-addition (bromine), Addition of HX (Markownikoff's and anti-Markownikoff's addition), Hydration, Ozonolysis, oxymercuration-demercuration, Hydroboration-oxidation.

Alkynes: (Upto 5 Carbons) *Preparation:* Acetylene from CaC_2 and conversion into higher alkynes; by dehalogenation of tetra halides and dehydrohalogenation of vicinal-dihalides. *Reactions:* formation of metal acetylides, addition of bromine and alkaline KMnO_4 , ozonolysis and oxidation with hot alk. KMnO_4 .

Learning Outcomes

Theory

At the end of the course students will be able to:

- Interpret the atomic structure based on postulates of Bohr's theory, Quantum mechanics.
- Evaluate the stability and magnetic property based on molecular diagrams of homonuclear and heteronuclear molecules.

- Identify and use the curved arrow notations in organic reaction mechanisms.
- Explain the concept of physical effects and electronic displacement with reference to organic molecules.
- Describe structure, shape and reactivity of organic molecules.
- Interpret strength of organic acids and bases.
- Identify if the given organic compound is aromatic.
- Classify isomers giving examples.
- Discuss the concept of stereoisomerism, configuration, chirality and optical rotation.
- Distinguish between conformational and configurational isomers and also geometrical and optical isomers, giving examples.
- Draw conformations with respect to ethane butane and cyclohexane.
- Draw and interconvert Wedge Formula, Newman, Sawhorse and Fischer representations.
- Give the nomenclature and assign configuration to configurational isomers.
- Give various methods of preparation and reactions of alkanes, alkenes and alkynes.

Reference Books:

Inorganic Chemistry

1. Lee, J.D. *Concise Inorganic Chemistry* ELBS, 1991.
2. Cotton, F.A., Wilkinson, G. & Gaus, P.L. *Basic Inorganic Chemistry*, 3rd ed., Wiley.
3. Douglas, B.E., McDaniel, D.H. & Alexander, J.J. *Concepts and Models in Inorganic Chemistry*,

John Wiley & Sons.

4. Huheey, J.E., Keiter, E.A., Keiter, R.L. & Medhi, O.K. *Inorganic Chemistry: Principles of Structure and Reactivity*, Pearson Education India, 2006.

Organic Chemistry

1. Graham Solomon, T.W., Fryhle, C.B. & Snyder, S.A. *Organic Chemistry*, John Wiley & Sons (2014).
2. McMurry, J.E. *Fundamentals of Organic Chemistry*, 7th Ed. Cengage Learning India Edition, 2013.
3. Sykes, P. *A Guidebook to Mechanism in Organic Chemistry*, Orient Longman, New Delhi (1988).
4. Eliel, E.L. *Stereochemistry of Carbon Compounds*, Tata McGraw Hill education, 2000.
5. Finar, I.L. *Organic Chemistry* (Vol. I & II), E.L.B.S.
6. Morrison, R.T. & Boyd, R.N. *Organic Chemistry*, Pearson, 2010.
7. Bahl, A. & Bahl, B.S. *Advanced Organic Chemistry*, S. Chand, 2010.
8. Francis Carey, *Organic Chemistry*; 3rd Edition, Tata McGraw Hill India.
9. Paula Yurkanis Bruice, *Organic Chemistry*; 3rd Edition, Pearson Education Asia.
10. Jerry March, *Advanced Organic Chemistry*; 4rd Edition, John Wiley

SEMESTER I

CHC-101 LAB: Inorganic and Organic Chemistry (Practicals)

PRACTICAL COURSE OBJECTIVE

- To estimate the metal ions by volumetric methods employing redox and acid-basetitration concepts.
- To get hands on experience for the systematic qualitative analysis of the organic compounds.
- To learn the purification and separation techniques for organic compounds.

Course Structure

Section A-(Inorganic Chemistry)

(30 Hours: 01 Credit)

Volumetric Analysis:

(5 x 6 Hours = 30 Hours)

1. Estimation of sodium carbonate and sodium hydrogen carbonate present in a mixture.
2. Estimation of oxalic acid by titrating with KMnO_4 .
3. Estimation of water of crystallization in Mohr's salt by titrating with standardised KMnO_4 .
4. Estimation of Fe (II) ions by titrating it with $\text{K}_2\text{Cr}_2\text{O}_7$ using internal indicator.
5. Estimation of Cu (II) ions iodometrically using $\text{Na}_2\text{S}_2\text{O}_3$.

Section B:(Organic Chemistry)

(30 Hours: 01 Credit)

1. Purification of organic compounds: (2 x 4 Hours = 8 Hours)
 - i) Solids by recrystallization process using water and ethanol as solvent. Determination of melting point.
 - ii) Liquids by distillation process, a) acetone b) nitrobenzene. Determination of boiling point.
2. Determination of chemical type, detection of elements, group test for any one compound.

(4 Hours)

3. Identification of unknown organic compounds. **(12 Hours)**

i) Water insoluble solids (Acid, Base, Phenol and Neutral)

ii) Water soluble solid (Acid and Neutral)

4. Thin layer chromatographic techniques: plate preparation, spotting, Separation of mixtures by thin layer Chromatography: Measure the R_f value in each case (combination of two compounds to be given eg. Mixture of o- and p-nitroaniline). **(6 Hours)**

PRACTICAL COURSE OUTCOMES

- The students will acquire the skill and knowledge to carry out volumetric estimation of inorganic constituents.
- The students will be able to get hands on experience for the systematic qualitative analysis of the organic compounds and the purification and separation techniques for organic compounds.

Reference Books:

Inorganic Chemistry

1. Svehla, G. *Vogel's Qualitative Inorganic Analysis*, Pearson Education, 2012.
2. Mendham, J. *Vogel's Quantitative Chemical Analysis*, Pearson, 2009.

Organic Chemistry

1. Vogel, A.I., Tatchell, A.R., Furnis, B.S., Hannaford, A.J. & Smith, P.W.G., *Textbook of Practical Organic Chemistry*, Prentice-Hall, 5th edition, 1996.
2. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry* Orient-Longman, 1960.
3. Pandey, O.P., Bajpai D. N. & Giri S. *Practical Chemistry, Revised Edition*, (For BSc. I, II, III Year Students of All Indian Universities) S. Chand Company Pvt Limited, 2014.

F.Y.B.Sc Chemistry

SEMESTER II

CHC-101: Inorganic and Organic Chemistry

THEORY COURSE OBJECTIVES

Section A

- To define the terms and state laws involved in thermodynamics, thermochemistry and chemical equilibrium.
- To explain the concept of enthalpies of solution, buffer solutions.
- To derive the thermodynamic derivation of the law of chemical standard state, enthalpies of solution, chemical equilibrium and relationships between different equilibrium constants based on ideal gases.
- To solve numerical based on chemical energetics, chemical equilibrium and ionic equilibrium.

Section B

- To learn the preparation methods and reactions of aromatic hydrocarbons, alkyl and aryl halides, phenols, ethers and carbonyl compounds.
- To learn the various named reactions mentioned in the syllabus.
- To understand reactivity and relative strength of C-halogen bond in alkyl, allyl, benzyl, vinyl and aryl halides.
- To understand Benzyne mechanism with respect to aromatic nucleophilic substitution.
- To understand Pinacol-pinacolone rearrangement with mechanism.

PRACTICALS: COURSE OBJECTIVES

- To understand and develop the problem-solving skills and hands on

experience with reference to concepts studied in theory pH metry, thermochemistry.

- To understand the mechanism of reactions involved in organic preparation experiments and develop hands on experience with reference to basic laboratory techniques required for organic preparations.

SYLLABUS

Theory:

Number of hours: 60

Section A (Physical Chemistry- I)

1. Chemical Energetics (10 H)

Need of thermodynamics and the laws of thermodynamics. Important principles and definitions of thermochemistry. Concept of standard state and standard enthalpies of formations, integral and differential enthalpies of solution and dilution. Calculation of bond energy, bond dissociation energy and resonance energy from thermochemical data. Variation of enthalpy of a reaction with temperature – Kirchhoff's equation. Statement of Third Law of thermodynamics and calculation of absolute entropies of substances.

2. Chemical Equilibrium (8 H)

Free energy change in a chemical reaction. Thermodynamic derivation of the law of chemical equilibrium. Definition of ΔG and ΔG° , Le Chatelier's principle. Relationships between K_p , K_c and K_x for reactions involving ideal gases.

3. Ionic Equilibria (12 H)

Strong, moderate and weak electrolytes, degree of ionization, factors affecting degree of ionization, ionization constant and ionic product of water. Ionization of weak acids and bases, pH scale, common ion effect. Salt hydrolysis-calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Buffer solutions. Solubility and solubility product of sparingly soluble salts.

Section B (Organic Chemistry – II)

4. Aromatic hydrocarbons (8 H)

Preparation (case benzene): from phenol, by decarboxylation, from acetylene, from benzene sulphonic acid.

Reactions: (case benzene): electrophilic substitution: nitration, halogenation and sulphonation. Friedel-Craft's reaction (alkylation and acylation) (upto 4 carbons on benzene). Side chain oxidation of alkyl benzenes (up to 4 carbons on benzene).

5. Alkyl and Aryl Halides (8 H)

Alkyl Halides (Upto 5 Carbons) Types of Nucleophilic Substitution (SN_1 , SN_2 and SN_i) reactions. Preparation: from alkenes and alcohols; reactions: hydrolysis, nitrite & nitro formation, nitrile & isonitrile formation; Elimination vs substitution. Aryl Halides Preparation: (chloro, bromo and iodo-benzene case): from phenol, Sandmeyer & Gattermann reactions; Reactions (Chlorobenzene): Aromatic nucleophilic substitution (replacement by $-OH$ group) and effect of nitro substituent. Benzyne Mechanism: KNH_2/NH_3 (or $NaNH_2/NH_3$); Reactivity and Relative strength of C-halogen bond in alkyl, allyl, benzyl, vinyl and aryl halides.

6. Alcohols, Phenols, Ethers and Carbonyl Compounds (14 H)

Alcohols: Preparation: Preparation of 1° , 2° and 3° alcohols: using Grignard reagent, Ester hydrolysis, Reduction of aldehydes, ketones, carboxylic acid and esters.

Reactions: With sodium, HX (Lucas test), esterification, oxidation (with PCC, alk. $KMnO_4$, acidic dichromate, conc. HNO_3). Oppeneauer oxidation Diols: oxidation of diols using HIO_4 . Pinacol-Pinacolone rearrangement with mechanism.

Phenols: (Phenol case) Preparation: Cumene hydroperoxide method, from diazonium salts. Reactions: Electrophilic substitution: Nitration, halogenation and sulphonation.

Reimer-Tiemann Reaction, Gattermann-Koch Reaction, Houben–Hoesch Condensation, Schotten –Baumann Reaction.

Ethers (aliphatic and aromatic): Williamson’s synthesis of ethers. Cleavage of ethers with HI.

Aldehydes and ketones (aliphatic and aromatic): (formaldehyde, acetaldehyde, acetone and benzaldehyde)

Preparation: from acid chlorides and from nitriles. *Reactions* – Reaction with HCN, ROH, NaHSO₃, NH₂-G derivatives. Iodoform test. Aldol Condensation, Cannizzaro’s reaction, Wittig reaction, Benzoin condensation. Clemmensen reduction and Wolff Kishner reduction. Meerwein-Ponndorf Verley reduction.

PRACTICALS

Number of hours: 60

Section A

1. Thermochemistry (Any three) (18 H)

- i. Determination of heat capacity of the calorimeter.
- ii. Determination of enthalpy of neutralization of hydrochloric acid with sodiumhydroxide.
- iii. Determination of enthalpy of ionization of acetic acid.
- iv. Study of the solubility of benzoic acid in water and determination of ΔH .

2. Chemical Kinetics: (10 H)

- i. To study the effect of nature of reactants on the rate of reactions
- ii. Determination of relative strength between HCl and Urea hydrochloride for hydrolysis of methyl acetate Ionic equilibria.

3. pH measurements (2 H)

Measurement of pH of different solutions like aerated drinks, fruit juices, shampoos and soaps (use dilute solutions of soaps and shampoos to prevent damage to the glass electrode) using ph meter.

Section B

4. Preparations (30 H)

Mechanisms involved in the following reactions to be discussed.

Recrystallisation, determination of melting point and calculation of quantitative yieldsto be done.

Each preparation for

- a. Bromination of Phenol/Aniline
- b. (b) Benzoylation of amines/phenols
- c. 2,4-dinitrophenylhydrazone of benzaldehyde/acetophenone
- d. Nitration of acetanilide to p-nitroacetanilide.
- e. (e) Oxime of Cyclohexanone
- f. Chalcone from benzaldehyde and acetophenone
- g. Iodoform from acetone

LEARNING OUTCOMES

Theory

At the end of the course students will be able to:

- ② Define the terms involved in chemical energetics, chemical equilibrium, ionic equilibrium and state the laws used in thermodynamics, thermochemical equilibrium.
- ② Describe enthalpy, buffer solutions, factors affecting ionization.
- ② Derive and use the equations thermochemistry, chemical equilibrium and ionic equilibria to solve the numericals.
- ② Give methods of preparation and reactions of aromatic hydrocarbons, alkyl and aryl halides, phenols, ethers and carbonyl compounds.
- ② Identify and give the named reactions mentioned in the syllabus.
- ② Explain reactivity and relative strength of C-halogen bond in alkyl, allyl, benzyl, vinyl and aryl halides.
- ② Explain benzyne mechanism with respect to aromatic nucleophilic substitution.

Practical

At the end of the course students will be able to

- ② Understand the concepts of thermochemistry, pH metry, chemical kinetics.
- ② Develop skills of working and set up of calorimeter.
- ② Solve numericals on and verify the graph of chemical kinetics
- ② Discuss the mechanisms involved in the organic preparation experiments.
- ② Develop skills of common laboratory techniques including recrystallisation, recording of melting point required for organic preparations and perform calculations for quantitative analysis.

REFERENCE BOOKS

Section A

1. Bahl, A. & Bahl, B.S. Advanced Physical Chemistry, S. Chand, 2010.
2. J. N. Gurtu and Aayushi Gurtu, Undergraduate Physical Chemistry, Vol I, Vol II and Vol III Pragati Prakashan.
3. Barrow, G.M. Physical Chemistry Tata McGraw-Hill (2007).
4. Castellan, G.W. Physical Chemistry 4th Ed. Narosa (2004).
5. Kotz, J.C., Treichel, P.M. & Townsend, J.R. General Chemistry Cengage Learning India Pvt. Ltd., New Delhi (2009).
6. Mahan, B.H. University Chemistry 3rd Ed. Narosa (1998).
7. Petrucci, R.H. General Chemistry 5th Ed. Macmillan Publishing Co.: New York (1985).

Section B

1. Graham Solomon, T.W., Fryhle, C.B. & Snyder, S.A. Organic Chemistry, John Wiley & Sons, (2014).
2. McMurry, J.E. Fundamentals of Organic Chemistry, 7th Ed. Cengage Learning India Edition, 2013.
3. Sykes, P. A Guidebook to Mechanism in Organic Chemistry, Orient Longman, New Delhi (1988).
4. Finar, I.L. Organic Chemistry (Vol. I & II), E.L.B.S.
5. Morrison, R.T. & Boyd, R.N. Organic Chemistry, Pearson, 2010.
6. Bahl, A. & Bahl, B.S. Advanced Organic Chemistry, S. Chand, 2010.
7. Francis Carey, Organic Chemistry; 3rd Edition, Tata McGraw Hill India.
8. Paula Yurkanis Bruice, Organic Chemistry; 3rd Edition, Pearson Education Asia.
9. Jerry March, Advanced Organic Chemistry; 4th Edition, John Wiley.
10. Vogel, A.I., Tatchell, A.R., Furnis, B.S., Hannaford, A.J. & Smith, P.W.G., Textbook of Practical Organic Chemistry, Prentice-Hall, 5th edition, 1996.
11. Mann, F.G. & Saunders, B.C. Practical Organic Chemistry Orient-Longman, 1960.
12. Pandey, O.P., Bajpai D. N. & Giri S. Practical Chemistry, Revised Edition, (For BSc. I, II, III Year Students of All Indian Universities) S. Chand Company Pvt

Limited, 2014.

