# **M.Sc. Applied Chemistry**

### **Programme Outcome**

Students would be able to get an in-depth knowledge in all disciplines of chemistry especially in fats and oils. Students would be able to employ the scientific method to design, carry out, record and analyze the results of chemical experiments and get an awareness of the impact of chemistry on the environment, society, and other cultures outside the scientific community.

## **Programme Specific Outcome**

The Program enable the students to develop

- Theoretical background and develop practical skills for analysing materials using modern analytical methods and instruments.
- Problem solving approach by coordinating the different branches of chemistry.
- Knowledge and skills to use oils and fats within their practice and to operate as a professional practitioner
- Professional skills for higher studies in research institutions and to work in chemical industries.
- In-depth knowledge helps to qualify in competitive exams.

# **Course Outcomes**

# SEMESTER 1 CH 50 01 01 ORGANOMETALLICS AND NUCLEAR CHEMISTRY

## UNIT 1. Organometallic Compounds: Synthesis, Structure, and Bonding

- CO 1a To demonstrate proficiency in Hapto nomenclature, synthesis, and bonding of organometallic compounds with linear pi donor ligands.
- CO 1b To analyze the synthesis and structural aspects of complexes with cyclic pi donors, metallocenes, and cyclic arene complexes.
- CO 1c To evaluate the properties, preparation, and bonding of metal carbonyls, including mono and binuclear metal carbonyls, metal nitrosyls, and metal cyanides.

## **UNIT 2. Reactions of Organometallic Compounds**

- CO 2a To understand nucleophilic ligand substitution, nucleophilic, and electrophilic attack on coordinated ligands.
- CO 2b To analyze addition and elimination reactions, oxidative addition, reductive elimination, and insertion reactions in organometallic compounds.
- CO 2c To explore redistribution reactions and fluxional isomerism in allyl, cyclopentadienyl, and allene systems.

### **UNIT 3. Catalysis by Organometallic Compounds**

- CO 3a To differentiate between homogeneous and heterogeneous organometallic catalysis.
- CO 3b To analyze catalytic reactions involving carbon monoxide and hydrogen, including the water gas shift and Fischer-Tropsch reactions.
- CO 3c To understand the processes of hydroformylation of olefins, polymerization using Ziegler Natta and metallocene catalysts, and various carbonylation reactions.
- CO 3d To explore applications of palladium catalysts in the formation of C-O and C-N bonds and oxidative coupling reactions.

#### **UNIT 4. Bioinorganic Compounds**

- CO 4a To evaluate the role of essential and trace elements in biological systems and recognize the toxic effects of metals.
- CO 4b To analyze the structure and functions of biological membranes, ion transport mechanisms, and redox metalloenzymes.
- CO 4c To explore the biochemistry of zinc and copper, including the functions of carbonic anhydrase, carboxypeptidase A, and superoxide dismutase.
- CO 4d To understand the significance of metal-containing biomolecules such as Vitamin B12 and chlorophyll in photosynthesis.

#### **UNIT 5. Nuclear Chemistry**

- CO 5a To analyze nuclear reactions, Q value, reaction threshold, and neutron capture cross-section.
- CO 5b To understand counting techniques using G.M. counters, proportional counters, ionization, and scintillation counters.
- CO 5c To explore the synthesis of transuranic elements and applications of radioisotopes in analytical chemistry.
- CO 5d To understand radiation chemistry, measure radiation doses, and recognize the relevance of radiation chemistry in various fields.

### CH 50 01 02 STRUCTURAL AND MOLECULAR ORGANIC CHEMISTRY

#### **UNIT 1. Basic Concepts in Organic Chemistry:**

CO 1a To understand and apply fundamental concepts in organic chemistry, including bonding, hybridization, and the molecular orbital picture of butadiene and allyl systems.

- CO 1b To analyze electron displacement effects, such as inductive effect, electromeric effect, resonance effect, hyperconjugation, and steric effects. Understand bonding weaker than covalent bonds.
- CO 1c To comprehend the concept of aromaticity, including delocalization of electrons, Hückel's rule, criteria for aromaticity, and examples of neutral and charged aromatic systems. Explore NMR as a tool and the significance of carbon nanotubes and graphene.
- CO 1d To analyze the mechanisms of electrophilic and nucleophilic aromatic substitution reactions, including arenium ion intermediates, SN1, SNAr, SRN1, and benzyne mechanisms.

### **UNIT 2. Physical Organic Chemistry:**

- CO 2a To understand energy profiles, kinetic versus thermodynamic control of product formation, Hammond postulate, and kinetic isotope effects. Apply linear free energy relationships, including the Hammet equation and Taft equation.
- CO 2b To analyze catalysis by acids, bases, and nucleophiles using examples from acetal, cyanohydrin, ester formation, and hydrolysis reactions. Understand the principles of hard and soft acids and bases (HSAB) and its applications in organic reactions.

### **UNIT 3. Organic Photochemistry:**

CO 3a To explore photoreactions of carbonyl compounds, including Norrish reactions, Paterno-Buchi reaction, Barton (nitrite ester reaction), di- $\pi$ -methane, Photo Fries rearrangements, and photochemistry of conjugated dienes and vision.

### **UNIT 4. Stereochemistry of Organic Compounds:**

- CO 4a To define stereoisomerism based on symmetry and energy criteria. Understand configuration, conformational stereoisomers, and the basic idea of Akamppt isomerism.
- CO 4b To analyze molecules with chiral centers, absolute configuration, enantiomers, racemic modifications, R and S nomenclature, and molecules with multiple centers of chirality. Understand diastereoisomers, constitutionally symmetrical and unsymmetrical chiral molecules, and erythro and threo nomenclature.
- CO 4c To explore axial, planar, and helical chirality with examples. Understand stereochemistry and absolute configuration of allenes, biphenyls, binaphthyls, ansa and cyclophanic compounds, spiranes, and exo-cyclic alkylidene cycloalkanes.
- CO 4d To analyze topicity and prostereo isomerism, including the nomenclature of ligands and faces. Understand NMR distinction of enantiotopic/diastereotopic ligands.

CO 4e To understand geometrical isomerism, including nomenclature, E-Z notation, methods of determination, and interconversion of geometrical isomers.

#### **UNIT 5. Conformational Analysis:**

- CO 5a To understand conformational descriptors and factors affecting the conformational stability of molecules. Analyze conformational analysis of substituted ethanes, cyclohexane and its derivatives, decalins, adamantane, norbornane, sucrose, and lactose.
- CO 5b To explore conformation and reactivity of elimination, substitution, and oxidation of 20 alcohols.
- CO 5c To analyze the chemical consequences of conformational equilibrium using the Curtin Hammett principle.