13. Khosla, B. D.; Garg, V. C. & Gulati, A. Senior Practical Physical Chemistry, R. Chand & Co.: New Delhi (2011).

S.Y.B.Sc Chemistry

SEMESTER III

CHC-103 Physical and Organic Chemistry

Course Objectives: THEORY COURSE OBJECTIVES

Section A (Physical Chemistry)

- To understand the difference between ideal and non-ideal solutions.
- To study phase diagrams of various systems and to apply the phase rule equation.
- To study the conductance of strong and weak electrolytes.
- To study reversible and irreversible cells and measurement of EMF.
- To solve the numerical problems based on standard electrode potentials and conductance measurement of solutions.

Section B (Organic Chemistry)

- To learn the preparation/synthesis and reactions of carboxylic acids and their derivatives, amines, diazonium salts, amino acids and simple peptides.
- To understand the mechanism of reactions.
- To compare Hofmann and Saytzeff elimination.
- To learn and remember the terms involved such as zwitterion, isoelectric point, electrophoresis with examples.
- To learn the laws, the terms involved and the principles in UV –Visible spectroscopy.
- To study various electronic transitions, λ_{\max} and effect of conjugation on colour.
- To know Woodward-Fieser rules for calculation of λ_{\max} for conjugated dienes and α, β unsaturated carbonyl compounds.
- To acquire knowledge to distinguish between *cis* and *trans* isomers using UV –Visible Spectroscopy
- To know classification of carbohydrates and their general properties.
- To know the open chain and cyclic structure of Glucose and Fructose.

- To gain knowledge of determining the configuration of monosaccharides.
- To study the terms involved with examples.
- To learn the synthesis involved.

Course Structure

Section A: Physical Chemistry-2

(30 Hours; 02 credits)

1. Solutions

(7 Hours)

Thermodynamics of ideal solutions: Ideal solutions and Raoult's law, deviations from Raoult's law – non-ideal solutions. Vapour pressure-composition and temperature composition curves of ideal and non-ideal solutions. Azeotropes.

Partial miscibility of liquids: Critical solution temperature, distillation and fractional distillation.

2. Phase Equilibrium

(8 Hours)

Phases, components and degrees of freedom of a system, criteria of phase equilibrium,

Phase diagrams of one-component systems (water, sulphur and CO₂) and two component systems involving eutectics, congruent and incongruent melting points (Zn-Mg, NaCl-H₂O).

3. Conductance

(5 Hours)

Conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes. Kohlrausch's law of independent migration of ions. Ionic mobility and factors affecting ionic mobility. Transference number and its experimental determination using moving boundary methods. Applications of conductance measurements: solubility and solubility products of sparingly soluble salts, ionic product of water, conductometric titrations (only acid-base).

4. Electrochemistry

(10 Hours)

Reversible and irreversible cells. Concept of EMF of a cell. Measurement of EMF of a cell. Nernst equation and its importance. Types of electrodes. Standard electrode potential.

Electrochemical series. Thermodynamics of a reversible cell, Concentration cells with transference and without transference. Liquid junction potential and salt bridge. pH

determination using hydrogen electrode and quinhydrone electrode.

Section B: Organic Chemistry-3

(30 Hours; 02 Credits)

1. Carboxylic acids and their derivatives

(6 Hours)

Carboxylic acids (aliphatic and aromatic) *Preparation:* Acidic and Alkaline hydrolysis of esters.

Reactions: Hell - Volhard - Zelinsky Reaction.

Carboxylic acid derivatives (aliphatic): (upto 5 carbons)

Preparation: Acid chlorides, Anhydrides, Esters and Amides from acids and their interconversions.

Reactions: Comparative study of nucleophilicity of acyl derivatives. Reformatsky reaction, Perkin condensation (mechanism).

2. Amines and Diazonium Salts

(6 Hours)

Amines (aliphatic and aromatic): (upto 5 carbons)

Preparation: from alkyl halides, Gabriel's phthalimide synthesis, Hofmann bromamide reaction (Hofmann rearrangement).

Reactions: Hofmann vs. Saytzeff elimination, Carbylamine test, Hinsberg test, with HNO_2 , Schotten – Baumann reaction. Electrophilic substitution (case aniline): nitration, bromination, sulphonation.

Diazonium salts: Preparation from aromatic amines, conversion to benzene, phenol, dyes.

3. Amino Acids and Peptides

(6 Hours)

Preparation of Amino Acids: Strecker synthesis, Gabriel's phthalimide synthesis.

Terms: Zwitterion, Isoelectric point and Electrophoresis.

Reactions of Amino acids: Ester of – COOH group, acetylation of –NH₂ group, complexation with Cu^{2+} ions, ninhydrin test. Synthesis of simple peptides (upto dipeptides) by N-protection (t-

butyloxycarbonyl and phthaloyl) & C-activating groups and Merrifield solid-phase synthesis.

4. UV –Visible Spectroscopy in Organic Chemistry (8 Hours)

Introduction to spectroscopy :

UV Spectroscopy: Beer-Lambert's law, Types of electronic transitions, λ_{\max} , Chromophores and Auxochromes, Bathochromic and Hypsochromic shifts, Intensity of absorption.

Visible Spectroscopy: Effect of conjugation on colour. Application of Woodward - Fieser rules for calculation of λ_{\max} for the following systems: α , β unsaturated aldehydes, ketones.

Conjugated dienes: alicyclic, homoannular and heteroannular, extended conjugated systems (aldehydes, ketones and dienes). Distinction between cis and trans isomers.

5. Carbohydrates: (4 Hours)

Classification and General Properties, Glucose and Fructose (open chain and cyclic structure), Determination of configuration of monosaccharides, absolute configuration of Glucose and Fructose, Mutarotation, Osazone formation, Killiani Fischer synthesis.

Reference Books:

1. Castellan, G.W. Physical Chemistry 4th Ed. Narosa (2004).
2. Kotz, J.C., Treichel, P.M. & Townsend, J.R. General Chemistry, Cengage Learning India Pvt. Ltd.: New Delhi (2009)
3. Undergraduate Physical Chemistry, Vol II, J.N. Gurtu, Pragati Prakashan.
4. Advanced Physical Chemistry, Gurtu and Gurtu, Pragati Prakashan
5. Mahan, B.H. University Chemistry, 3rd Ed. Narosa (1998).
6. Petrucci, R.H. General Chemistry, 5th Ed., Macmillan Publishing Co.: New York (1985).
7. Morrison, R. T. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson

Education).

8. Finar, I. L. Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
9. Finar, I. L. Organic Chemistry (Volume 2), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
10. Nelson, D. L. & Cox, M. M. Lehninger's Principles of Biochemistry 7th Ed., W. H. Freeman.
11. Berg, J. M., Tymoczko, J.L. & Stryer, L. Biochemistry, W.H. Freeman, 2002. Kemp, W. Organic Spectroscopy, Palgrave.
12. Pavia, D. L. et al. Introduction to Spectroscopy 5th Ed. Cengage Learning India
13. Silverstein, Bassler and Morill, Spectrometric Identification of Organic Compounds Ed. (2015).

SEMESTER III

CHC-103: LAB COURSE (Physical Chemistry & Organic Chemistry)

- ❑ **Course Objectives:** To understand and develop the problem-solving skills and hands on experience with reference to concepts studied in theory. (phase equilibria, conductometry and potentiometry)
- ❑ To get hands on experience for the preparation of derivatives.
- ❑ To gain knowledge of analyzing organic compounds.
- ❑ To learn to perform estimations.

COURSE STRUCTURE

Section A: Physical Chemistry-2

(30 Hours: 01 credit)

Phase Equilibria

12 Hours

- a) To draw the phase diagram of the binary system - diphenyl amine and α - Naphthol and find the eutectic temperature. (4 Hours)
- b) Study the mutual solubility of phenol and water at various temperatures and hence determine the critical solution temperature. (4 Hours)
- c) Study the effect of addition of NaCl on critical solution temperature of phenol water system and study of the effect of impurities on it. (4 Hours)

Conductance

10 Hours

- a) Determination of cell constant. (2 Hours)
- b) Determination of equivalent conductance, degree of dissociation and dissociation constant of a weak acid. (4 Hours)
- c) Conductometric titrations: (4 Hours)
 - i. Strong acid vs. strong base
 - ii. Weak acid vs. strong base

Potentiometry

08 Hours

Potentiometric titrations

- i. Strong acid vs. strong base (Quinhydrone method) (4 Hours)
- ii. Potassium dichromate vs. Ferrous Ammonium sulphate (4 Hours)

Section B: Organic Chemistry - 3**(30 Hours: 1 Credit)****I) Systematic Qualitative Organic Analysis: (6x2 =12 Hours)**

Analysis of Organic Compounds possessing monofunctional groups (carboxylic, aldehyde, ketone, amide, nitro, amines) and preparation of one derivative of each group. (Analysis of single compound and its derivative preparation)

II) Organic Preparations : (14 Hours)

Synthesis, yield, recrystallisation and Melting Point.

- (i) Hippuric acid from glycine (Benzoylation-Schotten Baumann reaction) (4 Hours)
- (ii) Osazone from Glucose (Nucleophilic addition) (2 Hours)
- (iii) Phthalic acid to Phthalic Anhydride to Phthalimide (4 Hours)
- (iv) Preparation of Azo dye (4 Hours)

III) Organic Estimations: (Any 2) (4 Hours)

- i. Estimation of glycine by formylation method (2 Hours)
- ii. Estimation of Glucose by oxidation (2 Hours)
- iii. Estimation of Acetamide by hydrolysis (2 Hours)

Course Outcomes:

At the end of the course students will be able to:

- ☐ Define the terms involved in Phase Equilibria, Solutions, Conductance and Electrochemistry.
- ☐ State the Raoult's Law and the Kohlrausch's law of independent migration of ions.
- ☐ Draw the schematic diagrams of instruments used in Conductance and Electrochemistry.
- ☐ Interpret the graphs based on Raoult's law and in Conductometric titrations.
- ☐ Define and explain the terms involved giving examples.
- ☐ Describe the preparation of various compounds involved.

- ❓ Classify carbohydrates.
- ❓ Draw the structures of carbohydrates.
- ❓ Predict and compare the mechanism of reactions involved.
- ❓ Explain and propose the mechanism of similar reactions.
- ❓ Predict the products, intermediates, reactants and reaction conditions for a given chemical reaction.
- ❓ State the laws involved in UV –Visible Spectroscopy and will be able to distinguish between cis and trans isomers.
- ❓ Calculate λ_{max} for Conjugated dienes and α , β unsaturated carbonyl compounds using Woodward–Fieser rules which will help them to predict the structure of organic compound with the help of other spectroscopic data.

Reference books:

1. Systematic experimental physical Chemistry by S.W. Rajbhoj, Dr. T. K. Chondhekar, Anjali Publication, Aurangabad.
2. Practical Chemistry by O.P. Pandey, D. N. Bajpai, S. Giri, S. Chand Publication
3. Khosla, B. D., Garg, V. C. & Gulati, A. Senior Practical Physical Chemistry, R. Chand & Co.: New Delhi (2011).

Organic Chemistry

1. Vogel, A.I., Tatchell, A.R., Furnis, B.S., Hannaford, A.J. & Smith, P.W.G., Textbook of Practical Organic Chemistry, Prentice-Hall, 5th edition, 1996.
2. Mann, F.G. & Saunders, B.C. Practical Organic Chemistry Orient-Longman, 1960.
3. Ahluwalia, V.K. & Aggarwal, R. Comprehensive Practical Organic Chemistry, Universities Press.

SEMESTER III

CHS101: (Natural Resources and Analysis)

THEORY: COURSE OBJECTIVES

- To define renewable, non-renewable and alternative energy sources.
- To define fuel, calorific value and the characteristics of a good fuel.
- To understand composition and uses of coal gas, producer gas and water gas.
- To study coal gasification (Hydrogasification and Catalytic gasification), coal liquefaction and solvent refining.
- To study different types of petroleum products and their applications.
- To understand idea about food processing and food preservation and adulteration.
- To understand the concept of pH and pH measurement with respect different types of soils...
- To study the use of different indicators for mapping various soil characteristics to improve soil fertility.
- To find out the sources responsible for contaminating water, study water sampling methods and methods employed for the purification of water.

Course Structure

(45 Hours: 3 Credit)

I. Review of energy sources (renewable and non-renewable). Classification of fuels and their calorific value.

2 Hours

II. Coal: Uses of coal (fuel and nonfuel) in various industries, its composition, carbonization of coal. Coal gas, Producer gas and Water gas—composition and uses. Fractionation of coal tar, uses of coal tar, requisites of a good metallurgical coke, coal gasification (Hydro gasification and Catalytic gasification), coal liquefaction and solvent refining.

10 Hours

III. Petroleum and Petrochemical Industry: Composition of crude petroleum, Refining and different types of petroleum products and their applications. Fractional Distillation (Principle and process), Cracking (Thermal and catalytic cracking), Reforming petroleum and non-petroleum fuels (LPG, CNG, LNG, bio-gas, fuels derived from biomass), fuel from waste, synthetic fuels (gaseous and liquids), clean fuels. Petrochemicals: Vinyl acetate, Propylene oxide, Isoprene, Butadiene, Toluene and its Derivatives.

10

Hours

M. Analysis of food products: Nutritional value of foods, idea about food processing and food

preservation and adulteration.

a) Identification of adulterants in some common food items like coffee powder, asafoetida, chilli powder, turmeric powder, coriander powder, pulses etc.

b) Analysis of preservatives and colouring matter. **10 Hours**

V. Analysis of soil: Composition of soil, Concept of pH and pH measurement, complexometric titrations, chelation, chelating agents, use of indicators. **7 Hours**

VI. Analysis of water: Definition of pure water, sources responsible for contaminating water, water sampling methods, water purification methods. **6 Hours**

CHS101: LAB COURSE (Natural Resources and Analysis)

PRACTICALS: COURSE OBJECTIVES

- To understand the different methods employed for the determination of various physico-chemical parameters of water.
- To understand the method of determination of soil pH.

COURSE STRUCTURE

(30 Hours: 1 Credit)

Instruction: Practicals/ demonstrations

1. Determination of pH of soil samples. **3 Hours**
2. Determination of pH of a water samples **3 Hours**
3. Estimation of Calcium and Magnesium ions as calcium carbonate by complexometric titration.
6 Hours
4. Determination of dissolved oxygen (DO) in a given water sample. **4 Hours**
5. Determination of acidity of a water sample **4 Hours**
6. Determination of alkalinity in a given water sample **4 Hours**
7. Measurement of dissolved CO₂. **4 Hours**

8. Percentage of available chlorine in bleaching powder.

2 Hours

At the end of the course students will be able to

LEARNING OUTCOMES

Theory

At the end of the course students will be able to:

- Define the terms renewable, non-renewable and alternative energy sources.
- Define fuel, its calorific value and know the properties of fuels.
- Understand production of coal gas, producer gas and water gas and their uses.
- Explain composition of crude petroleum, Refining and different types of petroleum products and their applications.
- Define Nutritional value of foods, idea about food processing and food preservation and adulteration.
- Apply the concept of pH to understand reactions in soil.
- Define chelate, chelating agent and know the method of preserving important cations in soil.
- Use different types of indicators for soil mapping to understand soil fertility.
- Identify various sources of water pollution and understand the use of water sampling methods to sample water.

Practical

At the end of the course students will be able to

- To determine various physico-Chemical parameters of water.
- To determine pH of any soil sample.

Reference Books for Theory and Practicals:

1. Svehla, G. Vogel's Qualitative Inorganic Analysis, Pearson Education, 2012.
2. Mendham, J. Vogel's Quantitative Chemical Analysis, Pearson, 2009.
3. Stocchi, E. Industrial Chemistry, Vol-I, Ellis Horwood Ltd. UK (1990). Jain, P.C. & Jain, M. Engineering Chemistry
4. Sharma, B.K. & Gaur, H. Industrial Chemistry, Goel Publishing House, Meerut (1996).
5. Skoog, D.A. Holler F.J. & Nieman, T.A. Principles of Instrumental Analysis, Cengage Learning India Ed.
6. Harris, D. C. Quantitative Chemical Analysis, W. H. Freeman.