### CH 50 01 03 QUANTUM CHEMISTRY AND GROUP THEORY

#### **Unit 1: Group Theory and Applications in Chemical Bonding**

- CO 1a To understand symmetry elements and symmetry operations in molecules.
- CO 1b To determine point groups of molecules and ions belonging to various point groups (Cn, Cs, Ci, Cnv, Cnh, C∞v, Dnh, D∞h, Dnd, Td, and Oh).
- CO 1c To recognize crystallographic point groups and Hermann-Mauguin symbols. Understand screw axis, glide planes, and elementary space group concepts.
- CO 1d To grasp mathematical group properties, including Abelian and cyclic groups, subgroups, similarity transformations, and classes (C2v, C3v, C2h).
- CO 1e To apply group multiplication tables (GMTs) for C2v, C3v, and C2h. Understand isomorphic groups.
- CO 1f To utilize matrix representation for elements and point groups. Understand trace/character and block-factored matrices.
- CO 1g To analyze reducible and irreducible representations. Apply the standard reduction formula. Understand the great orthogonality theorem (GOT). Construct character tables for C2v, C2h, C3v, and C4v.
- CO 1h To apply group theory in chemical bonding, including the projection operator, transformation properties of atomic orbitals, and construction of symmetry-adapted linear combinations of atomic orbitals (SALCs) for specific molecules.

#### **Unit 2: Quantum Mechanics and Applications**

- CO 2a: To explain the experimental observations that led to the development of quantum mechanics.
- CO 2b: To understand the key principles of quantum mechanics.
- CO 2c: To discuss the conditions of a well behaved wavefunction.
- CO 2d: To describe the operator algebra in quantum mechanics.
- CO 2e: To understand the basic principles of quantum mechanics.
- CO 2f: To analyze the quantum mechanical description of a particle with no external potential.
- CO 2g: To develop proficiency in the mathematical techniques used to solve problems related to translational motion in quantum mechanics.

- CO 2h: To understand the concept of a one-dimensional harmonic oscillator in classical and quantum mechanics.
- CO 2i: To derive and interpret the wave functions for the harmonic oscillator.
- CO 2j: To derive the wave equation in spherical polar coordinates.
- CO 2k: To analyze the quantum mechanics of a non-planar rigid rotor or a particle on a sphere.
- CO 21: To develop an understanding of quantum phenomena related to rotational motion.
- CO 2m: To solve problems related to angular momentum quantization and operators in different physical systems.
- CO 2n: To derive the wave equation for hydrogen-like atoms in spherical polar coordinates.
- CO 20: To solve the wave equations to obtain wave functions and energy levels for hydrogen-like atoms.

### CH 50 01 04THERMODYNAMICS, KINETIC THEORY AND STATISTICALTHERMODYNAMICS

#### **Unit 1: Classical Thermodynamics**

- CO 1a To understand the mathematical foundations of thermodynamics, including variables, extensive and intensive quantities, and exact differentials.
- CO 1b To comprehend thermodynamic equations of state, Maxwell relations, and the significance of irreversible processes.
- CO 1c To analyze free energy, thermodynamic equilibria, and the temperature dependence of free energy using the Gibbs-Helmholtz equation.
- CO 1d To understand partial molar quantities, chemical potential, and Gibbs-Duhem equations. Determine partial molar volume and enthalpy.
- CO 1e To explore fugacity, its relation to pressure, and determination of fugacity for real gases. Understand activity and its dependence on temperature and pressure.
- CO 1f To Study the thermodynamics of mixing, Gibbs-Duhem-Margules equation, and excess thermodynamic functions.
- CO 1g To analyze chemical affinity, thermodynamic functions, and the effect of temperature and pressure on chemical equilibrium.
- CO 1h To understand the Third Law of Thermodynamics, Nernst heat theorem, and the determination of absolute entropies.
- CO 1i To explore three-component systems, solid-liquid equilibria, ternary solutions, hydrate and compound formation, and liquid-liquid equilibria.

### **Unit 2: Kinetic Theory of Gases**

- CO 2a To derive Maxwell's law of distribution of velocities, understand collision diameter, frequency, and mean free path. Explore effusion and the law of corresponding states.
- CO 2b To analyze transport properties of gases and the time dependence of pressure in effusing gases.

### **Unit 3: Statistical Thermodynamics**

- CO 3a To understand the macroscopic and microscopic approaches, permutation, probability, and the concept of macrostates and microstates.
- CO 3b To explore Boltzmann distribution law, partition function, and their physical significance. Understand distinguishable and indistinguishable particles.
- CO 3c To calculate thermodynamic functions and equilibrium constants. Explore thermodynamic probability, entropy, and the statistical formulation of the third law of thermodynamics.
- CO 3d To understand quantum statistics, Bosons and Fermions, Bose-Einstein and Fermi-Dirac statistics, and their applications.
- CO 3e To analyze the heat capacity of solids, vibrational properties, and the theories of Einstein and Debye.

### SEMESTER 2 CH 50 02 01COORDINATION CHEMISTRY

### **Unit 1: Structural Aspects and Bonding**

- CO 1a To classify complexes based on coordination numbers and geometries. Understand sigma and pi bonding ligands, stability of complexes, and thermodynamic aspects of complex formation.
- CO 1b To explain the splitting of d orbitals in various fields, LFSE, Dq values, Jahn-Teller effect, and evidence of covalency in metal-ligand bonds.

### **Unit 2: Spectral and Magnetic Properties**

- CO 2a To understand electronic spectra of complexes, term symbols, Racah parameters, and d-d transitions. Interpret electronic spectra using Orgel and Tanabe-Sugano diagrams.
- CO 2b To analyze the interpretation of electronic spectra, including Orgel diagrams, Tanabe-Sugano diagrams, and charge transfer spectra. Explore magnetic properties and temperature dependence.

### **Unit 3: Kinetics and Mechanism of Reactions**

- CO 3a To analyze thermodynamic and kinetic stability, kinetics, and mechanisms of nucleophilic substitution reactions in square planar complexes. Understand the trans effect and its applications.
- CO 3b To explore kinetics and mechanisms of octahedral substitution, water exchange, dissociative and associative mechanisms, solvolytic reactions, and electron transfer reactions.

### **Unit 4: Stereochemistry of Coordination Compounds**

- CO 4a To understand geometrical and optical isomerism in octahedral complexes. Analyze the resolution of optically active complexes, determination of absolute configuration, and stereoselectivity in chelate rings.
- CO 4b To explore linkage isomerism, factors affecting it, and the symbiosis concept. Understand Prussian blue and related structures, as well as macrocycles-crown ethers.

## Unit 5: Coordination Chemistry of Lanthanoids and Actinoids

- CO 5a To understand term symbols for lanthanide ions, electronic spectra, magnetic properties, and organometallic complexes of lanthanoids.
- CO 5b To explore general characteristics of actinoids, coordination complexes, organometallic compounds of thorium and uranium, and comparative coordination chemistry of lanthanoids and actinoids.

## CH 50 02 02 ORGANIC REACTION MECHANISMS

#### **Unit 1: Review of Organic Reaction Mechanisms**

- CO 1a To analyze organic reaction mechanisms, emphasizing nucleophilic and electrophilic substitutions, eliminations, and addition reactions. Distinguish between E1, E2, SN1, SN2, SNi, SE1, and SE2 mechanisms.
- CO 1b To investigate the influence of substrate, reagent, leaving group, solvent, and neighboring group on nucleophilic substitution and elimination reactions. Differentiate between elimination and substitution pathways.

### **Unit 2: Chemistry of Carbanions**

- CO 2a To understand the formation, structure, and stability of carbanions. Explore reactions of carbanions, including aldol and Michael reactions, alkylation, and acylation.
- CO 2b To investigate nucleophilic additions to carbonyl groups, including Claisen, Dieckmann, Knoevenagel, Stobbe, Darzen, and acyloin condensations. Study the Shapiro reaction, Julia elimination, and Favorski rearrangement.

### **Unit 3: Chemistry of Carbocations**

- CO 3a To explore the formation, structure, and stability of carbocations, including classical and non-classical types.
- CO 3b To investigate C-X bond formations involving carbocations and various molecular rearrangements, such as Wagner-Meerwein, Pinacol-pinacolone, and benzilic acid rearrangements.

### Unit 4: Carbenes, Carbenoids, Nitrenes, and Arynes

- CO 4a To understand the structure of carbenes, their generation, and reactions. Explore reactions such as Wolff rearrangement and Reimer-Tiemann reaction.
- CO 4b To investigate the structure, generation, and reactions of nitrenes and related electron-deficient intermediates. Explore Hoffmann, Curtius, Lossen, Schmidt, and Beckmann rearrangements. Understand the generation and reactions of arynes.

### **Unit 5: Radical Reactions**

- CO 5a To analyze the generation of radical intermediates, their addition to alkenes, alkynes, fragmentation, and rearrangements. Understand Baldwin's rules and autooxidation.
- CO 5b To investigate name reactions involving radical intermediates, including Barton deoxygenation, decarboxylation, and McMurry coupling.

### **Unit 6: Chemistry of Carbonyl Compounds**

- CO 6a To understand reactions of carbonyl compounds, including oxidation, reduction, addition, Aldol condensation, Cannizzaro reaction, and Grignard reactions.
- CO 6b To explore the structure and reactions of  $\alpha$ ,  $\beta$ -unsaturated carbonyl compounds, involving electrophilic and nucleophilic addition reactions such as Michael addition and Mannich reaction.

### **Unit 7: Concerted Reactions**

- CO 7a To classify and understand concerted reactions, including electrocyclic, sigmatropic, cycloaddition, chelotropic, ene, and dyotropic reactions. Apply Woodward-Hoffmann rules and the PMO method.
- CO 7b To explore pericyclic reactions in organic synthesis, including Claisen, Cope, Wittig, and Diels-Alder reactions. Understand dipolar cycloaddition (introductory).
- CO 7c To analyze unimolecular pyrolytic elimination reactions, such as Cheletropic elimination and decompositions involving cyclic transition states.

## CH 50 02 03 CHEMICAL BONDING AND COMPUTATIONAL CHEMISTRY

### **Unit 1: Application of Group Theory in Spectroscopy**

- CO 1a To analyze vibrational modes using group theory, focusing on examples like H<sub>2</sub>O, NH<sub>3</sub>, and trans-N<sub>2</sub>F<sub>2</sub>. Predict IR and Raman activities, apply the rule of mutual exclusion, and understand redundant modes.
- CO 1b To apply group theory in UV-visible spectroscopy, discussing selection rules, orbital selection rules, and predicting electronic transitions in various point groups. Explore spin selection rules and relaxation in selection rules.
- CO 1c To apply group theory in hybridization, determining hybridization and hybrid functions in molecules like CH<sub>4</sub>, BF<sub>3</sub>, and PCl<sub>5</sub>.
- CO 1d To understand the role of group theory in optical activity, providing a brief study on its applications.

### **Unit 2: Approximation Methods in Quantum Mechanics**

- CO 2a: To understand the challenges posed by the many-body problem in quantum mechanics.
- CO 2b: To extend quantum mechanical treatment of single body problem to many body problems.
- CO 2c: To understand the necessity of employing approximation methods to address complex quantum systems.
- CO 2d: To understand and apply the variation theorem to specific examples.
- CO 2e: To analyze and evaluating the effectiveness of the variation method in approximating solutions for different quantum systems.
- CO 2f: To understand the concept of perturbation theory in quantum mechanics.
- CO 2g: To learn how to calculate the first-order correction to the energy and wave function using the perturbation method.
- CO 2h: To solve the first-order corrections to energy and wave function for specific systems.

- CO 2i: To gain a qualitative understanding of the Hellmann-Feynman theorem.
- CO 2j: To understand the Hartree-Fock method as an approach to solving the quantum mechanical problem for systems with multiple electrons.
- CO 2k: To understanding Roothan's concept of basis functions as a set of mathematical functions used to represent the atomic orbitals in the Hartree-Fock method.

#### **Unit 3: Chemical Bonding**

- CO 3a: To extend the Schrödinger equation to describe the quantum mechanical behavior of molecules.
- CO 3b: To understand the Born-Oppenheimer approximation as a key simplifying assumption in molecular quantum mechanics.
- CO 3c: To apply valence bond theory to describe the formation of the hydrogen molecule through the overlap of atomic orbitals.
- CO 3d: To understand the fundamental principles and concepts of Molecular Orbital theory.
- CO 3e: To recognize the key features that distinguish MO theory from other theories, such as Valence Bond (VB) theory.
- CO 3f: To apply MO theory to analyze the electronic structures of heteronuclear diatomic molecules.
- CO 3g: To understand the construction of spectroscopic term symbols for diatomic molecules.
- CO 3h: To recognize the role of hybrid orbitals in forming molecular geometries.
- CO 3i: To employ Huckel molecular orbital theory to analyze the electronic structure of ethene, allyl systems, butadiene, and benzene.