7. Dean, J. A. Analytical Chemistry Notebook, McGraw Hill.
8. Day, R. A. & Underwood, A. L. Quantitative Analysis, Prentice Hall of India

CHC- 104 Physical Chemistry and Organic Chemistry

THEORY COURSE OBJECTIVES

Section A –Physical Chemistry

- ☐ To study the postulates of kinetic theory of gases and understand the deviations of real gases from ideal behaviour.
- ☐ To understand properties of liquids such as surface tension and viscosity and the methods to measure them.
- ☐ To study the structures of cubic crystals and the laws explaining their structure.
- ☐ To understand rates of chemical reactions of zero, first and second orders.
- ☐ To apply reaction rate theories for chemical reactions.

Section B-Inorganic Chemistry

- ☐ To understand electronic configuration, variable valency, color, magnetic and catalytic properties of 3d series.
- ☐ To understand the complexing ability and stability of various oxidation states (Latimer diagrams) for Mn, Fe, and Cu.
- ☐ To understand electronic configurations, oxidation states, color, magnetic properties of lanthanides.
- ☐ To explain lanthanide contraction, separation of lanthanides (ion exchange method only).
- ☐ To understand the IUPAC system of nomenclature for coordination compounds.
- ☐ To understand the bonding in complexes using valence bond theory.

- ❑ To study the different types of isomerism's associated with coordination compounds.
- ❑ To understand the factors affecting the magnitude of $10Dq$.
- ❑ To study the effect of strong field and weak field ligands on CFSE.
- ❑ To study crystal field splitting in tetrahedral and octahedral complexes and to calculate CFSE.

PRACTICALS COURSE OBJECTIVES

- ❑ To understand and develop the problem-solving skills and hands on experience with reference to concepts studied in theory.
- ❑ To systematically analyse the cations and anions in a given mixture.

- ② To quantitatively estimate several metal ions using the gravimetric and volumetric techniques.
- ② To determine the concentration of coloured compounds using the colorimetric technique.

SYLLABUS

Theory:

Number of hours: 60

Section A

1. Kinetic Theory of Gases (8H)

Postulates of Kinetic Theory of Gases, deviation of real gases from ideal behaviour, compressibility factor, causes of deviation. van der Waals equation of state for real gases. Boyle temperature (derivation not required). Critical phenomena, critical constants and their calculation from van der Waals equation. Andrew's isotherms for CO₂. Maxwell Boltzmann distribution laws of molecular velocities and molecular energies (graphic representation – derivation not required) and their importance. Temperature dependence of these distributions. Most probable, average and root meansquare velocities (no derivation), collision number, collision frequency, collision diameter and mean free path of molecules.

2. Liquids (6 H)

Surface tension and its determination using stalagmometer. Effect of temperature on surface tension. Viscosity of a liquid and determination of coefficient of viscosity using Ostwald viscometer and factors affecting viscosity.

3. Solids (8 H)

Forms of solids, symmetry elements, unit cells, crystal systems, Bravais lattice. Laws of crystallography - Law of constancy of interfacial angles, Law of rational indices. Miller indices, X-Ray diffraction by crystals, Bragg's law. Particle size determination using powder method. Structures of NaCl, KCl and CsCl (qualitative treatment only)

4. Chemical Kinetics (8 H)

The concept of reaction rates. Effect of temperature, pressure and catalyst on reaction rates. Order and molecularity of a reaction. Derivation of integrated rate equations for zero, first and second order reactions (both for equal and unequal concentrations of reactants). Half-life of a reaction. General methods for determination of order of a reaction. Concept of activation energy and its calculation from Arrhenius equation. Theories of Reaction Rates: Collision theory and Activated Complex theory of bimolecular reactions.

Section B

5. Transition Elements (10 H)

General characteristic properties of 3d series with special reference to electronic configuration, variable valency, color, magnetic and catalytic properties. Ability to form complexes and stability of various oxidation states (Latimer diagrams) for Mn, Fe, and Cu. Lanthanides: Electronic configurations, oxidation states, color, magnetic properties,

lanthanide contraction, separation of lanthanides (ion exchange method only). Actinides: Electronic configuration and general characteristics.

6. Coordination Chemistry (10 H)

IUPAC system of nomenclature. Bonding in complexes based on Valence Bond Theory (VBT), Inner and outer orbital complexes of Cr, Fe, Co, Ni, and Cu (coordination numbers 4 and 6). Different types of structural and stereo-isomerism including optical isomerism in complexes with coordination numbers 4 and 6. Drawbacks of VBT.

7. Crystal Field Theory (10 H)

Crystal field splitting in octahedral complexes. Crystal field stabilization energy (CFSE), Crystal field effects for weak and strong fields. Spectrochemical series. Crystal Field Splitting in Tetrahedral complexes. Calculation of CFSE. Comparison of CFSE for Oh and Td complexes. Factors affecting the magnitude of $10Dq$. Merits and Demerits of Crystal Field Theory.

PRACTICALS

Number of hours: 60

Section A (Physical Chemistry)

I. Surface Tension measurement (4 H)

Determination of the surface tension of a liquid or a dilute solution using stalagmometer.

II. Solutions of Solids in Liquids (4 H)

Determine solubility curve for KCl from 25°C to 50°C.

III. Viscosity measurement (10 H)

- a. Determination of the viscosity of a liquid or dilute solution using an Ostwald's viscometer.
- b. Study of the variation of viscosity of an aqueous solution with concentration of solute.

IV. Chemical Kinetics (12 H)

- a. To determine the rate constant and order of reaction between KI and K₂S₂O₈.
- b. Study of saponification of ethyl acetate with sodium hydroxide at equal concentration of ester and alkali.
- c. Compare the strengths of HCl and H₂SO₄ by studying kinetics of hydrolysis of methyl acetate.

Section B (Inorganic Chemistry)

I. Semi-micro qualitative analysis: not more than four ionic species (two anions and two cations): (4 Mixtures) (12 H)

Cations: NH₄⁺, Pb²⁺, Ag⁺, Bi³⁺, Cu²⁺, Cd²⁺, Sn²⁺, Fe³⁺, Al³⁺, Co²⁺, Cr³⁺, Ni²⁺, Mn²⁺, Zn²⁺, Ba²⁺, Sr²⁺, Ca²⁺, K⁺.

Anions: CO₃²⁻, S²⁻, SO₄²⁻, SO₃²⁻, NO₂⁻, Cl⁻, Br⁻, I⁻, NO₃⁻, PO₄³⁻, F⁻

II. Gravimetric/Volumetric (12 H)

1. Estimate the amount of Nickel present in a given solution as bis(dimethylglyoximate) Nickel(II) gravimetrically by counterpoise filter paper.
2. Estimation of (i) Mg²⁺ or (ii) Zn²⁺ by complexometric titrations using EDTA.
3. To estimate the amount of Bismuth present in the given solution of Bi(NO₃)₃·5H₂O by complexometric titration.
4. To estimate the amount of Nitrite present in the given NaNO₂ solution by titrating v/s Ceric ammonium sulphate /Ceric sulphate.

III. Colorimetric Experiments (6 H)

1. Draw calibration curve (absorbance at λ_{max} v/s concentration) for various concentrations of a given coloured compound (KMnO₄/ CuSO₄) and estimate the concentration of the same in a given solution.
2. Determine the composition of the Fe³⁺-salicylic acid complex solution by Job's method.

LEARNING OUTCOMES

Theory

Section A: Physical Chemistry

At the end of the course students will be able to:

- Define the terms involved in Kinetic Theory of Gases, Liquids, Solids, and Chemical Kinetics.
- Draw the schematic diagrams of stalagmometer, Ostwald viscometer and cubic crystal structures.
- Draw the graphs for first order and second order reactions.
- Explain the terms involved like unit cell, space lattice, activation energy, surface tension, viscosity, average velocity, root mean square velocity.

Section B: Inorganic Chemistry

- ☐ Explain general characteristics and electronic configuration of 3d Lanthanide and Actinide elements.
- ☐ Explain oxidation states, colour, and magnetic properties of 3d and lanthanide elements.
- ☐ Understand the Latimer diagram for Mn, Fe, and Cu.
- ☐ Name coordination compounds using IUPAC nomenclature.
- ☐ Explain inner and outer orbital complexes.
- ☐ Identify the different types of isomerism's associated with coordination complexes.
- ☐ Calculate crystal field stabilization energy of coordination complexes. Understand the effect of strong field and weak field ligands on the crystal field splitting of coordination complexes.

Practical

At the end of the course, students will be able to:

- ☐ Understand the concepts of surface tension, viscosity, and solubility.

- ② Develop skills for doing chemical kinetics titrations.
- ② Draw graphs and determine order of reactions.
- ② Understand on how to use a stalagmometer and Ostwald's viscometer.
- ② Develop skills in the identification and analysis of cations and anions.
- ② Perform gravimetric, volumetric and colorimetric experiments for quantitative interpretation of substances/metal ions.
- ② Carry out quantitative estimations of various metal ions.

REFERENCE BOOKS

Section A: Physical Chemistry

1. Mendham, J. Vogel's Quantitative Chemical Analysis, Pearson, 2009.
2. Khosla, B. D.; Garg, V. C. & Gulati, A. Senior Practical Physical Chemistry, R. Chand & Co.: New Delhi (2011).
4. Systematic experimental physical Chemistry by S.W. Rajbhoj, Dr. T. K. Chondhekar, Anjali Publication.
5. Practical Chemistry by O.P. Pandey, D. N. Bajpai, S. Giri, S. Chand Publication.
6. Senior Practical Physical Chemistry, B.D. Khosla, V.C. Garg, A. Gulati, R. Chand & Comp, New-Delhi.

Section B: Inorganic Chemistry

1. Cotton, F.A. & Wilkinson, G. Basic Inorganic Chemistry, Wiley.
2. Shriver, D.F. & Atkins, P.W. Inorganic Chemistry, Oxford University Press.
3. Wulfsberg, G. Inorganic Chemistry, Viva Books Pvt. Ltd.
4. Rodgers, G.E. Inorganic & Solid State Chemistry, Cengage Learning India Ltd., 2008.
5. Kotz, J.C., Treichel, P.M. & Townsend, J.R. General Chemistry Cengage Learning India Pvt. Ltd., New Delhi (2009).
6. Mahan, B.H. University Chemistry 3rd Ed. Narosa (1998).

7. Petrucci, R.H. General Chemistry 5th Ed. Macmillan Publishing Co.: New York (1985).
8. Principles of Inorganic chemistry by B.R. Puri, S. Sharma, and Kalia,
VallabhPublication.
9. Inorganic Chemistry Principles of Structure and Reactivity James E Huheey,
Ellen A.Keiter, Richard L.Keiter, Okhil K Medhi

CHS-102: Chemistry of Cosmetics and Perfumes(Semester IV)

Credits: 04 (Theory: 03 & Practical: 01)

THEORY COURSE OBJECTIVES

- ❑ To explain the term cosmeticology.
- ❑ To give examples of marketed products and describe the preparation formulation and packaging of various cosmetic products.
- ❑ To define herb and other terms involved.
- ❑ To describe the preparation of herbal drug.
- ❑ To classify herbal cosmetics.
- ❑ To describe the development of Ayurvedic and Herbal formulations and their evaluation by physical methods, chemical methods and microscopical techniques.
- ❑ To describe the formulation and preparation of Herbal cosmetics for skin care and haircare products.
- ❑ To define the terms involved in perfumes and flavours.
- ❑ To understand the classification of perfumes and categorise as per the ingredients.
- ❑ To understand the importance of essential oils in cosmetic industries.
- ❑ To describe the general methods of obtaining volatile oils from plants. To describe the composition of volatile oils.

PRACTICALS COURSE OBJECTIVES

- ❑ To understand the concept of cosmetics and develop preparation and skills of working and preparation of various cosmetic products.

SYLLABUS

Theory:**Number of hours: 45**

- 1. Cosmetic Formulation, principles and preparations (15 H)**

Introduction to cosmeticology. Definition of cosmetics as per EU and Indian guidelines. Cleansing and care needs for face, eye lids, lips, hands, feet, nail, scalp, neck, body, and underarms. Examples of marketed products. A general study including preparation and uses of the following: Hair dye, hair spray, sunscreen lotions, face powder, lipsticks, talcum powder, nail enamel, creams (cold, vanishing and shaving), Formulation, preparation and packaging of cosmetics for hair - Shampoo and conditioners. Examples from marketed products.
- 2. Herbal Cosmetics (15 H)**

Definition of herb, herbal medicine, herbal medicinal product, herbal drug preparation. Classification of herbal cosmetics. Development of Ayurvedic and Herbal formulations and their evaluation by physical methods, chemical methods and microscopical techniques. Herbal cosmetics for skin care (lotions, vanishing cream, foundation creams, anti sunburn preparations, face packs, lipsticks, face powders, soaps). Herbal cosmetics for hair care: Henna and Hibiscus.
- 3. Perfumes and Flavors (15 H)**

Classification of perfumes. Perfume ingredients listed as allergens. Deodorants, antiperspirants and artificial flavours. Essential oils and their importance in cosmetic industries with reference to Eugenol, Geraniol, sandalwood oil, eucalyptus, rose oil, 2-phenyl ethyl alcohol, Jasmone, Civetone, Muscone. Volatile Oils: General methods of obtaining volatile oils from plants; Study of volatile oils of Mentha, Lemon peel, Orange peel, Lemon grass, Eucalyptus, Musk, Sandal wood.

PRACTICALS**Number of hours: 30**

- 1) Demonstration/Practicals
- 2) Preparation of talcum powder.
- 3) Preparation of shampoo.
- 4) Preparation of enamels.
- 5) Preparation of hair remover.
- 6) Preparation of cold cream.
- 7) Preparation of nail polish and nail polish remover.
- 8) Preparation of vanishing cream.
- 9) Preparation of shaving cream.
- 10) Herbal preparations and evaluations of lotions.
- 11) Herbal preparations and evaluations of face packs.
- 12) Herbal preparations and evaluations of soaps.
- 13) Extraction of volatile oil from lemon peel.
- 14) Extraction of volatile oil from lemon grass.
- 15) Extraction of volatile oil from orange peel.

LEARNING OUTCOMES

THEORY

At the end of the course students will be able to

- ☐ Define cosmetics as per EU and Indian guidelines
- ☐ Describe the preparation and uses of various cosmetic products mentioned.
- ☐ Describe the formulation and packaging of cosmetics for hair - Shampoo and conditioners.
- ☐ Classify herbal cosmetics.
- ☐ Explain the terms herbal medicine and herbal medicinal products.
- ☐ Describe the preparation of herbal drug.
- ☐ Describe the development of Ayurvedic and Herbal formulations and their evaluation by physical methods, chemical methods and microscopical techniques.

- ☐ Describe the formulation and preparation of Herbal cosmetics for skin care and hair care.
- ☐ Classify the perfumes and categorize the perfume ingredients.
- ☐ Explain the importance of essential oil in cosmetic industries.
- ☐ Describe the composition of different volatile oils and methods of obtaining them.

PRACTICAL

At the end of the course students will be able to:

- ☐ Understand the concepts various cosmetic products.
- ☐ Prepare various cosmetic products.

REFERENCE BOOKS

1. E. Stocchi: *Industrial Chemistry*, Vol -I, Ellis Horwood Ltd. UK.
2. P.C. Jain, M. Jain: *Engineering Chemistry*, Dhanpat Rai & Sons, Delhi.
3. Sharma, B.K. & Gaur, H. *Industrial Chemistry*, Goel Publishing House, Meerut (1996).
4. G.L. Patrick: *Introduction to Medicinal Chemistry*, Oxford University Press, UK. 65.
5. Hakishan, V.K. Kapoor: *Medicinal and Pharmaceutical Chemistry*, Vallabh Prakashan, Pitampura, New Delhi.
6. Keith Wilson and John Walker: *Practical Biochemistry*.
7. Thomas M. Devlin: *Textbook of Biochemistry*.
8. Talwar, G.P. & Srivastava, M. *Textbook of Biochemistry and Human Biology*, 3rd Ed. PHI Learning.
9. *Textbook of herbal cosmetics* by Vimaladevi M. CBS Publishing 1st Ed. 2015.
10. *The complete technology book on herbal beauty products with formulation and processes* by H. Panda, Asia Pacific Business Press Inc. 2005.
11. *Essential oils: A practical guide* by John Gordon, Aetheric Publishing.