### **Unit 4: Computational Quantum Chemistry**

- CO 4a To introduce and understand the scope of computational chemistry, exploring potential energy surfaces and conformational searches.
- CO 4b To review ab initio methods, basis sets, and post-Hartree-Fock methods. Discuss Density Functional Theory (DFT) methods, including Hohenberg-Kohn theorems.
- CO 4c To compare ab initio, semi-empirical, and DFT methods. Understand the molecular geometry input and features of molecular mechanics force fields.
- CO 4d To gain hands-on experience in performing calculations using GAMESS/Firefly software. Understand Koopmans' theorem and molecular mechanics force fields like AMBER and CHARMM.

### CH 50 02 04 MOLECULAR SPECTROSCOPY

#### **Unit 1: Foundations of Spectroscopic Techniques**

- CO 1a To demonstrate an understanding of different regions of the electromagnetic spectrum.
- CO 1b To explain the origin of the spectrum and factors influencing the intensity of absorption.
- CO 1c To analyze and assess the signal-to-noise ratio in spectroscopy.
- CO 1d To comprehend natural line width and its significance in spectroscopy.

CO 1e To understand Doppler broadening, Lamb dip spectrum, and the Born-Oppenheimer approximation.

#### **Unit 2: Microwave Spectroscopy**

- CO 2a To calculate principal moments of inertia and classify molecules into linear, symmetric tops, spherical tops, and asymmetric tops.
- CO 2b To apply selection rules and analyze the intensity of rotational lines.
- CO 2c To derive Jmax, evaluate the effect of isotopic substitution, and calculate intermolecular distances.
- CO 2d To analyze rotational spectra of polyatomic molecules, understand the Stark effect, and its application in chemical analysis.
- CO 2e To comprehend nuclear spin and electron spin interaction in microwave spectroscopy.

#### **Unit 3: Infrared and Raman Spectroscopy**

- CO 3a To interpret Morse potential energy diagrams and understand fundamental vibrations, overtones, and hot bands.
- CO 3b To analyze vibrational spectra of polyatomic molecules and understand normal modes of vibrations.
- CO 3c To comprehend combination and difference bands, Fermi resonance, and the breakdown of the Born-Oppenheimer approximation.
- CO 3d To explain the classical theory of Raman spectrum, understand scattering of light, and analyze rotational and vibrational Raman spectra.
- CO 3e To understand the complementarities of Raman and IR spectra, mutual exclusion principle, and polarization features.

#### **Unit 4: Electronic Spectroscopy**

- CO 4a To determine term symbols of diatomic molecules and interpret electronic spectra.
- CO 4b To apply selection rules and understand vibrational coarse structure and rotational fine structure of electronic spectra.
- CO 4c To comprehend the Franck-Condon principle, predissociation, and calculate the heat of dissociation using the Birge and Sponer method.
- CO 4d To analyze electronic spectra of polyatomic molecules and transitions localized in a bond or group.

### **Unit 5: Nuclear Magnetic Resonance Spectroscopy**

- CO 5a To understand the theory of NMR spectroscopy, including the interaction between nuclear spin and applied magnetic fields.
- CO 5b To analyze important magnetically active nuclei, nuclear energy levels, and the population of energy levels.
- $\begin{array}{c} \text{CO 5c} \\ \text{shift on the } \delta \text{ scale of PMR and CMR.} \end{array}$
- CO 5d To apply spin-spin coupling theory, illustrating with the AX system.

- CO 5e To understand the instrumentation of NMR techniques and apply Fourier Transformation (FT) NMR Spectroscopy.
- CO 5f To comprehend solid-state NMR and its applications, including Magic Angle Spinning (MAS).

# **Unit 6: Other Magnetic Resonance Techniques**

- CO 6a To understand the principles of EPR Spectroscopy, including electron spin interactions and the g factor.
- CO 6b To analyze factors affecting g values, determine g values (g || and  $g^{\perp}$ ), and comprehend fine structure and hyperfine structure.
- CO 6c CO28: Students w To ill comprehend the theory and important applications of NQR Spectroscopy.
- CO 6d To understand the principles of Mossbauer Spectroscopy, including the Doppler effect, recording of spectra, and factors determining chemical shift.
- CO 6e To apply Mossbauer Spectroscopy to metal complexes.

# CH 50 02 05 INORGANIC CHEMISTRY PRACTICAL-1

- 1a Employ qualitative analysis methods (flame tests, complex formation, etc.) for the identification of cations.
- 1b Develop analytical skills to identify both familiar and less familiar metal ions in mixtures.
- 1c Utilize selective precipitation techniques for separating cations in complex mixtures.
- 1d Apply theoretical knowledge of cation properties and reactions to design effective separation schemes.
- 1e Develop colorimetric methods for the estimation of Fe, Cu, Ni, Mn, Cr, NH<sub>4</sub><sup>+</sup>, nitrate, and phosphate ions.
- 1f Calibrate spectrophotometers and use them to measure absorbance for quantitative analysis.
- 1g Perform concentration determination of ions using calibration curves and absorbance measurements.
- 1h Synthesize the specified complexes (Tris(thiourea)copper(I), Potassium tris(oxalate)aluminate(III), Hexammine cobalt(III) chloride, Tetrammine copper(II) sulfate, Schiff base complexes of divalent metal ions, Bis(dimethylglyoximato)nickel(II), Prussian blue).
- 1i Utilize IR spectroscopy to identify functional groups and confirm the formation of the complexes.
- 1j Apply NMR spectroscopy to gain insights into the molecular structure of the complexes.
- 1k Analyze electronic spectra to understand electronic transitions and coordination environments in the complexes.
- **11** Develop a comprehensive understanding of coordination chemistry principles through practical applications.

# CH 50 02 06 ORGANIC CHEMISTRY PRACTICAL-1

# PART 1: General Methods of Separation and Purification of Organic Compounds

- 1a Understand the principles of solvent extraction in separating organic compounds.
- 1b Apply solvent extraction techniques for the isolation of specific compounds from mixtures.
- 1c Comprehend the continuous extraction process in Soxhlet extraction.
- 1d Gain insights into the theory and application of fractional crystallization.
- 1g Understand the principles of TLC and paper chromatography in separation.
- 1h Apply TLC and paper chromatography for qualitative analysis of organic mixtures.
- 1i Master the technique of column chromatography for the separation of organic compounds.
- 1k Understand the principles of membrane dialysis for separation based on molecular size.

PART II: Separation of Organic Binary Mixtures and Quantitative Separation

- 2a Apply chemical and solvent separation methods for the efficient separation of binary mixtures.
- 2b Understand the factors influencing the choice of separation methods.

2c Gain proficiency in quantitative separation using column chromatography.

2d Assess the purity of separated components using TLC.

# PART III: Drawing Reaction Schemes and Spectra

- 3a To Draw reaction schemes of reactions using chemsketch
- 3b Generate accurate structures and spectroscopic data for substrates and products using chemsketch or chemdraw
- 3c Students will demonstrate proficiency in drawing reaction schemes, generating structures, and interpreting spectroscopic data for a variety of organic reactions.

# CH 50 02 07 PHYSICAL CHEMISTRY PRACTICAL-1.

# **PART A: Experimental Chemistry Experiments**

- 1a Verification of Freundlich and Langmuir adsorption isotherms using the Charcoal-Acetic Acid or Charcoal-Oxalic Acid system.
- 1b Determination of the concentration of a given acid using the adsorption isotherm.
- 1c Construction of the phase diagram of simple eutectics.
- 1d Investigation of the effect of KCl/Succinic acid on the Critical Solution Temperature of the phenol-water system.
- 1e Construction of the phase diagram of a three-component system with one pair of partially miscible liquids.

- 1f Measurement of the distribution coefficient of iodine between an organic solvent and water.
- 1g Determination of the equilibrium constant
- 1h Determination of the unknown concentration of KI.
- 1i Determination of the surface tension of a liquid using: (a) Capillary rise method (b) Drop number method (c) Drop weight method
- 1j Determination of Parachor values.
- 1k Determination of the composition of two liquids by surface tension measurements.
- 11 Determination of the Critical Micelle Concentration (CMC) of surfactants by surface tension measurements.

# **PART B: Computational Chemistry Experiments**

- 2a To calculate single point energy and vibrational frequencies and to optimize geometry of molecules, .
- 2e Conformational analysis of ethane and transition state search.
- 2f To calculate Molecular orbitals, ionization energy, and electron affinity.
- 2g To calculate Dipole moment, free valence, and bond order determination.
- 2h Determination of inversion barriers of simple molecules like NH<sub>3</sub>, H<sub>2</sub>O, H<sub>2</sub>O<sub>2</sub>.
- 2i Determination of Z-matrices/Cartesian coordinates of furan, thiophene, pyrrole, and benzene using structure drawing programs like Chemsketch and MacMolPlt.
- 2j Students will acquire practical skills in various experimental techniques related to adsorption, phase diagrams, distribution law, surface tension, and heat of solution determination.
- 2k Students will gain hands-on experience in computational chemistry using modern open-source tools for calculations related to energy, molecular structures, and properties.

## SEMESTER 3 CH 03 03 01 ESSENTIAL OILS AND AROMATICS Credit 4 Contact Hours: 72Hrs

## Unit 1: Essential oils

- CO 1a Demonstrate knowledge of various isolation techniques
- CO 1b Identify sources, nature, and chemical constituents of specific essential oils.
- CO 1c Analyze the uses of the identified essential oils.

# **Unit 2: Terpenoids**

CO 2a Define terpenoids and discuss their classification.

- CO 2b Explain the isoprene rule and general methods for determining the structure of terpenoids.
- CO 2c Describe the biosynthesis of terpenoids, emphasizing the formation of mevalonic acid as an intermediate.

### Unit 3: Study of Essential oil constituents-I

- CO 1- Describe the natural sources of ocimene,  $\alpha$ -pinene, p-cymene, and caryophyllene.
- CO 2-Explain the methods employed for the production of ocimene,  $\alpha$ -pinene, pcymene, and caryophyllene.
- CO 3-Illustrate the molecular structures of ocimene,  $\alpha$ -pinene, p-cymene, and caryophyllene.
- CO 4-Summarize the physical and chemical properties of ocimene,  $\alpha$ -pinene, pcymene, and caryophyllene.
- CO 5-Outline the major reactions involving ocimene,  $\alpha$ -pinene, p-cymene, and caryophyllene.
- CO 6-Explain the synthetic methods for obtaining ocimene,  $\alpha$ -pinene, p-cymene, and caryophyllene.
- CO 7-Identify the natural sources of geraniol, citronellol, terpineol, and menthol.
- CO 8-Discuss the production techniques for geraniol, citronellol, terpineol, and menthol.
- CO 9-Analyze the physical and chemical properties of geraniol, citronellol, terpineol, and menthol.
- CO 10-Describe the synthetic pathways for geraniol, citronellol, terpineol, and menthol.
- CO 11-Identify the natural sources of citral.
- CO 12-Explain the methods used for the production of citral.
- CO 13-Illustrate the molecular structure of citral.
- CO 14-Summarize the physical and chemical properties of citral.
- CO 15-Interpret UV-visible spectra of ocimene,  $\alpha$ -pinene, geraniol, citral, and camphor.
- CO 16-Interpret infrared spectra of ocimene,  $\alpha$ -pinene, geraniol, citral, and camphor.
- CO 17-Analyze mass spectra of ocimene, α-pinene, geraniol, citral, and camphor.

### Unit 4: Study of essential oil constituents- II

- CO 4a Comprehend the natural sources, production, structure, properties, and uses of aromatic and essential oil constituents.
- CO 4b Study specific compounds, including alcohols (Cinnamyl alcohol, leaf alcohol), aldehydes (Anisaldehyde, Vanillin), phenols (Eugenol, Isoeugenol, Methyl eugenol), esters (Cinnamyl acetate, Geranyl acetate, Linalyl acetate), and miscellaneous compounds (Coumarin, Muscone, Civetone, Artificial Musk).

## Unit 5: Spices and spice oils

CO 5a Identify sources, production, nature, and chemical constituents of various spices.

CO 5b Understand the uses of spices such as cardamom, pepper, clove, nutmeg, mace, cinnamon, ginger, turmeric, coriander, garlic, vanilla, saffron, curry leaf, and peppermint.

CO 5c Demonstrate knowledge of methods of production, chemistry of constituents, and uses of spice oils and oleoresins, specifically pepper, ginger, and turmeric.

### CH 03 03 02 ADVANCED SYNTHETIC ORGANIC CHEMISTRY Credit:4 Contact Hours : 72 Hrs

### **Unit 1: Asymmetric Synthesis**

- CO 1a To classify stereoselectivity and define relevant terminology and principles.
- CO 1b To demonstrate the application of stereoselectivity, asymmetric induction, and asymmetric synthesis principles in practical organic synthesis.
- CO 1c To discuss double diastereoselection and double asymmetric induction concepts.
- CO 1d To provide examples illustrating the use of chiral auxiliaries and the chiral pool in asymmetric synthesis.
- CO 1e To introduce the use of chiral auxiliaries and the chiral pool in asymmetric synthesis.
- CO 1f To examine the principles of asymmetric aldol condensation.
- CO 1g To understand the principles and applications of asymmetric diels-alder reactions.
- CO 1h To apply these methods in the synthesis of complex organic molecules.