Bachelor of Science (Honours) Programme

Physical Chemistry (Semester V)

Credits: 06 (Theory: 04 & Practical: 02)

THEORY COURSE OBJECTIVES

Section A & B

- To study the mathematical concepts (integration, derivation, exponential trigonometric function.)
- To solve the numerical wrt Nernst equation, to study electrochemical series and applications.
- To study optical activity, polarization, dipole moment and methods of determination of dipole moments and structure of molecules
- To classify different nuclides. Binding energy and nuclear forces. To study nuclear models, radioactivity.
- To study emf and its measurements. To study concentration cell, its measurements, applications,
- To study decomposition potential, overvoltage and factors affecting them.
- Molecular structure and molecular spectra
- To define the principles, hypothesis, postulates of quantum mechanics in Quantum chemistry.
- To apply the basic mathematical concepts in quantum chemistry.
- To draw the wave functions, orbital diagrams and the graphs involved.
- To solve the numerical, explain and interpret the wave functions.
- To study the electromagnetic spectrum, terms, principles involved. To study Rotational spectra of diatomic molecules, determination of bond lengths and qualitative description
- To study counters used in measurement of radioactivity

PRACTICALS COURSE OBJECTIVES

- To understand and develop the problem-solving skills and hands on experience with reference to concepts studied in theory (potentiometry, pH metry, Solubility, Chemical kinetics)

SYLLABUS

Theory:

Number of hours: 60

SECTION A

1. Nuclear Chemistry I (10 H)

Composition of the nucleus, nuclear binding forces and energy, nuclear stability, nucleon –nucleon forces and their equality, characteristics and theory of nuclear forces, nuclear models, radioactive disintegration, decay constant, half- life and average life, units of radioactivity, artificial radioactivity, detection and measurement of radioactivity, GM counter, semiconductor and proportional counter, Scintillation counter, characteristics of suitable scintillator. (numericals to be solved)

2. Electrochemistry I (20 H)

Ion-selective electrodes: Fixed-site membrane, mobile-site membrane, site-free membrane, construction of ion selective electrodes, applications of ion selective electrodes. Decomposition potential, experimental determination of decomposition potential, application of decomposition potential, overvoltage and overpotential, theory of overvoltage, experimental determination of overvoltage, factors affecting overvoltage, hydrogen overvoltage, oxygen overvoltage, metal overvoltage. Fuel cells; H₂-O₂, Molten Carbonate Fuel cell, Proton exchange membrane fuel cell, Solid Oxide Fuel cell, Electrochemical Sensors; sensors, Principle, advantages and applications.

SECTION B

3. Quantum Chemistry I (16 H)

Mathematical Concepts: Derivatives and integrations, trigonometric functions, exponential functions, second derivatives of the functions. De-Broglie hypothesis, Heisenberg Uncertainty principle, sinusoidal wave function, terms involved in Quantum mechanics: Normalisation, orthogonality, observables, operators, stationary states, and variables. Schrodinger equation and its application to free particle and “particle in a box”(rigorous treatment) quantisation of energy levels, zero – point energy, Schrodinger equation in Cartesian and spherical polar (derivation not required), Extension to two- and three-dimensional boxes, separation of variables, degeneracy. Operators (Hermitian, non-Hermitian), eigen value and eigen functions, physical significance of wave function, examples of operators, Hamiltonian operators, Quantum mechanical operators and commutation rules Postulates of quantum mechanics, wave functions, probability distribution functions, nodal properties.

4. Molecular Spectroscopy I (14 H)

Interaction of electromagnetic radiation with molecules and various types of spectra, Born Oppenheimer approximation. Rotational Spectroscopy: selection rules, intensities of spectral lines, determination of bond lengths of diatomic and linear triatomic molecules, isotopic substitution. Vibrational spectroscopy: Classical equation of vibration, computation of force constant, amplitude of diatomic molecular vibrations, anharmonicity, Morse potential, dissociation energies, fundamental frequencies, overtones, hot bands, degree of freedom for polyatomic molecules, modes of vibration, concept of group frequencies. Vibration –rotation spectroscopy: Diatomic vibrating rotator, P, Q, R branches Raman spectroscopy: Qualitative treatment of Rotational Raman effect, Vibrational Raman spectra, Raman effect, Stokes and Anti-stokes lines, their intensity difference, Quantum and Classical theories of Raman effect rule of mutual exclusion principle.

1. To study the kinetics of iodine clock reactions.
2. To determine the strength of mixture containing weak acid and salt of weak base by titrating against standard 0.1N NaOH solution conductometrically.
3. To determine the dissociation constant of a weak monobasic acid using pH metry.
4. To determine the percentage composition and amount of halides from a mixture (any two halide) using standard 0.1N AgNO₃ solution.
5. To study the adsorption of Acetic acid by charcoal and to verify Freundlich adsorption isotherm.
6. To determine the energy of activation of hydrolysis of ethyl acetate (unequal concentration)
7. To determine degree of hydrolysis and hydrolysis constant of CH₃COONa/ NH₄Cl.

Minor Experiments

- 1) Using vibrational-rotational spectra of HCl molecule;
 - (A) Assign the rotational lines to various transitions.
 - (B) Calculate
 - (I) The value of B₀ and B₁, for R and P branches of spectra.
 - (II) Vibrational frequency and
 - (III) Inter nuclear distance
- 2) Using vibrational-rotational spectra of HBr molecule:
 - (A) Assign the rotational lines to various transitions.
 - (B) Calculate
 - (I) The value of B₀ and B₁, for R and P branches of spectra.
 - (II) Vibrational frequency and
 - (III) Inter nuclear distance
- 3) To determine Standard Reduction Potential of Zn⁺⁺/Zn.
- 4) To determine Standard Reduction Potential of Cu⁺⁺/Cu.
- 5) To determine the solubility product of AgCl of 0.1 M AgNO₃.
- 6) To determine the solubility product of AgCl of 0.05 M AgNO₃.
- 7) To determine the solubility product of AgCl of 0.01 M AgNO₃.

LEARNING OUTCOMES:

THEORY

At the end of the course students will be able to

- Define the terms involved in Quantum chemistry, electrochemistry, molecular structure and nuclear chemistry.
- State the laws, principles of quantum chemistry, electrochemistry, molecular structure and nuclear chemistry. postulates of quantum mechanics
- Draw the schematic diagrams, diagrams of instruments, wave functions, orbital diagrams and the graphs involved.

- Distinguish between types of nuclear forces, types of polarisations.

- Explain the terms involved in quantum chemistry, electrochemistry, molecular structure and nuclear chemistry with suitable examples, interpret the graph of binding energy, neutron energy.
- Explain classification of electrochemical cells, nuclear models, working of counters used in measurement of radioactivity, electrodes used in electrochemical cells.
- Derive and use the equations to solve the numerical in quantum chemistry, electrochemistry, molecular structure and nuclear chemistry.
- Interpret the wave function, compare the various methods involved in measurement of dipole moment.
- To solve the numerical in quantum chemistry using basic mathematical concepts (definite integrals, derivatives, trigonometric functions and exponential functions.)

PRACTICAL

At the end of the course students will be able to

- Understand the concepts of adsorption isotherms and activation energy solubility product.
- Develop skills of working and set up of electrochemical cells (potentiometry and pH-metry, conductometry).
- Solve numericals on standard electrode potential and verify the graph of adsorption isotherms.

REFERENCE BOOKS

Textbooks

1. J. N. Gurtu, Physical Chemistry Vol-III, A Pragati edition.
2. N. B. Laxmeshwar, S. M. Malushte, A. S. Mulye, V. N. Kulkarni, Concepts of Physical Chemistry, Chetana Prakashan.
3. P. C. Jain, Monica Jain, Engineering Chemistry 15th Edition, Dhanpat Rai Publishing Co.

Reference Books

1. Barnwell, C.N. & McCash, E.M., Fundamentals of Molecular Spectroscopy, 4th Ed. Tata McGraw Hill, New Delhi (2006)
2. U. N. Dash, Nuclear Chemistry, S. Chand Publication
3. H. J. Arnikar, Essentials of Nuclear Chemistry, New Age International Publishers, 4th Revised Edition
4. Gurdeep Raj, Advanced Physical Chemistry Goel Publication.
5. Chandra, A.K., Introductory Quantum Chemistry, Tata McGraw –Hill (2001).
6. House., J.E., Fundamentals of Quantum Chemistry, 2ND Ed. Elsevier: USA (2004)
7. Lowe. J.P. & Peterson., K., Quantum Chemistry, Academic Press (2005)
8. Kakkar., R., Atomic and Molecular Spectroscopy, Cambridge University Press (2015)
9. Ira N. Levine, Quantum Chemistry, Seventh Edition, Pearson
10. Chemistry for degree students Semester V and VI by R. L. Madan, S. Chand Publication
11. Quantum Chemistry by Donald A McQuarrie, viva student edition

Bachelor of Science (Honours) Programme

CHC-106

CORE COURSE

Inorganic Chemistry (SEMESTER V)

Credits: 06 (Theory: 04 & Practical: 02)

THEORY COURSE OBJECTIVES

Section A

- To define the various periodic properties like atomic and ionic radii, electron affinity and electronegativity and determine the trends of the periodic properties in the groups and the periods of the periodic table.
- To define the terms, Interhalogens, Oxyacids of Halogens, Polyhalides and Pseudo halogens and generalize their properties.
- To evaluate the structure and bonding in Interhalogens, Oxyacids of Halogens, Polyhalides and Pseudohalogens.
- To discuss the occurrence and general properties of Noble gases.
- To discuss the uses and hydrates and Clathrates of Noble gases.
- To interpret the structure and bonding in various xenon compounds.
- To introduce concept of defects in solids, define Schottky and Frenkel defects, Color center, extended defects and Non-stoichiometry.
- To introduce basic synthesis concepts of solid-state chemistry and to provide introductory knowledge on concept of band gap and classification of materials based on it.

Section B

- To define Primary valency, Secondary valency, Chelate effect, Stability of Complexes.
- To generalize Werner's Co-ordination Theory, Ligand field Theory and Molecular Orbital Theory (σ as well as π bonding).
- To draw molecular orbital diagrams and to discuss the evidences for Covalent bonding in Complexes and factors affecting stability of complexes.
- To define the basic concepts of oxidation and reduction and the study of electrochemical series.
- To define and draw Frost, Latimer and Pourbaix diagrams for various types of reactions and to study the principles involved in extraction of elements
- To introduce Nano chemistry and explain nano particles, their properties and applications
- To know the classification of elements as essential or trace and their uses in

biological processes.

- To study the roles of myoglobin and hemoglobin and to define and study metalloenzymes

PRACTICALS: COURSE OBJECTIVES

- To understand and to get hands on experience on the various steps involved in gravimetry for quantitative estimations of desired metal ions in the presence of other interfering ions in the mixture of salt solutions by precipitating method and preparation of some inorganic complexes.

SYLLABUS

Theory:

Number of hours: 60

SECTION A

1. Periodicity of Elements (10 H)

Detailed discussion of the following:

Properties of the elements with their trends in the periodic table.

- Atomic radii (van der Waals)
- Ionic radii and Covalent radii.
- Effective nuclear charge, shielding or screening effect, Slater rules.
- Ionization Energy, Successive ionization energies and factors affecting ionization energy.
- Electron Affinity.
- Electronegativity, Pauling's/ Mulliken's/ Alfred and Rochow's. Calculation of Electronegativity (Pauling's Method), Factors affecting Electronegativity.

2. Chemistry of halogens (8 H)

General methods of preparation, structure, bonding and chemical properties of: i) Interhalogens ii) Polyhalides ions iii) Oxoacids of halogens in different oxidation states iv) Pseudo halogens.

3. Noble Gases (4 H)

Occurrence and uses, inertness of noble gases, Clathrates; preparation properties and structure (VSEPR) of XeF_2 , XeF_4 and XeF_6 .

4. Inorganic Solid-State Chemistry (8 H)

Defects in solids, Point defects; Schottky and Frenkel defects, Colour Centre, Extended defects and Non-stoichiometry. Band Theory of solids: Band gaps, Metals, Insulators and Semi-conductors.

SECTION B

5. Bonding in Co-ordination Compounds (12 H)

Werner's theory and its experimental verification Evidences for Covalent bonding in complexes; Stereochemistry of Co-ordination Compounds with different co-ordination Numbers

- Ligand Field Theory (Adjusted Crystal Field Theory) –Brief Introduction; Comparison of the CFT and MOT.
- Molecular Orbital Theory as applied to Octahedral Complexes. Stability of complexes and factors affecting stability.

C. Molecular orbitals diagrams of $[\text{Ti}(\text{H}_2\text{O})_6]^{+3}$, $[\text{Fe}(\text{CN})_6]^{-3}$, $[\text{FeF}_6]^{-3}$ and $[\text{Co}(\text{NH}_3)_6]^{+3}$ Complexes. Effect of π - bonding on splitting parameter.

6. Oxidation and Reduction (8 H)
Oxidation number, single electrode potential, Standard electrode potential and Electrochemical series. Energy cycle for electrode potential. Application of Electrochemical series to check feasibility of reaction. Hydrogen overvoltage and Oxygen overvoltage. The use of reduction potentials, redox cycle, redox stability in water. The diagrammatic presentation of potential data - Frost, Latimer and Pourbaix diagrams. Principles involved in the extraction of the elements.
7. Selected Topics
- A) Nano chemistry (5 H)
Introduction to Nano particles, their properties, carbon nanotubes, SWCNT, MWCNT, different types of nanomaterials and their applications.
- B) Bio-inorganic Chemistry (5 H)
Overview, essential and trace elements in biological processes, Metalloporphyrins with special reference to haemoglobin and myoglobin. The role of Model systems, The alkali and alkaline earth metals, Metalloenzymes, Nitrogen fixation: Bacterial nitrogenase system (The biological nitrogen cycle).

PRACTICALS

Number of hours: 60

Gravimetric Estimations

1. To estimate the amount of Al as Al_2O_3 in the given solution of aluminum sulphate.
2. To estimate the amount of Fe as Fe_2O_3 in the given solution of ferric chloride containing barium chloride and free HCl.
3. To estimate the amount of nickel as Ni-DMG in the solution of nickel chloride containing copper chloride and free HCl.
4. To estimate the amount of barium as BaCrO_4 in the solution of barium chloride containing ferric chloride and free HCl.
5. To estimate the amount of Zinc as $\text{Zn}_2\text{P}_2\text{O}_7$ in the given solution of zinc sulphate containing copper sulphate and free H_2SO_4 .

Inorganic Preparations

1. Preparation Potassium trioxalatoferate (III).
2. Preparation of potassium trioxalatoaluminate (III).
3. Preparation of Trithiourecopper (I) sulphate.
4. Guignet's green (hydrated chromium oxide).
5. Cobalt blue (azure).

LEARNING OUTCOMES

Theory

At the end of the course students will be able to

- Define the terms involved in the chapter Periodic Properties, derive the equations for the various periodic properties and follow the trends within groups and periods of the various periodic properties.
- Discuss the general properties and evaluate bonding in different compounds of halogens like Interhalogens, Oxyacids, Pseudohalogens and Polyhalides.
- Understand the reactivity of Noble gas elements and their compound formation.
- Define and differentiate different types of defects.
- Explain non-molecular solids and their preparation methods.
- To understand the Werner's Co-ordination Theory, Ligand field Theory and Molecular Orbital Theory to interpret the properties, bonding and stability in Co-ordination Compounds.
- Define the concepts of oxidation and reduction and draw Frost, Latimer and Pourbaix diagrams and apply them for various reactions
- Describe nanomaterials, their properties and applications
- To study the roles of myoglobin and hemoglobin with respect to the transfer and storage of oxygen in biological systems and the process of respiration.
- Define the roles metalloenzymes in biological systems.

Practical

- Understand the methods to quantitatively estimate with precision the desired amount of the precipitate..
- Understand the various conditions to be undertaken to acquire the desired yield.
- Understand various methods to estimate inorganic complexes of various ions.

REFERENCE BOOKS

Textbooks

1. J. D. Lee, *Concise Inorganic Chemistry*, 5th Edn. Wiley India.
2. B. R. Puri, L. R. Sharma, and K. C. Kalia, *Principles of Inorganic Chemistry*, 33rd Edn.

Reference books

1. F. Albert Cotton, Geoffrey Wilkinson, and Paul L. Gaus, *Basic inorganic chem.* 3rd Edn. Wiley India
2. James E. Huheey, Ellen A. Keiter, Richard L. Keiter and Okhil K. Medhi, *Inorganic Chemistry, Principles of Structure and Reactivity.* 4th Edn. Pearsons
3. K. V. S. Laxmi Devi, N. C. Patel, S.S. Dhume, A. Venkatachalam, S. P. Turakhia, Chhaya Dixit and R. A. Mirji, *College Inorganic Chemistry for T.Y. B. Sc.* 21st Edn, Himalaya Publishing House.
4. Solid State Chemistry, Third edition By- Lesley E. Smart, Elaine A. Moore, Pub- Taylor and Francis.
5. Shriver, P.W. Atkins and C.H. Langford, *Inorganic Chemistry*, Oxford.

6. G.D. Tuli, S. K. Basu and R.D. Madan, Advance inorganic chemistry, Satya Prakash, S. Chand Publication.
7. F. A. Cotton, Chemical Applications of Group Theory, Wiley India
8. P.K Bhattacharya, Group Theory and its Chemical Applications Himalaya Publications.

Bachelor of Science (Honours) Programme

CHC-107

CORE COURSE

Organic Chemistry (Semester V)

Credits: 06 (Theory: 04 & Practical: 02)

THEORY COURSE OBJECTIVES

Section A

- To understand the concept of aromaticity.
- To understand mechanistic aspects of electrophilic and nucleophilic aromatic substitution.
- To understand the concept related to reactivity and orientation of activating and deactivating groups.
- To study methods for structure elucidation of Nicotine, Papaverine and Hygrine.
- To learn the synthesis of Nicotine from Succinimide, synthesis of Papaverine using Bischler-Napieralski reaction and synthesis of Hygrine from Pyrrole.
- To understand important concepts in IR, NMR and Mass spectroscopic methods.
- To learn interpretation of IR, NMR and MS spectra.

Section B

- To study heterocyclic compounds and bicyclic heterocycles with examples.
- To learn classification with examples of oxygen, sulphur and nitrogen containing heterocycles (up to 6 membered).
- To understand structure, resonance, stability and reactivity of furan, pyrrole, thiophene, pyridine, indole, quinoline and isoquinoline and also learn about their industrial source and preparation methods.
- To study structure elucidation of Vitamin A, Vitamin C, Thyroxine and Adrenaline and also learn their synthesis from β -ionone, xylose, tyrosine and catechol respectively.
- To learn classification of dyes with one example and structure of each class.
- To understand reasons for colour of some molecules.
- To learn synthesis and understand chemistry of phenolphthalein, congo-red, crystal violet and methyl orange.

PRACTICAL COURSE OBJECTIVES

- To understand theoretical concepts required for experiments and develop hands on experience with reference to basic laboratory techniques required for organic preparations, estimations and identification and separation of organic binary mixtures.

- To learn the interpretation of Infra-Red and proton NMR spectra by applying the concepts studied in theory.

SYLLABUS

Theory:

Number of hours: 60

Section A

1. Aromaticity, Aromatic hydrocarbons and Reactivity (6 H)

Huckel's rule of Aromaticity ($4n+2$) Rule, $4n$ Rule for antiaromaticity, Electrophilic Aromatic substitution (w.r.t Benzene): Mechanism of Nitration, Sulphonation, Halogenation, Friedel – Crafts alkylation and acylation. Reactivity and orientation of activating, deactivating groups (ortho, para and meta effects). Nucleophilic aromatic substitution of Aryl halides (S_NAr mechanism)

2. Alkaloids (6 H)

Ziesel's Method, Herzig-Meyer's method, Hoffman's exhaustive methylation method. Structure elucidation of Nicotine, Papaverine and Hygrine. Synthesis of Nicotine from Succinimide. Synthesis of Papaverine using Bischler-Napieralski reaction. Synthesis of Hygrine from Pyrrole.

3. Spectroscopic methods in Organic Chemistry (18 H)

Infra-Red Spectroscopy: Principle of I.R Spectroscopy (Hooke's law), types of molecular vibrations (Stretching and bending). Source, instrumentation and working of I.R spectrophotometer. Functional group region and Fingerprint region. Applications of I. R. Spectroscopy: Functional group analysis, detection of purity of sample, establishing the identity of an unknown molecule, Effect of H-bonding, conjugation, resonance and ring size on IR absorptions. To study the progress of a reaction. Problems based on I.R. spectroscopy (ketone, aldehyde, ester, acid & alcohol).

Nuclear Magnetic Resonance Spectroscopy:

Basic Principles of 1H NMR spectroscopy, Number of signals (Homotopic, Enantiotopic, diastereotopic protons). Position of signals, Chemical shift: Reference standard, Solvent effect, Shielding and de-shielding effect, anisotropic effects in alkenes, alkynes, aldehydes, aromatic compounds, factors affecting chemical shift. Intensity of signals: Peak area and proton counting. Spin-Spin coupling: Coupling constant (J). Interpretation of NMR spectra of simple compounds. (acetone, acetaldehyde, toluene, ethyl bromide, anisole, acetic acid, t-butylbenzene, 2-butanone, propene). Simple problems based on NMR spectral data for identification of molecule. Carbon-13 Nuclear Magnetic Resonance Spectroscopy and Mass Spectrometry: Principle of ^{13}C spectroscopy. Number of signals: Proton coupled and decoupled spectra (off-resonance). Position of signals. Factors affecting position of signals (hybridisation). Problems based on ^{13}C spectroscopy. Principle, theory, instrumentation of Mass spectrometry. Base Peak, Molecular ion, Metastable ion. Fragmentation pattern for alkanes. Fragmentation pattern of ketones: α cleavage and McLafferty rearrangement. Isotopic effect of alkyl halides.

Section B

4. Chemistry of Heterocyclic Compounds (18 H)

Definition of heterocyclic compounds: Organic compounds containing oxygen, sulphur, nitrogen. Classification with examples for three, four, five and six membered heterocycles. Structure, resonance, stability and industrial source of furan, pyrrole, thiophene and pyridine. Preparation of furan, pyrrole and thiophene using Paal Knorr Synthesis. Reactivity of furan, pyrrole and thiophene: Electrophilic substitution at 2/5 position. Preparation of pyridine using Hantzsch synthesis. Reactivity of pyridine: Electrophilic substitution at 3 position, Nucleophilic substitution at 2 and 4 position. Definition of bicyclic heterocycles with examples. Structure, resonance, stability and industrial source of indole, quinoline, isoquinoline. Preparation of indole using Fischer indole synthesis. Reactivity of Indole: Electrophilic substitution at 3 position. Skraup synthesis of quinoline and Bischler Napieralski synthesis of isoquinoline. Reactivity of quinoline and isoquinoline: Electrophilic substitution at 5/8 position, Nucleophilic substitution at 2 and 4 position. Oxidation and Reduction of quinoline and Isoquinoline.

5. Vitamins and Hormones (6 H)

Structure elucidation of Vitamin A, Vitamin C, Thyroxine and Adrenaline. Synthesis :Vitamin A from β -ionone ,Vitamin C from xylose , Adrenaline from Catechol and thyroxine from tyrosine.

6. Dyes (6 H)

Classification of dyes: Acidic, basic, azo, reactive, Vat, mordant, direct, disperse with one example and structure of each class. Reasons for colour of some molecules: Resonance effect in p-nitroaniline and nitrobenzene, conjugation effect in β -carotene and graphite. Synthesis and chemistry of phenolphthalein, congo-red, crystal violet, methyl orange.

PRACTICALS

Number of hours: 60

1. Organic Preparations (Two steps): (Any 5)

Synthesis, yield, recrystallisation and Melting Point.

- i) Nitrobenzene to m-nitroaniline
- ii) Phthalimide to 2-iodobenzoic acid
- iii) Acetanilide to p-nitroaniline
- iv) Benzamide to m-nitrobenzoic acid
- v) Benzoin to benzilic acid
- vi) Acetophenone to acetanilide
- vii) Benzophenone to benzanilide

2. Organic Estimations (Any 3)

- a) Acid+ Amide
- b) Acid + Ester
- c) Estimation of the number of acetyl groups in an acetyl ester. (Triacetyl glycerol,Hexaacetyl mannitol or Pentaacetyl glucose) (Any one) .
- d) Estimation of nitro group by reduction using stannous chloride

3. Synthesis of dyes

- a) Diazoaminobenzene
- b) Picric acid

4. Interpretation of Infra-Red, and proton NMR spectra
a) IR spectra of the following: aldehyde, alcohol, ketone, carboxylic acid, amine, nitrile.
b) Proton NMR of simple organic compounds (6 compounds)

5. Identification and Separation of following Organic binary mixtures

Water insoluble –water insoluble (Acid-Base, Acid-Phenol, Base-Neutral, Acid-Neutral, Phenol-Base, Phenol-Neutral), Water soluble- water insoluble (Acid-Acid, Acid-Neutral, Neutral-Neutral), Liquid-Liquid (2 mixtures), Solid-liquid (2 mixtures).

LEARNING OUTCOMES

Theory

At the end of the course students will be able to

- Explain the concept of aromaticity and distinguish between aromatic and anti-aromatic compounds.
- Explain the mechanism of electrophilic and nucleophilic aromatic substitution.
- Explain the concept related to reactivity and orientation of activating and deactivating groups.
- Explain structure elucidation of nicotine, papaverine and hygrine using suitable methods and give their synthesis.
- Explain important concepts in IR, NMR and mass spectroscopic methods.
- Identify functional group based on IR spectra.
- Predict the structure of simple organic compounds based on IR, NMR, MS data.
- Define and classify oxygen, sulphur and nitrogen containing heterocyclic compounds with examples.
- Explain structure, resonance, stability and reactivity of furan, pyrrole, thiophene, pyridine, indole, quinoline and isoquinoline and give their industrial source and preparation methods.
- Explain structure elucidation of vitamin A, vitamin C, thyroxine and adrenaline and also give their synthesis from β -ionone, xylose, tyrosine and catechol respectively.
- Classify dyes, giving one example and structure of each class.
- Explain reasons for colour of some molecules.
- Give synthesis and explain the chemistry of phenolphthalein, congo-red, crystal violet and methyl orange.

Practical

At the end of the course students will be able to

- Discuss the theory behind experiments.
- Understand stoichiometric requirements during organic preparations.
- Develop skills of common laboratory techniques including reflux, recrystallisation, recording of melting point, distillation, titration and chemical analysis.
- Identify the separation technique for binary mixture separation and perform chemical nature analysis.
- Perform calculations for quantitative analysis.

- To interpret infra-red and proton NMR spectra of simple organic compounds.

Textbooks

1. I.L.Finar, Organic Chemistry Vols I and II, Orient Longman.
2. Morrison and Boyd, Organic Chemistry; 6th Edn. Prentice Hall India.
3. J. March, Advanced Organic Chemistry: Reaction, Mechanism and Structure, Wiley, 2010, 4th Ed.
4. P.S. Kalsi, Spectroscopy of Organic compounds, New Age International Pub. Ltd. & Wiley Eastern Ltd., Second edition, 1995.

Reference books

1. Francis Carey, Organic Chemistry, 10th Edition.
2. Paula Yurkanis Bruice, Organic Chemistry; 3rd Edn. Pearson Education Asia.
3. Silverstein, Bassler and Morill, Spectrometric Identification of Organic Compounds.
4. J. Clayden, N. Greeves, S. Warren & Wothers, Organic Chemistry, Oxford University Press, 2012, 2nd Ed.
5. I.L. Finar Stereochemistry and Chemistry of Natural products, ELBS, Longmans, 1963, Vol. 2, 3rd Ed.
6. E.S. Gould et al., Mechanism and structure in Organic Chemistry, 1965.
7. F. A. Carey, Organic Chemistry, 2000, 4th Ed.
8. S.H. Pine, Organic Chemistry, McGraw-Hill International Edn. 2010, 5thEd.
9. F.A. Carey and R.J. Sundberg, Advanced Organic Chemistry, Part A and Part B. Plenum Press, Springer, 1977.
10. J. M. Harris & C.C. Wamser, Fundamentals of Organic Reaction Mechanisms, John Wiley & Sons. Inc. 1976.
11. F.M. Menger, D.J. Goldsmith & L. Mendell, Organic Chemistry, A concise approach, 1975, 2nd Ed.
12. J. R. Dyer, Applications of Absorption Spectroscopy of Organic compounds, Prentice Hall of India, 1987.
13. V.M. Parikh, Absorption spectroscopy of organic Molecules, Addison Wesley Longman Publishing Co., 1974.
14. D.H Williams & I. Fleming, Spectroscopic methods in organic chemistry, 6th Ed., Tata Mcgraw Hill Education, 2011.
15. William Kemp, Organic spectroscopy, 3rd Ed., Palgrave Macmillan, 1991.
16. R. O. C. Norman and J. M. Coxon, Principles of Organic Syntheses, 3rd Ed., CRC Press Inc, 1993.
17. J A Joule and G F Smith, Heterocyclic Chemistry, ELBS, Advances in Heterocyclic Chemistry, Edited by A R Katritzky etal, Vol. 1 to 50, Academic Press.
18. Gurdeep Chatwaal, Synthetic dyes, Himalaya Publishers.

Practical

Textbooks

1. A. I. Vogel, A. R. Tatchell, B. S. Furniss, A. J. Hannaford, Vogel's Textbook of Practical Organic Chemistry, 5th Ed., Prentice Hall; 2011.

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2. F G Mann and B C Saunders, Practical organic chemistry, Orient Longman, 4th ed.

Reference Books

1. D. Pasto, C. Johnson and M. Miller, Experiments and Techniques in Organic Chemistry, 1st Ed., Prentice Hall, 1991.
2. L. F. Fieser, K. L. Williamson "Organic Experiments" 7th edition D. C. Heath, 1992.
3. K. L. Williamson, K.M. Masters, Macroscale and Microscale Organic Experiments, 6th Edition, Cengage Learning, 2010
4. R.K. Bansal, Laboratory Manual in Organic Chemistry, New Age International, 5th Edition, 2016.
5. Morrison and Boyd, Organic Chemistry, 6th Edition, Prentice Hall, India.
6. Ahluwalia, V. K. & Aggarwal, R. Comprehensive Practical Organic Chemistry, Universities Press.
7. Silverstein, Bassler and Morill, Spectrometric Identification of Organic Compounds.
8. S. Kalsi, Spectroscopy of Organic compounds, New Age International Pub. Ltd. & Wiley Eastern Ltd., Second edition, 1995.

Bachelor of Science (Honours) Programme

CHD-101

Discipline Specific Elective

Basic Topics in Analytical Chemistry (SEMESTER V)

Credits: 04 (Theory: 03 & Practical: 01)

THEORY COURSE OBJECTIVES

- To define the terms involved in analytical chemistry, sampling techniques, data handling, chromatographic Techniques and electroanalytical methods.
- To explain scope and importance of analytical chemistry, different types of sampling and the types of solvent extractions.
- To classify different types of chromatographic techniques and errors with examples.
- To study the principles of volumetric analysis and gravimetric analysis and the basic principles of instrumentation of electrogravimetry, coulometry and polarographic analysis.
- To interpret steps involved in chemical analysis.
- To describe the basic components of instruments of electroanalytical methods.
- To draw the schematic diagrams of different electroanalytical methods.
- To solve numericals of evaluation of data and solvent extractions.
- To discuss the applications of different chromatographic techniques and electroanalytical methods.