#### **Unit 2 : Retrosynthetic Analysis and Construction of rings**

- CO 2a To Define the basic principles and terminology of retrosynthesis.
- CO 2b To Explain the key concepts involved in retrosynthetic analysis.
- CO 2c To Explore Important Strategies of Retrosynthesis:
- CO 2d To Describe one-group and two-group C-X disconnection strategies for the synthesis of aromatic compounds.
- CO 2e To Discuss the one-group C-C disconnection approach for alcohols and carbonyl compounds.
- CO 2f To Illustrate the synthesis of amines and alkenes using this retrosynthetic approach.
- CO 2g To Explain the two-group C-C disconnection strategies.
- CO 2h To Illustrate the application of these strategies with examples.
- CO 2i To Different Approaches Towards the Synthesis of Three, Four, Five, and Six-Membered Rings:
- CO 2j To Explore the strategic considerations in planning the retrosynthesis of ring systems.
- CO 2k To discuss the Photochemical Approaches for the Synthesis of Four-Membered Rings
- CO 21 To Discuss the ketene cycloaddition reactions in retrosynthetic planning.
- CO 2m To Discuss the Demjenov reaction and its application in the inter-conversion of ring systems, including contraction and expansion.
- CO 2n To discuss the mechanism and applications of Cyclisation Reactions
- CO 20 To apply the retrosynthetic strategies for the synthesis of 5-membered ring heterocyclic compounds.
- CO 2p To Apply retrosynthetic analysis to the synthesis of complex molecules, including (+) Heliotridine, Juvabione, and Luciferin.

## Unit 3: Organic Synthesis via Oxidation and Reduction (18 Hrs)

- 3a To develop a comprehensive understanding of oxidation reactions in organic chemistry, with a specific focus on metal-based and non-metal-based oxidations.
- 3b To explore various oxidation methods for converting alcohols to carbonyls, including reactions with Chromium, Manganese, Aluminium, and DMSO-based reagents.
- 3c To investigate reactions transforming alkenes into epoxides, including peroxides/per acids-based methods, Sharpless asymmetric epoxidation, Jacobsen epoxidation, and Shi epoxidation.
- 3d To analyze the oxidative processes converting alkenes to diols, utilizing Manganese and Osmium-based reagents, and explore specific reactions like Prevost and Woodward modification.
- 3e To Study methods for converting alkenes to carbonyls with bond cleavage, focusing on Manganese and Lead-based ozonolysis.
- 3f To Examine reduction reactions that convert alkenes to alcohols or carbonyls without bond cleavage, including hydroboration-oxidation, Wacker oxidation, and Selenium/Chromium-based allylic oxidation.
- 3g To Understand the Baeyer-Villiger oxidation method for transforming Explore heterogeneous and homogeneous catalytic hydrogenation, involving metals such as Pd, Pt, Rh, Ni, and Wilkinson's catalyst.
- 3h To Investigate metal-based reductions using Li, Na, Ca in liquid ammonia, Sodium, Magnesium, and Zinc, covering reactions like Birch reduction, Pinacol formation, McMurry reaction, Acyloin formation, dehalogenation, and deoxygenations.
- 3i To Examine hydride transfer reactions using Group III and Group IV hydride reagents, including NaBH4, triacetoxyborohydride, LiAlH4, DIBAL-H, Meerwein-Pondorff-Verley reduction.
- 3j To understand stereo- and enantioselective reductions, focusing on chiral boranes and the Corey-Bakshi-Shibata method.

## Unit 4: Modern Synthetic Methods and Reagents (9 Hrs)

4a To Understand the Baylis-Hillman reaction mechanism, its applications, and synthetic utility in the formation of allylic alcohols.

4b To Explore the Henry reaction, its mechanism, and its significance in the synthesis of nitroalkanes, with emphasis on the catalytic and asymmetric variants. 4c To Analyze the Nef reaction and its synthetic applications in the conversion of  $\alpha$ -halo ketones to  $\alpha$ -keto acids.

4d To Investigate the Sakurai reaction and its role in the synthesis of organosilanes, particularly in the context of metal-catalyzed coupling reactions.

4e To Understand the Tischenko reaction and its significance in the synthesis of carboxylic esters from aldehydes.

4fTo Explore a variety of metal-mediated coupling reactions, including Heck, Stille, Suzuki, Negishi, Sonogashira, Nozaki-Hiyama, Buchwald-Hartwig,

Ullmann, and Glaser coupling reactions. Understand the mechanism and applications of each.

4g To Familiarize with the usage and applications of specific reagents such as N-bromosuccinimide (NBS), 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ), dicyclohexylcarbodiimide (DCC), and Gilman reagent in organic synthesis.

4h To Define and understand the concept of multicomponent reactions, focusing on their efficiency in generating complex molecules in a single reaction vessel.

4iTo Explore three-component reactions, including the Mannich reaction, Passerini reaction, and Biginelli reaction. Understand the key steps and applications of each.

4jTo Analyze four-component reactions, particularly the Ugi reaction. Understand the reaction mechanism and its versatility in synthesizing diverse chemical compounds.

4k To Introduce the concept of click reactions, providing an elementary understanding of their principles and applications in synthetic chemistry

# Unit 5: Molecular Recognition and Supramolecular Chemistry (9 Hrs)

5a To grasp the concept of molecular recognition, including the principles and significance of host-guest complex formation in supramolecular chemistry.

5b To explore the various forces involved in molecular recognition, such as hydrogen bonding, van der Waals forces, and electrostatic interactions, and understand their roles in stabilizing host-guest complexes.

5c To understand the structures and functions of molecular receptors, including cyclodextrins, crown ethers, cryptands, spherands, and tweezers. Analyze their applications and selectivity.

5d To explore the properties and applications of other molecular receptors like carcerands, cyclophanes, calixarenes, and carbon nanocapsules. Understand their roles in molecular recognition and supramolecular chemistry.

5e To examine the importance of molecular recognition in biological systems, particularly in DNA and protein interactions. Understand how supramolecular chemistry principles contribute to the functioning of biological molecules.

5fTo investigate the role of molecular recognition in controlled release phenomena, including drug delivery systems and other applications in medicine.

5g To analyze the applications of supramolecular complexes in medicine, focusing on drug design, targeted drug delivery, and diagnostics.

5h To explore how supramolecular complexes are utilized in the perfumery industry, including the design of fragrance molecules and controlled release of scents.

## **Unit 6: Chemistry of Natural Products and Biomolecules**

CO 6a To Illustrate the key reactions and methods involved in the synthesis of these natural products.

CO 6b To Explain the methods used for determining the primary structure of peptides, proteins, and nucleic acids.