PRACTICALS COURSE OBJECTIVES

- To understand and develop the problem-solving skills and hands on experience with reference to concepts studied in theory (ion exchange chromatography, colorimetry, statistical data).

SYLLABUS

Theory:

Number of hours: 60

1. Introduction (3 H)
Scope and importance of analytical chemistry, chemical analysis and analytical chemistry.
Classification of instrumental methods, analytical process (steps involved in chemical analysis): defining the problem, sampling, separation of desired components, actual

analysis, presentation and interpretation of results.

2. Quantitative analysis (8 H)
 - A. Principles of volumetric analysis: Theories of acid-base, redox, complexometric, iodometric and precipitation titrations - choice of indicators for these titrations.
 - B. Principles of gravimetric analysis: precipitation, coagulation, peptization, coprecipitation, post precipitation, digestion, filtration and washing of precipitate, drying and ignition.
3. Sampling Techniques (4 H)

Terms encountered in sampling: the population or the universe, Sample, Sampling unit, increment, the gross sample, the sub sample, Analysis sample, Bulk ratio, Size to weight ratio, Random sampling, Systematic sampling, Multistage sampling, Sequential sampling. Sampling of Gases, Liquids and Solids. Preservation, storage and preparation of sample solution.
4. Evaluation of analytical data (10 H)

Significant figures and rounding off, accuracy and precision Errors: determinate and indeterminate error, constant and proportionate errors, minimization of errors. Measures of central tendency and dispersion. Standard deviation, Gaussian distribution curve and its characteristics, Histogram and Frequency polygon. Confidence limit. Test of significance: Students t, F test, Rejection of the results: 2.5d & 4d rule and Q test. Linear least squares and Method of averages (Numerical problems are expected to be solved)
5. Solvent Extraction (4 H)

Basic Principle, percentage extraction, role of complexing agents in solvent extraction, separation factor, types of extraction (continuous, batch) (Numerical problems are to be solved)
6. Chromatography (7 H)

Principles Classification of chromatographic techniques

 1. Column chromatography: Principle, experimental details, theory of development, factors affecting column efficiency and applications.
 2. Paper and thin layer chromatography: Principles, techniques and applications of paper and thin layer chromatography.
 3. Ion exchange chromatography: Principles, classification of ion exchange materials, Nature of exchanging ions, Ion exchange capacity, applications in analytical chemistry.
7. Electroanalytical methods (9 H)

Electro gravimetric analysis: Introduction, principles, instrumentation, Electrolysis at constant current, apparatus, determination of copper by constant current electrolysis. Coulometry: Introduction, constant Current measuring device, Hydrogen-Oxygen coulometer, Silver coulometer. General characteristics of coulometric method, applications of coulometry in Neutralization, complexation, precipitation and redox titrations. Polarography: Introduction, Basic principles of instrumentation, Deposition potential, Dissolution potential, Polarization of electrode, Polarographic wave, Ilkovic equation, Supporting electrolytes, Interference of oxygen, Applications of polarography – inorganic and organic.

1. Determination of iron by salicylic acid by colorimetry.
2. Determination of nitrite in water by colorimetry.
3. Separation of organic compounds by TLC. (Demonstration)
4. Zn^{2+} / Mg^{2+} separation by an anion exchanger & volumetric estimation of Magnesium with standard EDTA.
5. Zn^{2+} / Mg^{2+} separation by an anion exchanger & volumetric estimation of Zinc with standard EDTA.
6. Estimation of Na^+ in NaCl by cation exchange resin using standard NaOH.
7. Estimation of Ca in calcium tablet by oxalate method and titration with $KMnO_4$.
8. Determination of hardness of water by EDTA i.e. estimate Ca as $CaCO_3$ and report analysis in ppm. (The candidate should record more than 5 observations and carry out statistical analysis to find out mean, median, range, standard deviation, absolute error, relative error and possibly Q test.

LEARNING OUTCOMES

Theory

At the end of the course students will be able to

- Define the terms, state the laws and principles involved in sampling techniques, data handling, chromatographic techniques, solvent extractions, volumetric analysis and gravimetric analysis.
- Explain sampling of liquid, solid and gases, different types of tests related to data handling, scope and importance of analytical chemistry.
- Draw and describe the basic components of instruments of electroanalytical methods.
- Classify and explain different types of errors, sampling and chromatographic techniques.
- Derive and use the equations of linear least squares and method of averages and solvent extraction to solve numerical.
- Interpret steps involved in chemical analysis.
- To discuss the applications of different chromatographic techniques and electroanalytical methods

Practical

At the end of the course students will be able to

- Understand the concepts based on ion exchange chromatography, colorimetry and to estimate acidic and basic radicals quantitatively.
- Develop skills to prepare different plates of thin layer chromatography.
- Solve numericals based on statistical data obtained from experimental results.

REFERENCE BOOKS

Textbooks

1. Baliga and Shetty, College Analytical Chemistry, 15th edition, Himalaya Publishing House, 2004
2. K. Raghuraman, D. V. Prabhu, C. S. Prabhu and P. A. Sathe, 5th Edn., Sheth Publishers

Pvt. Ltd.

Reference Books:

1. G. D. Christan Analytical Chemistry by, 5th edition Wiley publications.
2. G. Chatwal and S. Anand, Instrumental Methods of Chemical Analysis 5th edition (reprint 2003), Himalaya publication.
3. Vogels Textbook of Quantitative Inorganic Analysis 4th edition ELBS.
4. Willard, Meritt and Dean. Instrumental Methods of Analysis
5. Skoog and Leary, Principles of Analytical Chemistry 4th International edition.
6. B. K. Sharma. Instrumental Methods of Chemical Analysis: Goel Publishing House, Meerut
7. Mendham, J. Vogel's Quantitative Chemical Analysis (6th Edition) Pearson.

Bachelor of Science (Honours) Programme

CHD-102

Discipline Specific Elective

Green Methods and Safety Aspects in Chemistry (Semester V)

04 Credits (4 + 0)

COURSE OBJECTIVES

Section A

- To understand the need of Green Chemistry.
- To know the 12 principles of Green Chemistry and their importance in Green chemistry.
- To know the Green chemistry institutes and organizations in the world.
- To study green techniques in chemistry including the use of greener solvents, solvent-free reactions, grinding technique, ball milling techniques, use of various catalysts, microwave, and ultrasound techniques.
- To understand the mechanism of Phase Transfer Catalysis.
- To learn the green methods of preparation of metallophthalocyanine complexes, Grignard reagent, Schiff's base, 1-acetylferrocene, and bis(acetylacetonato) copper (II).
- To study the real-world cases in chemistry.

Section B

- To study the various risks and hazards involved in a chemical laboratory.
- To study the personnel protective equipment and emergency equipment to be used in a chemical laboratory.
- To understand the risks and hazards associated with a specific chemical.
- To distinguish between SDS and MSDS

- To study the toxic hazards involved in a chemical laboratory
- To study the types and working of fire extinguishers.
- To study the different types of waste and their hazards associated in a chemical laboratory.
- To study the precautions to be taken while working with water-dependent, electrical, and heating devices.
- To study the handling of solid waste.

SYLLABUS

Theory:

Number of hours: 60

Section A

1. Green Chemistry (10 H)

Introduction. Why there is a need for green chemistry? A brief overview of twelve green chemistry principles as proposed by Paul Anastas and John Warner. Explanation with examples, with special emphasis on atom economy, designing of less hazardous substances, reducing toxicity, use of greener solvents, catalysis, Energy efficiency, alternative sources of energy, accident prevention, and green Chemistry for better sustainability. Brief on green chemistry institutes and organizations in the world.

2. Green techniques in Chemistry (10 H)
Greener solvents: Water as solvent-Diels Alder Reaction, supercritical liquids-extraction of D-limonene from orange pill, ionic liquids and deep eutectic solvents-properties- one application. Solvent free reaction: Grinding techniques - Aldol condensation between 3,4-dimethoxybenzaldehyde and 1-indanone. and Ball milling techniques in synthesis. Catalysts: Definition: Solid supported reagents- NaBH₄-Alumina and PCC-silica. natural catalysts-Thiamine hydrochloride, L-Proline. Phase transfer catalysis: Phase Transfer catalyst, Mechanism of PTC, Advantages and application in Chemistry-Using 18-crown-6 ether or ammonium salt. Microwave and Ultrasound techniques: Principles and advantages, Green synthesis of metallophthalocyanine complexes by Microwave method. Preparation of Grignard reagent by ultrasonication method. Solid-solid synthesis of Schiff's base. (p-toluidine and o-vanillin). Green preparation of 1-acetylferrocene and bis(acetylacetonato) copper (II).
3. Real world Cases in Green Chemistry (10 H)
Surfactants for carbon dioxide – Replacing smog producing and ozone depleting solvents with CO₂ for precision cleaning and dry cleaning of garments. Designing of environmentally safe marine antifoulant. Right fit pigment: Synthetic azo pigments to replace toxic organic and inorganic pigments. An efficient, green synthesis of a compostable and widely applicable plastic (polylactic acid) made from corn. Greening of acetic acid manufacture, EPDM rubbers and Vitamin C. Eco-friendly pesticides.

Section B

4. **Introduction to Laboratory Safety (10 H)**
Risks in a Chemical Laboratory, Health Effects Due to “Hazardous” Chemical Exposure (How Does One Determine the Hazards Associated with Specific Chemicals? ; Exposure Routes, Toxicity Risk Assessment), Personal Protective Equipment (PPE) Proper Attire (Eye/Face Protection, Lab Coats, Gloves, Respirators, Disposal/Removal of PPE), Emergency Equipment Safety Showers/Eye Washes.
5. Laboratory Emergencies (10 H)
Spills and Fires, Handling the Accidental Release of Hazardous Materials, Spill Containment, and Clean-up, Leaking Gas Cylinders, Fires. Fire Extinguisher (how they work, types), Risk Assessment. Chemical Hazards, The New Safety Data Sheets (SDS) versus the Old Material Safety Data Sheets (MSDS), Assessment of Chemical Toxicity, Toxic Hazards (Dose, Risk Assessment, Types of Toxins, Flammable Hazards, Flammability Characteristics, Flammability Classes, Causes of Ignition, Reactive Hazards, Explosives).

6. Waste Handling and Laboratory equipment (10 H)
Characterization of Waste, Collection, and Storage (Lids, Leaks, Labels, Location, Containers). Consequences of Mixing Incompatibles. Solid Wastes (Chemicals, Broken Glass, Sharps, Cylinders, Pick-up). Special Cases. Hazardous Waste Minimization. Laboratory Equipment. Working with Electricity, Working with Water (liquid)-dependent Equipment (Hazards, Proper Use, Heating Baths), Working with High Pressure/Vacuum, Working with Vacuum Pumps, Working with Stirring and Mixing devices, Working with Heating Devices (Variacs, Oil, Salt, Sand baths, Microwave Oven).

LEARNING OUTCOMES

At the end of the course, students will be able to

Section A

- Explain concepts in Green Chemistry.
- State and explain the principles of Green Chemistry.
- Name the Green chemistry institutes and organizations in the world.
- Explain green techniques in chemistry including the use of greener solvents, solvent-free reactions, grinding technique, ball milling technique, use of various catalysts, microwave, and ultrasound techniques.
- Explain the mechanism of Phase Transfer Catalysis.
- Give and discuss the green methods of preparation of metallophthalocyanine complexes, Grignard reagent, Schiff's base, 1-acetylferrocene and bis(acetylacetonato) copper (II).
- Describe the real-world cases in chemistry.

Section B

- Identify the various risks involved in a chemical laboratory.
- Identify the Hazards Associated with Specific Chemicals.
- Understand the various personnel protective equipment and emergency equipment to be used in a chemical laboratory.
- Explain the working and types of fire extinguishers.
- Understand about the Flammable Hazards, Flammability Classes, and causes of ignition.
- Explain how New Safety Data Sheets are different from the Old Material Safety Data Sheets.
- Explain the hazards associated with water-dependent, pressure-dependent equipment, and heating devices.
- Explain the collection, storage, and minimization of hazardous waste chemicals.

REFERENCE BOOKS

Textbooks

1. Vogel's textbook of Practical Organic Chemistry, ELBS Publishers,1996.

2. Anastas, P.T. & Warner, J.K. Green Chemistry- Theory and Practical, Oxford University Press (1998).
3. Sharma, R. K.; Sidhwani, I. T. & Chaudhari, M. K. Green Chemistry Experiments: A monograph I.K. International Publishing House Pvt Ltd. New Delhi, Bangalore.
4. Green Chemistry: Environmentally Benign Reactions, V. K. Ahluwalia, Anne Books India, New Delhi, 2006.

Reference Books

1. Cann, M. C. & Connely, M.E. Real-World cases in Green Chemistry, American Chemical Society, Washington (2000).
2. Phase Transfer Catalysis, Waber and Gokel, springer-verlag, 1977.
3. Organic Synthesis-Special Techniques, V.K. Ahluwalia and R. Aggarwal, Narosa Publishing House, New Delhi, 2001.
4. Kappe, C. O. & Stadler, A. Microwaves in Organic and Medicinal Chemistry (Wiley-VCH, Weinheim) 2005.
5. New trends in Green Chemistry, V. K. Ahluwalia and M. Kidwai, Kluwer Academic Publishers, 2004.
6. Laboratory Safety for Chemistry students, Robert H. Hill, David C Finster, Wiley, July, 2010.
7. Laboratory safety: Theory and Practice, 1st Edition, Elseviers.

Bachelor of Science (Honours) Programme

CHC-108

CORE COURSE

Physical Chemistry (Semester VI)

Credits: 06 (Theory: 04 & Practical: 02)

THEORY COURSE OBJECTIVES

Section I

- To study the molecular orbital theory diagrams and the graphs involved.
- To interpret the physical picture of bonding and antibonding wavefunction.
- To define terms involved in electrochemistry, pH, pOH, pKa, pKb. Buffer solution, buffer capacity. Measurement of pH using different electrodes by potentiometric methods.

- To describe the mechanism of buffer action.
- To derive and solve numerical on Henderson's equation.
- To study energy released in nuclear fission, fission products.
- To classify various nuclear reactors. To describe the working of reactors and its parts.
- To know nuclear reactors in India.
- To define the terms and laws involved in photochemistry.
- To draw and interpret Jablonski diagrams.
- To study photochemical and photosensitized reactions with examples

Section II

- To describe types of theories in corrosion
- To explain the types of energy sources
- To study vibrational spectroscopy, IR, harmonic and anharmonic oscillator, Raman spectroscopy.
- Define terms, force constants, bond energy, polarizability.
- To study stokes and antistock lines, Raman shift and selection rules involved.
- Chain reactions, terms involved and units of radioactivity, applications of radioactiveisotopes Biological effects of radiations.

PRACTICAL COURSE OBJECTIVES

- To understand and develop the problem-solving skills and hands on experience withreference to concepts studied in theory.

Theory:**Number of hours: 60**

SECTION A

1. Quantum chemistry II (20 H)

Qualitative treatment of hydrogen atom and hydrogen – like ions/harmonic oscillator; setting up of Schrodinger equation in spherical polar co-ordinates, radial part, quantization of energy (only final energy expression). Average and most probable distances of electron from nucleus. Setting up of Schrodinger equation for many-electron atoms (He, Li) Need for approximation methods. Statement of variation theorem and application to simple systems. Chemical Bonding: Covalent bonding, valence bond and molecular orbital approaches, LCAO-MO treatment of H₂⁺ Bonding and antibonding orbitals, qualitative extension to H₂.

2. Nuclear Chemistry II (10 H)

Nuclear Fission, discovery, energy released in fission, fission products, neutron emitted in fission, nuclear reactors, classification of reactors, Breeder reactor, nuclear reactors in India, chain Reactions & its control, reprocessing of spent fuels Units of radiation energy, applications of radio-isotopes, radioisotopes as tracers, biological effects of radiation.