CO 6c To Discuss the principles and techniques involved in the characterization of these biomolecules.

CO 6d To Describe the process of DNA replication, emphasizing the key enzymes and steps involved.

CO 6e To Understand the significance of DNA replication in cellular processes.

CO 6f To Explain the processes of transcription and translation in protein biosynthesis.

CO 6g To Illustrate the role of RNA in transferring genetic information and the formation of polypeptide chains.

CO 6h To Understand the importance of DNA sequencing in deciphering genetic information.

CO 6i To Describe the principles and applications of the Polymerase Chain Reaction (PCR).

CO 6j To Understand the goals and significance of the Human Genome Project. CO 6k To Demonstrate an understanding of the interplay between synthetic chemistry and biomolecular research in the synthesis of natural products.

CO 61 To Critically analyze and evaluate the synthetic strategies employed in the synthesis of specific natural products.

CO 6m To Discuss the challenges and advancements in synthetic approaches to complex biomolecules.

CO 6n To Understand how molecular biology techniques, such as DNA sequencing and PCR, contribute to the understanding and manipulation of biomolecules.

#### CH 03 03 03 PHYSICAL CHEMISTRY Credit: 4 Total Hours: 72

#### **Unit 1: Chemical Kinetics and Catalysis**

- CO 1a To Apply ARRT to simple bimolecular processes.
- CO 1b Study mechanisms of photochemical reactions.
- CO 1c Explore oscillatory reactions.
- CO 1d Examine chain reactions, particularly the kinetics of the H2 Br2 reaction and the decomposition of acetaldehyde and N2O5.
- CO 1e Investigate H2 O2 explosive reactions.
- CO 1f Understand the theory of unimolecular reactions using Lindemann-Hinshelwood, RRKM, and Slater treatments.
- CO 1g Apply steady state approximation, principle of microscopic reversibility, and detailed balancing.
- CO 1h Study kinetic isotope effect and primary/secondary kinetic salt effect.
- CO 1i Analyze the influence of solvents on reaction rates.
- CO 1j Understand the significance of volume and entropy of activation.
- CO 1k Investigate fast reactions using the stopped flow method.
- CO 11 Explore specific and general acid-base catalysis, including Bronsted catalysis law, acidity functions, and enzyme catalysis (Michaelis-Menton kinetics).

## **Unit 2: Surface Chemistry**

- CO 2a Understand different types of surfaces.
- CO 2b Explore the thermodynamics of surfaces.
- CO 2c Study adsorption isotherms, including Freundlich and Langmuir isotherms.
- CO 2d Derive BET theory and understand surface area determination.
- CO 2e Investigate Temkin adsorption isotherm and adsorption on liquid surfaces.
- CO 2f Explore colloids, including Zeta potential and electrokinetic phenomena.
- CO 2g Understand sedimentation potential and streaming potential.
- CO 2h Analyze Donnan membrane equilibrium.
- CO 2i Study Surface Enhanced Raman Scattering (SERS) and experimental methods of studying surfaces (Augar, LEED, and ESCA).

## **Unit 3: Electrochemistry**

- CO-1: Demonstrate a comprehensive understanding of the fundamental principles of electrochemistry, including electrochemical cells, electrode kinetics, and thermodynamics of electrochemical processes.
- CO-2: Analyze redox reactions at electrodes, including the identification of halfreactions, determination of cell potential, and understanding the role of standard electrode potentials.
- CO-3: Apply the Nernst equation to calculate cell potentials under non-standard conditions and understand its implications in real-world applications.
- CO-4: Study electrode kinetics, including the determination of rate constants, mechanisms of electrode reactions, and the influence of mass transport.
- CO-5: Investigate various electroanalytical techniques, including cyclic voltammetry, chronoamperometry, and impedance spectroscopy, and understand their applications in chemical analysis.
- CO-6: Explore the principles underlying batteries and fuel cells, including electrochemical energy storage and conversion mechanisms, and evaluate the efficiency and limitations of these devices.
- CO-7: Study corrosion processes and methods for corrosion protection, including the use of sacrificial anodes, coatings, and inhibitors.
- CO-8: Understand the principles of bioelectrochemistry, including electron transfer in biological systems, electrochemical sensors, and applications in biotechnology.

## **Unit 4: Photochemistry**

- CO-1: Demonstrate a comprehensive understanding of the fundamental principles of photochemistry, including electronic transitions, Jablonski diagrams, and the concept of singlet and triplet states.
- CO-2: Analyze and interpret photochemical reactions, including the identification of photochemical pathways, photophysical processes, and the role of excited states.
- CO-3: Apply quantum mechanical concepts to describe electronic transitions, explain the selection rules for absorption and emission, and calculate transition probabilities.
- CO-4: Study photophysics, including fluorescence and phosphorescence phenomena, and understand the factors influencing the emission of light from excited states.
- CO-5: Explore various photochemical mechanisms, such as Norrish Type I and Type II reactions, and understand the factors affecting the efficiency and selectivity of photochemical processes.

- CO-6: Investigate the principles of photoredox catalysis, including the use of photoexcited species as catalysts in chemical transformations, and evaluate their synthetic applications.
- CO-7: Study photochromic materials, including photochromic dyes and molecular switches, and assess their applications in responsive materials and devices.
- CO-8: Apply laser spectroscopy techniques, such as laser-induced fluorescence and time-resolved spectroscopy, for the investigation of ultrafast processes and transient species in photochemical reactions.
- CO-9: Explore the role of photochemistry in photobiology, including the study of photosynthesis, photodamage to biological molecules, and applications in medicine.

## CH 50 03 04 SPECTROSCOPIC METHODS IN CHEMISTRY Credit :4 Contact Lecture Hours: 54

## Unit 1: Ultraviolet-Visible and Chiro-optical Spectroscopy

- CO 1a Understand the principles of energy levels and selection rules in UV-Visible spectroscopy.
- CO 1b Apply Woodward-Fieser and Fieser-Kuhn rules.
- CO 1c Analyze the influence of substituents, ring size, and strain on spectral characteristics.
- CO 1d Explore solvent effects, stereochemical effects, and non-conjugated interactions.
- CO 1e Understand chiro-optical properties including ORD, CD, octant rule, axial haloketone rule, and Cotton effect.
- CO 1f Apply chiro-optical properties in practical applications.
- CO 1g Solve problems based on energy levels, selection rules, and chiro-optical properties.

## **Unit 2: Infrared Spectroscopy**

- CO 2a Understand fundamental vibrations and characteristic regions in the infrared spectrum.
- CO 2b Analyze the influence of substituents, ring size, hydrogen bonding, vibrational coupling, and field effect on frequency.
- CO 2c Interpret IR spectra of C=C bonds (olefins and arenes) and C=O bonds.
- CO 2d Solve problems related to spectral interpretation with examples.