SECTION B

3. Electrochemistry II (12 H)

Definition of pH, pOH, pK_a, and pK_b, Determination of pH using glass electrodes by potentiometric method, Buffer solution, types, buffer action, buffer capacity, mechanics of buffer action, Henderson equation for acidic and basic buffer, amphoteric electrolyte, existence of dipolar ions, isoelectric point, strong electrolytes, Debye Huckel theory of strong electrolytes. Variation of activity coefficient with concentration, ionic strength, Debye Huckel limiting law. Energy sources: Primary and Secondary batteries. Acid and Alkaline battery, Ni-Cd cell, , solar cells. Construction, working, advantages and CdS solar Cell.

4. Molecular Spectroscopy II (18 H)

Electronic Spectroscopy: Franck-Condon principle, electronic transitions, singlet and triplet states, fluorescence and phosphorescence, dissociation and predissociation, calculation of electronic transitions of polyenes using free electron model. Nuclear Magnetic Resonance (NMR) spectroscopy: Principles of NMR spectroscopy, Larmor precession, Chemical shift and low-resolution spectra, different scales (Delta and T), Spin-spin coupling and high-resolution spectra, interpretation of PMR spectra of organic molecules. Electron Spin Resonance (ESR) spectroscopy: Principle, hyperfine structure, ESR of simple radicals.

1. Conductometric titration of Lead Nitrate against Sodium Sulphate and to determine the solubility of Lead Sulphate.
2. To investigate the influence of Ionic strength on the rate constants between Potassium Persulphate and Potassium Iodide.
3. To determine the dissociation constant of a weak dibasic acid using pH metry.
4. To study the Kinetics of ethyl acetate by NaOH at two different temperatures and hence determine the energy of activation.
5. To determine the percentage concentration and strength of a strong acid and weak acid present in a mixture by potentiometric titration.
6. Preparation of aniline hydrochloride and to determine hydrolysis and hydrolysis constant of aniline hydrochloride.
7. Adsorption of Oxalic acid by charcoal and verifying Freundlich adsorption isotherm.
8. Verification of Debye-Huckel-Onsager equation to dilute solutions of KCl by conductometric method.
9. To determine composition of Zinc Ferrocyanide complex by potentiometric titration.

Minor Experiments

1. Using vibrational-rotational spectra of NO molecule:
 - a. Assign the rotational lines to various transitions.
 - b. Calculate
 - i) the value of B_0 and B_1 , for R and P branches of spectra.
 - ii) Vibrational frequency and
 - iii) Inter nuclear distance
2. Using vibrational-rotational spectra of CO molecule.
 - a. Assign the rotational lines to various transitions.
 - b. Calculate
 - i. The value of B_0 and B_1 , for R and P branches of spectra.
 - ii. Vibrational frequency and
 - iii. Inter nuclear distance
3. To Calculate ionic strength at different concentration of potassium persulphate and potassium iodide.
4. Calculate the potentials by supplying the values of pH using the equation $pH = 0.457 - E_{cell}/0.0592$ and plot the graph.
5. Calculate the rate constants and energy of activation by using the given titre values.
6. Determine the hydrolysis and hydrolysis constant of aniline hydrochloride at any two concentrations, given the conductance values at these concentrations.
7. Provide any five values for $\log x/m$ and $\log C_e$ and plot a graph of $\log x/m$ against $\log C_e$ and determine the constant values n and k .

LEARNING OUTCOMES

THEORY

At the end of the course students will be able to

- Define the terms involved in Quantum chemistry, electrochemistry, spectroscopy and nuclear chemistry.
- Derive Schrodinger's equation in spherical polar coordinates.
- Apply Schrödinger equation to many electron system apply the concept in valence bond chemical bond and molecular orbital.
- Draw the schematic diagrams, diagrams of reactors, energy sources, molecular orbital diagrams and the graphs involved.
- Describe the working of reactors, electrochemical cells and energy sources.
- Explain the terms involved giving examples, classify the types of nuclear reactors, energy sources and corrosion types.
- Derive and use the equations to solve the numerical in electrochemistry, spectroscopy,
- Interpret the physical picture of bonding and antibonding wave function.
- Discuss the principles involved in electronic spectroscopy (NMR PMR ESR)

PRACTICAL

At the end of the course students will be able to

- Understand the concepts of conductance adsorption isotherms and activation energy solubility product.
- Develop skills of working and set up of electrochemical cells and electrodes.
- Solve numericals on and verify the graph of adsorption isotherms.
- Interpret vibrational spectra of NO CO molecule.
- Determine potential with respect to pH.

REFERENCE BOOKS

Textbooks

1. J. N. Gurtu, Physical Chemistry Vol-III, A Pragati edition.
2. N. B. Laxmeshwar, S. M. Malushte, A. S. Mulye, V. N. Kulkarni, Concepts of Physical Chemistry, Chetana Prakashan.
3. P. C. Jain, Monica Jain, Engineering Chemistry 15th Edition, Dhanpat Rai Publishing Co.

Reference Books

1. Barnwell, C. N. & McCash, E.M., Fundamentals of Molecular Spectroscopy, 4th Ed. Tata McGraw Hill, New Delhi (2006)
2. U. N. Dash, Nuclear Chemistry, S. Chand Publication
3. H. J. Arnikar, Essentials of Nuclear Chemistry, New Age International Publishers, 4th Revised Edition
4. Gurdeep Raj, Advanced Physical Chemistry Goel Publication.

5. Chandra, A. K., Introductory Quantum Chemistry, Tata McGraw –Hill (2001).
6. House., J. E., Fundamentals of Quantum Chemistry, 2ND Ed. Elsevier: USA (2004)
7. Lowe. J. P. & Peterson., K., Quantum Chemistry, Academic Press (2005)
8. Kakkar., R., Atomic and Molecular Spectroscopy, Cambridge University Press (2015)
9. Ira N. Levine, Quantum Chemistry, Seventh Edition, Pearson
10. Chemistry for degree students Semester V and VI by R. L. Madan, S. Chand Publication
11. Quantum Chemistry by Donald A McQuarrie, viva student edition.

Bachelor of Science (Honours) Programme

CHC-109

CORE COURSE

Inorganic Chemistry (Semester VI)

Credits: 06 (Theory: 04 & Practical: 02)

THEORY COURSE OBJECTIVES

Section A

- To define the terms Organometallic compounds, mononuclear, polynuclear metal carbonyls.
- To state the Effective atomic number rule, 18 electron rule for metal carbonyls and organometallic compounds.
- To discuss the IUPAC nomenclature, of metal carbonyls and organometallic compounds.
- To discuss the methods of preparation, properties and bonding in metal carbonyls and Ferrocene.
- To study the different types of magnetic behavior
- To discuss the measurement of magnetic susceptibility.
- Calculate the magnetic moments of transition metal complexes.
- To prepare by various methods alkyls and aryls of Li, Al, Hg and Ti.
- To study the effect of crystal field splitting on magnetic and spectral properties of octahedral complexes
- To study the types of electronic transitions like d-d, charge transfer and ligand-ligand.
- To study the selection rules for transitions to take place like Laporte, Orbital and Spin selection rules.
- To study the applications to determine ligand field strength, color of complexes, Cis-trans isomerism and Geometry of complexes.

Section B

- To study stability constants of reactions in terms of thermodynamic and kinetic stability.
- To study the substitution reaction mechanisms of octahedral complexes and the trans effect observed in square planar complexes.
- To define various acid-base theories.
- To know the several types of solvents and their typical characteristics.

- To explain the distinct types of reactions occurring in liquid ammonia and liquid Sulphur dioxide solvents.

- To introduce concept of Symmetry elements: Centre of symmetry, Rotation axis, Mirror plane, rotation – reflection axis and Identity To apply concepts of symmetry and point groups to different molecules.

PRACTICAL COURSE OBJECTIVES

- To estimate the metal ions by volumetric methods employing redox, argentometric and complexometric titration concepts.
- To prepare complexes and estimate the metal ion by volumetric analysis.
- To determine the alkalinity of water samples.

SYLLABUS

Theory:

Number of hours: 60

SECTION A

1. Organometallic chemistry (15 H)

Definition, nomenclature and classification of organometallic compounds, EAN rule, 18 electron rule.

- Mononuclear metal carbonyls: Preparation, properties, structure and bonding of $\text{Ni}(\text{CO})_4$, $\text{Fe}(\text{CO})_5$ and $\text{Cr}(\text{CO})_6$ (Orbital diagram not expected)
- Polynuclear metal carbonyl: Preparation and structures of $\text{Mn}_2(\text{CO})_{10}$, $\text{Co}_2(\text{CO})_8$, $\text{Fe}_2(\text{CO})_9$ and $\text{Fe}_3(\text{CO})_{12}$ (Orbital diagram not expected)
- Sandwich compounds like Ferrocene: preparation, properties, reactions, structure and Bonding (MOT).
- Preparation and properties of alkyl and aryls of Li, Al, Hg and Ti.

2. Spectra and Magnetic properties (15 H)

- Effect of Crystal Field Splitting on properties of Octahedral Complexes: Magnetic, Spectral. Measurement of 10 Dq for $[\text{Ti}(\text{H}_2\text{O})_6]^{+3}$ Complex.
- Determination of ground state term for d1 to d10 metal ions
- Electronic Spectra of transition Metal Complexes. Introduction, Types of Electronic transitions. The d-d transitions (d1/d9 and d2/d8), Charge transfer transitions and Ligand- Ligand transitions. Selection Rules (LaPorte Orbitals and Spin). Applications: Ligand field strength, Colour of complexes, Cis – Trans isomerism and Geometry of complexes.
- Types of magnetic behaviour, Methods of determining magnetic susceptibility (Gouy's method); Spin only formula; application of magnetic moment data for 3d – Metal complexes.

SECTION B

3. Reaction Kinetics and Mechanism (10 H)

A brief outline of thermodynamic stability of metal complexes and factors affecting the stability. Thermodynamic and Kinetic stability, Lability and inertness of octahedral complexes, Taube's classification. Kinetics of octahedral complexes: Electrophilic and Nucleophilic substitution. Mechanism of ligand substitution in octahedral complexes: acid hydrolysis, base hydrolysis and annation reaction. Trans- effect with respect to square planar Platinum complexes.

4. Acid Bases and Non-aqueous Solvents (12 H)

Bronsted theory, Lux – Flood Solvent systems and Lewis concept of Acids and Bases. Classification and physical properties of solvents, their general characteristics and levelling effect. Reactions in non-aqueous solvents with respect to liquid NH_3 , liquid SO_2 and liquid HF .

5. Symmetry and Term Symbols (8 H)

Symmetry elements like Centre of symmetry, Rotation axis. Mirror Plane, Rotation Reflection Axis, Identity. Determination of Point group and its application to H_2O , Ethylene, Trans dichloro ethylene, NH_3 , BCl_3 , $[\text{PtCl}_4]^{2-}$, SiCl_4 , Benzene, SF_6 .

PRACTICALS

Number of hours: 60

Volumetric Exercise

1. Volumetric estimation of Nitrite in the given solution of sodium nitrite using KMnO_4 .
2. Estimation of Fe(III) by dichromate method in the given solution of ferric alum by using SnCl_2 .
3. Preparation of Tetraamine copper(II) sulphate complex and estimate the amount of copper from Tetraamine copper(II) sulphate complex by iodometry.
4. Preparation of Triethylenediaminenickel(II) chloride complex and estimate the amount of Ni by EDTA.
5. Estimate volumetrically the amount of cobalt in $\text{CoCl}_2 \cdot \text{H}_2\text{O}$ by EDTA method using hexamine indicator.
6. To estimate amount of ferrous(Fe^{2+}) and ferric(Fe^{3+}) ions in the given solution containing ferric chloride and ferrous sulphate by using potassium dichromate.
7. To estimate aluminum by back titration using zinc sulphate.
8. Estimation of manganese in presence of iron in ferromanganese by EDTA titration.
9. Determine the strength in grams per litre of a given AgNO_3 solution being provided $\text{N}/30\text{NaCl}$ solution by Mohr's Method.
10. Determination of alkalinity of a given mixture of OH^- and CO_3^{2-} using phenolphthalein and methyl orange indicator.

LEARNING OUTCOMES

Theory

At the end of the course students will be able to

- To interpret the stability of metal carbonyls and organometallic compounds. To generalise the methods of preparation, properties and bonding in organometallic compounds.
- To study the different types of magnetic behaviour.
- Discuss the measurement of magnetic Susceptibility.
- Calculate the magnetic moments of transition metal complexes.
- Define stability constants of reactions in terms of thermodynamic and kinetic stability.
- Know the various factors affecting the stability constants of complexes.
- Know the types of substitution reaction mechanisms of octahedral complexes and understand the trans effect to apply it to square planar complexes.
- Define and understand various acid-base theories with various examples
- Understand the behaviour of non- aqueous solvents like liquid ammonia and liquid Sulphur dioxide with the help of the distinct reactions taking place in these solvents.
- Explain Symmetry elements: Centre of symmetry, Rotation axis, Mirror plane, rotation – reflection axis and
 - Identify symmetry elements in various molecules and assign them to different pointgroups.

Practical

- The students will acquire the skill to effectively prepare complexes and carry out their quantitative analysis.
- Acquire skills to effectively prepare complexes and carry out their quantitative analysis.
- Learn methodology to determine the alkalinity of water samples.

REFERENCE BOOKS

Theory

Textbooks

- 1) J. D. Lee, Concise Inorganic Chemistry, 5th Edn. Wiley India.
- 2) B. R. Puri, L. R. Sharma and K. C. Kalia, Principles of Inorganic Chemistry, 3rd Edn.

Reference books

- 1) F. Albert Cotton, Geoffrey Wilkinson and Paul L. Gaus, Basic inorganic chem. 3rd Edn. Wiley India
- 2) James E. Huheey, Ellen A. Keiter, Richard L. Keiter and Okhil K. Medhi, Inorganic Chemistry, Principles of Structure and Reactivity. 4th Edn. Pearsons
- 3) K. V. S. Laxmi Devi, N. C. Patel, S.S. Dhume, A. Venkatachalam, S. P. Turakhia, Chhaya Dixit and R. A. Mirji, College Inorganic Chemistry for T.Y. B. Sc. 21st Edn, Himalaya Publishing House.
- 4) Solid State Chemistry, Third edition By- Lesley E. Smart, Elaine A. Moore, Pub- Taylorand Francis.
- 5) D. E. Shriver, P. W. Atkins and C.H. Langford, Inorganic Chemistry, Oxford.

- 6) G. D. Tuli, S. K. Basu and R.D. Madan, Advance inorganic chemistry, Satya Prakash, S. Chand Publication.

- 7) F. A. Cotton, Chemical Applications of Group Theory, Wiley India
- 8) P. K. Bhattacharya, Group Theory and its Chemical Applications Himalaya Publications.

Practical

Textbooks

- 1) G. H. Jeffery, J. Bassett, J. Mendham, R. C. Denney, Vogel's Textbook of Quantitative Chemical Analysis, 5th Edn. ELBS.

Reference books:

1. J. Mendham, R. C. Denney, J.D. Barnes, M. Thomas, B. Sivasankar, Vogel's Textbook of Quantitative Chemical Analysis, 6th Edn. Pearson
2. S. Ratan, Experiments in Applied Chemistry, 3rd Edn. S.K. Kataria & Sons
3. O. P. Pandey, D. N. Bajpai and S. Giri, Practical Chemistry, Revised Edn. S. Chand.

Bachelor of Science (Honours) Programme

CHC-110

CORE COURSE

Organic Chemistry (Semester VI)

Credits: 06 (Theory: 04 & Practical: 02)

THEORY COURSE OBJECTIVES

Section A

- To understand the reactions and mechanism of name reactions and rearrangements mentioned in the syllabus.
- To know the definition of the enolate ion and understand the concept of acidity and pK_a values of carbonyl compounds.
- To understand the generation of enolate ions and their use in synthetic organic chemistry.
- To study Keto-enol tautomerism of ethylacetoacetate.
- To study Jablonskii diagram and understand fluorescence, phosphorescence, intersystem crossing, and vibrational relaxation.
- To learn and understand photochemical reactions.

Section B

- To learn the structure elucidation of terpenes.
- To learn the synthesis of terpenes.
- To understand the reactions of glucose and determination of ring size of Glucose and sucrose.
- To understand the open chain reactions of sucrose and inversion of cane sugar.
- To know the evidence of presence of glucose and fructose unit in sucrose.
- To understand the stereospecific and stereoselective reactions.
- To understand the mechanistic aspects of addition, substitution and elimination reactions.

PRACTICALS COURSE OBJECTIVES

- To get hands on experience for the preparation of derivatives using the reactions learnt in theory and binary mixture separation followed by analysis of individual compound.

Theory:**Number of hours: 60**

SECTION A

1. Name Reactions and Rearrangements (18 H)

Reaction and mechanism of the following: Benzoin, Aldol, Knoevenagel, Wittig and Darzens Glycidic ester. Rearrangement with mechanism: Beckmann, Wolff Rearrangement and Hofmann. Only Reaction and applications (2) of the following: Baeyer Villiger, Appel, Diekmann and Stobbe. Rearrangements: Schmidt, Claisen, Favorskii, Curtius. Comparison of Clemmensen reduction and Wolff Kishner reduction.

2. Chemistry of Enolates (8 H)

Definition of enolate ion, acidity of carbonyl compounds, pKa values, generation of enolate ion, role of bases in enolate ion formation, alkylation of carbonyl compounds with reference to cyclohexanone, acetone, ethylacetoacetate, malonic ester. Claisen condensation for preparation of ethylacetoacetate (reaction and mechanism). Keto-enol tautomerism of ethylacetoacetate. Malonic ester synthesis of carboxylic acids, ethylacetoacetate synthesis of ketones. Alkylation of 1,3-dithianes. Alkylation via enamine synthesis. Michael addition reaction.

3. Photochemistry (4 H)

Jablonski diagram, fluorescence, phosphorescence, intersystem crossing and vibrational relaxation. Norrish Type I and Type II cleavage reactions of ketones. Paterno Buchi and Barton reaction.

SECTION B

4. Terpenes (16 H)

Structure elucidation of Citral, α -Terpineol, α -Pinene and Camphor. Synthesis of Methylheptenone, Terebic acid and terpenylic acid. Synthesis of Citral from Methylheptenone. Synthesis of α -Terpineol from p-toluic acid. Synthesis of Norpinic acid, camphoric acid, camphoronic acid. Commercial synthesis of camphor.

5. Carbohydrates (6 H)

Open chain reactions of Glucose, Ruff degradation, determination of ring size of Glucose (pyranose and furanose using methylation method). Open chain reactions of sucrose, inversion of canesugar, Evidence of presence of glucose and fructose unit in sucrose. Determination of ring size of Sucrose. (using methylation method).

6. Stereochemistry (6 H)

Stereospecific and stereoselective reactions. Addition of bromine to 3-Hexene with mechanism. Addition of hydrogen halides to alkenes: Markownikoff's and anti-Markownikoff's addition rule. Substitution reactions: SN1, SN2, SNi reactions with mechanisms. Elimination reactions: E1, E2, E1cb reactions with mechanism.

1. Preparation of Derivatives (any 4)
 - i. Oxime derivative of Benzophenone.
 - ii. Acetyl derivative of Salicylic acid
 - iii. Osazone of Fructose
 - iv. Aldol derivative (using benzaldehyde and acetone to give dibenzalpropanone)
 - v. Benzoyl derivative of p-nitroaniline
 - vi. Demonstration of Knoevenagel condensation between Salicylaldehyde and ethylacetoacetate.

2. Binary mixture separation and analysis (Microscale)
(Any 10 Mixtures to be analysed)
 - i) Water insoluble –water insoluble (4 mixtures)
(Acid-Base, Acid-Phenol, Base-Neutral, Acid-Neutral, Phenol-Base, Phenol-Neutral.
 - ii) Water soluble –water insoluble (2 mixtures) (Acid-Acid, Acid-Neutral, Neutral-Neutral).
 - iii) Liquid-Liquid (2 mixtures)
 - iv) Solid-liquid mixture. (2 mixtures)

LEARNING OUTCOMES

Theory

At the end of the course students will be able to

- Explain and give the reactions and mechanism of reactions mentioned in the syllabus.
- Draw Jablonskii diagram and explain various processes.
- Discuss and illustrate photochemical reactions.
- Define enolate ion.
- Explain the acidity of carbonyl compounds, pK_a values, Keto-enol tautomerism.
- Describe the use of enolate ion in organic synthesis
- Elucidate the structure of terpenes.
- Describe the synthesis of terpenes.
- Illustrate the reactions of glucose, open chain reactions of sucrose and determination of ring size of Glucose and sucrose.
- Give the evidence of presence of glucose and fructose unit in sucrose.
- Describe stereospecific and stereoselective reactions and mechanism w.r.t. addition, substitution and elimination reactions.

Practical

At the end of the course students will be able to

- Perform reactions and prepare derivatives.
- Develop skills of separation of binary mixture and the analysis of separated

compound at microscale level.

REFERENCE BOOKS

THEORY

Textbooks

1. I. L. Finar, Organic Chemistry Vols I and II, Orient Longman
2. Morrison and Boyd, Organic Chemistry; 6th Edn. Prentice Hall India
3. J. March, Advanced Organic Chemistry: Reaction, Mechanism and Structure, Wiley, 2010, 4th Ed.
4. I. L. Finar, Stereochemistry and Chemistry of Natural products, ELBS, Longmans, 1963, Vol. 2, 3rd Ed.
5. P. S. Kalsi, Spectroscopy of Organic compounds, New Age International Pub. Ltd. & Wiley Eastern Ltd., Second edition, 1995.Press.

Reference books

1. Francis Carey, Organic Chemistry, 10th Edition.
2. Paula Yurkanis Bruice, Organic Chemistry; 3rd Edn., Pearson Education Asia
3. Silverstein, Bassler and Morill, Spectrometric Identification of Organic Compounds.
4. P Sykes, A guidebook to mechanisms in organic chemistry, 6th Ed., Pearson Edu., 1996.
5. J. Clayden, N. Greeves, S. Warren & Wothers, Organic Chemistry, Oxford University Press, 2012, 2nd Ed.
6. E. S. Gould et al., Mechanism and structure in Organic Chemistry, 1965
7. F. A. Carey, Organic Chemistry, 2000, 4th Ed.
8. S. H. Pine, Organic Chemistry, McGraw-Hill International Edn., 2010, 5thEd.
9. F. A. Carey and R. J. Sundberg, Advanced Organic Chemistry, Vol. I & II. Plenum Press, 1977.
10. D. Nasipuri, Stereochemistry of Organic compounds - Principles and Application, Wiley Eastern Limited, 2013, 4th Ed. Kent, [England]: New Academic Science Limited, 2013.
11. E. L. Eliel, Stereochemistry of carbon compounds, Tata Mac Graw Hill Publishing Company Ltd. (1990)
12. V. M. Potapov, Stereochemistry, MIR Publishers, Moscow, 1979
13. Organic Photochemistry- A Visual Approach, J Kopecky, VCH Pub., 1992.
14. Applications of Absorption Spectroscopy of Organic compounds, J. R. Dyer, Prentice Hall of India, 1987.
15. V. M. Parikh, Absorption spectroscopy of organic Molecules, Addison Wesley Longman Publishing Co., 1974.
16. D. H Williams & I. Fleming, Spectroscopic methods in organic chemistry, 6th Ed., Tata Mcgraw Hill Education, 2011.
17. William Kemp, Organic spectroscopy, 3rd Ed., Palgrave Macmillan, 1991.
18. R. O. C. Norman and J. M. Coxon, Principles of Organic Syntheses, 3rd Ed., CRC Press Inc, 1993.
19. R. Bruckner, Advanced Organic Chemistry – Reaction Mechanisms, San Diego, CA: Harcourt /Academic Press, San Diego, 2002.
20. M. B. Smith, Organic Synthesis, McGraw – HILL International Edition, NewYork,1994.
21. W. Caruthers, Modern Methods of Organic Synthesis, 4th Ed., Cambridge University Press, 2004.

22. Heterocyclic Chemistry, J A Joule and G F Smith, ELBS, Advances in Heterocyclic Chemistry, Edited by A R Katritzky et al, Vol. 1 to 50, Academic P.

PRACTICAL

Textbooks

1. A.I. Vogel, A.R. Tatchell, B. S. Furniss, A.J. Hannaford, Vogel's Textbook of Practical Organic Chemistry, 5th Ed., Prentice Hall; 2011.
2. Practical organic chemistry, F G Mann and B C Saunders, Orient Longman, 4th ed.
3. Ahluwalia, V. K. & Aggarwal, R. Comprehensive Practical Organic Chemistry, Universities Press.

Reference books

1. D. Pasto, C. Johnson and M. Miller, Experiments and Techniques in Organic Chemistry, 1st Ed., Prentice Hall, 1991.
2. L. F. Fieser, K.L. Williamson "Organic Experiments" 7th edition D. C. Heath, 1992.
3. K. L. Williamson, K.M. Masters, Macroscale and Microscale Organic Experiments, 6th Edition, Cengage Learning, 2010
4. R. K. Bansal, Laboratory Manual in Organic Chemistry, New Age International, 5th Edition, 2016.

Bachelor of Science (Honours) Programme

CHD-103

Discipline Specific Elective

Selected Instrumentation in Chemistry (Semester VI)

Credits: 04

THOERY: COURSE OBJECTIVES

- To define the terms involved in chromatographic techniques and spectroscopic methods.
- To explain working of chromatographic techniques and detectors, spectrophotometer, Atomic spectroscopy, DTA, DSC.
- To classify different types of chromatographic methods.
- To study the principles of GC, HPLC,
- To interpret steps involved in chemical analysis.
- To describe the basic components of instruments.
- To draw the schematic diagrams of different instruments.
- To solve numerical on chromatographic techniques
- To discuss the applications of different chromatographic techniques and spectroscopic methods.

SYLLABUS

Theory:

Number of hours: 60

SECTION A

1. Introduction (4 H)

Overview of instruments in chemical analysis, Basic components of instruments for analysis: Signal generators, detectors (input transducers) Signal processors, read out devices, circuits & electrical devices in the instruments, advantages of instruments interfaced with computers.

2. Chromatographic techniques (12 H)

Classification of chromatography methods. Gas chromatography: Basic principles of GSC and GLC. Terms involved: Distribution equilibria, rate of travel, retention time,

retention volume, relative retention, Height Equivalent to a Theoretical Plate(HETP), Van Deemter equation. Instrumentation: carrier gas, column, injections systems,

explanations of factors affecting separation, thermal conductivity and flame ionization detectors. Qualitative and Quantitative analysis: internal standards, determination of peak area. HPLC: Instrumentation, description of pumps, detector choice (UV absorption and refractive index detectors), columns, injection system, packing materials, applications. Introduction to hyphenated techniques: Basic principles of GC-MS and LC-MS. (Numerical problems are to be solved)

3. Mass spectrometry (8 H)

Introduction, theory, making the gaseous molecule into an ion (electron impact, chemical ionization), making liquids and solids into ions (electro spray, electrical discharge), separation of ions on basis of mass to charge ratio. Instrumentation: schematic diagram of single and double focusing. Advantages of Quadrupole Mass Spectrometer, sample introduction, sample purity, spectrum resolution. Applications of mass spectrometry in structure elucidation. Peak matching.

4. X-ray diffraction methods (6 H)

Introduction to X-ray absorption and emission methods, Bragg's law, Diffraction of X-rays, production and detection of X-rays, sample preparation, identification of powder diffraction patterns of ZnO, NiO and MgAl₂O₄.

SECTION B

5. UV-Visible Spectroscopy (10 H)

Interaction of electromagnetic radiation with matter, Quantitative calculations- Beer's and Lambert's law, derivation of Beer-Lambert's law, deviations from Beer's law. Principles of instrumentation: Sources, monochromators, cells. Types of instruments: Photoelectric colorimeters and Spectrophotometers: Single & Double beam; comparison between colorimeter and spectrophotometer; applications: qualitative control of purity, quantitative analysis; identification of structural groups in a molecule; study of co-ordination compound, cis-trans isomerism; chemical kinetics. Photometric titrations (numerical problems are expected to be solved).

6. Atomic spectrometric methods (14 H)

Atomic absorption Spectroscopy: Introduction, principle, instrumentation, applications, limitations. Flame photometry and introduction, principle, instrumentation, applications, limitations. Differences between flame photometry and atomic absorption spectroscopy. Fluorimetry: principles of fluorescence, chemical structure and fluorescence. Relationship between concentration & fluorescence intensity, instrumentation & applications. (numerical problems are expected to be solved)

7. Analysis of drug in solid state (6 H)

Concepts of particle size, size distribution shown as cumulative undersize curve. Thermal methods of analysis: Basic principles of differential thermal analysis (DTA) and Differential Scanning Calorimetry (DSC), Differential Thermal Analysis - apparatus and methodology, factors affecting DTA results, quantitative DTA, interpretation of results.

Applications to detect polymorphism and pseudo polymorphism in pharmaceuticals by DSC or DTA.

LEARNING OUTCOMES

At the end of the course students will be able to

- Discuss the principles behind the basic components of instruments (signal generators processors and detectors) and their advantages interfaced with computers.
- Define the terms, and principles involved in involved gas chromatography (GC) liquid chromatography (HPLC).GC-MS, LC-MS and solve the numericals with reference to the techniques.
- Explain sampling and working of X ray absorption and emission techniques.
- Describe the working and principles in photoelectric colorimeters and spectrophotometers and its application in isomerism photometric titrations and chemical kinetics.
- Explain principles, instrumentation, applications and limitations of AAS, fluorimetry, flame photometry and solve the numerical with reference to the technique.
- Interpret steps involved in thermal methods of analysis- DTA, DSC and its applications in pharmaceuticals.
- To discuss the applications of advantages of different chromatographic techniques and spectroscopic methods.

REFERENCE BOOKS

Textbooks:

1. B. K. Sharma. Instrumental Methods of Chemical Analysis: Goel Publishing House, Meerut.
2. K. Raghuraman, D. V. Prabhu, C. S. Prabhu and P. A. Sathe, Basic principles in Analytical Chemistry, 5th edition, Shet Publications Pvt. Ltd.

Reference books:

1. G. Chatwal and S. Anand, Instrumental Methods of Chemical Analysis, 5th edition (reprint 2003), Himalaya publication.
2. Willard, Meritt and Dean. Instrumental Methods of Analysis.
3. Skoog and Leary, Principles of Instrumental analysis, Saunders College Publication.

(Semester V &VI)

Credits: 04

PROJECT COURSE OBJECTIVES

Students will gain knowledge and understanding of

- **Basic research:** The objective of basic research is to gain more comprehensive knowledge or understanding of the subject under study, without specific applications in mind. In industry, basic research is defined as research that advances scientific knowledge but does not have specific immediate commercial objectives, although it may be in fields of present or potential commercial interest.
- **Applied research:** Applied research is aimed at gaining knowledge or understanding to determine how a specific, recognized need may be met. In industry, applied research includes investigations oriented to discovering new scientific knowledge that has specific commercial objectives with respect to products, processes, or services.

This Project course is in lieu of one of the DSE course. The project work is to be started in the beginning of semester V and to be completed at the end of semester VI.

LEARNING OUTCOMES

Students will be able to learn the following:

- Students will have a firm foundation in the fundamentals and application of current chemical and scientific theories including those in Analytical, Inorganic, Organic and Physical Chemistries. Majors to be certified by the American Chemical Society will have extensive laboratory work and knowledge of Biological Chemistry.
- Students will be able to design and carry out scientific experiments as well as accurately record and analyse the results of such experiments.
- Students will be skilled in problem solving, critical thinking and analytical reasoning as applied to scientific problems.
- Students will be able to clearly communicate the results of scientific work in oral, written, and electronic formats to both scientists and the public at large.
- Students will be able to explore new areas of research in both chemistry and allied fields of science and technology.

- Students will appreciate the central role of chemistry in our society and use this as a basis for ethical behaviour in issues facing chemists including an understanding of safe handling of chemicals, environmental issues and key issues facing our society in energy, health and medicine.
- Students will be able to explain why chemistry is an integral activity for addressing social, economic, and environmental problems.
- Students will be able to function as a member of an interdisciplinary problem-solving team.