## **Unit 3: Nuclear Magnetic Resonance Spectroscopy**

- CO 3a: To understand the principles of nuclear magnetic resonance and its application to nuclei, with a special focus on 1H and 13C.
- CO 3b: To understand relaxation processes in NMR spectroscopy.
- CO 3c: To define and understand spin-spin splitting phenomena.
- CO 3d: To understand the Karplus curve and its implications for coupling constants.
- CO 3e: To understand the principles and applications of 2D NMR techniques.

CO 3f: To apply the learned concepts to solve problems related to spectral interpretation in NMR spectroscopy.

### **Unit 4: Mass Spectrometry**

- CO 4a Understand molecular ion production methods, including EI, and soft ionization methods (SIMS, FAB, CA, MALDI-TOF, PD, field desorption electrospray ionization).
- CO 4b Analyze fragmentation patterns for various compound classes.
- CO 4c Explore McLafferty rearrangement, HRMS, MS-MS, LC-MS, GC-MS.
- CO 4d Solve problems on spectral interpretation with examples.

## **Unit 5: Structural Elucidation Using Spectroscopic Techniques**

- CO 5a Identify structures of unknown organic compounds based on UV-Vis, IR, 1H NMR, and 13C NMR spectroscopy.
- CO 5b Interpret given UV-Vis, IR, and NMR spectra.
- CO 5c Analyze the spectral data for reactions/functional transformations including Pinacol-Pinacolone rearrangement, Benzoin condensation, (4+2) cycloaddition, Beckmann rearrangement, Cis-trans isomerisation of azo compounds, Benzil-benzilic acid rearrangement, and Fries rearrangement.

### SEMESTER 4 ELECTIVE COURSES CH 84 04 01 INDUSTRIAL OILS AND FAT PRODUCTS UNIT – 1 EXTRACTION AND PROCESSING OF OILS AND FATS

- CO 1: To understand different heat treatment methods applied to oil-bearing materials and their effects on extraction efficiency.
- CO 2: To apply the principles and methods of mechanically expressing oils from oilbearing materials.
- CO 3: To understand the practical aspects of solvent extraction techniques.
- CO 4: To gain a comprehensive understanding of the mechanical and chemical processes involved
- in oil extraction from various sources.
- CO 5: To understand various purification processes in oils.
- CO 6: To study of the sources, composition, characteristics of different oils.

## Unit 2: Oils and Fats as Food Materials (9 Hrs)

- 2a To explain the different types of cooking oils, salad oils, and salad dressings, highlighting their characteristics and uses in culinary applic
- 2b To demonstrate the ability to evaluate the quality of cooking oils and salad oils, considering factors such as smoke point, flavor stability, and nutritional content.
- 2c To analyze the composition and properties of margarine and shortenings, and discuss their roles in cooking and baking.
- 2d To define  $\omega$ -3 and  $\omega$ -6 fatty acids, identify their dietary sources, and explain their significance in human nutrition and overall health.

- 2e To assess the importance of EFAs in maintaining cellular health, brain function, and hormone regulation, emphasizing their essential role in a balanced diet
- 2f To investigate the relationship between dietary fats and the development of atherosclerosis and arthritis, exploring the mechanisms and impact on overall health.
- 2g To explain the role of HDL, LDL, and VLDL in the context of fat-related diseases, and evaluate their implications on cardiovascular health.
- 2h To discuss strategies for preventing fat-related diseases through dietary choices, and explore nutritional interventions for managing conditions associated with these diseases.

## **Unit 3.Hydrogenation of Oils**

CO3.1 To defin eand Overview of Catalytic Hydrogenation

CO3.2 To apply in Industry and Chemistry

- CO3.3To understand chemical Reactions Involved in Hydrogenation
- CO3.4To analyse different types of Substrates Subjected to Hydrogenation

CO3.5 To understand mechanisms of Hydrogenation Reactions

- CO 3.6 To understand factors Influencing Reaction Rates
- CO 3.7.To analyse thermodynamics of Hydrogenation

Co 3.8.To understand hydrogenolysis

CO3.9.To analyse catalyst Synthesis Methods

CO 3.10.To understand catalyst Characterization Techniques

CO 3.11.To understand hydrogenation of Vegetable and Marine Oils

CO 3.12.To understand manufacture of Vanaspati

## **Unit 4:Fat Splitting and Esterification**

CO 1-Describe the Twitchell process for fat splitting.

- CO 2-Explain the principles and mechanisms involved in the Twitchell process.
- CO 3-Analyze the low-pressure fat splitting process with catalysts.
- CO 4-Discuss the role of catalysts in enhancing the efficiency of low-pressure splitting.
- CO 5-Examine the medium-pressure autoclave splitting process with catalyst.
- CO 6-Discuss the advantages and limitations of medium-pressure autoclave splitting.
- CO 7-Evaluate the continuous uncatalyzed high-pressure counter-current splitting method.
- CO 8-Compare and contrast this method with other fat splitting processes.
- CO 9-Explain the enzymatic fat splitting process.
- CO 10-Discuss the specificity and selectivity of enzymes in fat splitting.
- CO 11-Outline the methods for recovering glycerine from the fat splitting process.
- CO 12-Analyze the recovery process for spent lye.
- CO 13-Classify and describe different grades of glycerine.
- CO 14-Discuss the factors influencing the quality of glycerine.
- CO 15-Illustrate the chemical structure and synthesis pathways of glycerine.
- CO 16-Explain the chemical reactions involved in glycerine synthesis.
- CO 17-Enumerate and discuss the various industrial and commercial uses of glycerine.
- CO 18-Analyze the versatility of glycerine in different applications.

CO 19-Identify and describe substitutes for glycerine.

CO 20-Discuss the properties and applications of glycerine substitutes.

CO 21-Explain the mechanisms involved in esterification and ester hydrolysis.

CO 22-Illustrate the key steps in these chemical processes.

CO 23-Discuss the esterification of fatty acids with glycerol.

CO 24-Explore alternative esterification reactions with different alcohols.

CO 25-Define and explain inter esterification.

CO 26-Discuss the significance and applications of inter esterification reactions.

CO 27-Differentiate between acidolysis, alcoholysis, glycolysis, and glycerolysis.

CO 28-Discuss the specific conditions and outcomes of each type of reaction.

CO 29-Explain the mechanism of transesterification.

CO 30-Discuss the applications and significance of transesterification reactions.

CO 31-Explore the various applications of esterification in different industries.

CO 32-Discuss the industrial relevance of inter esterification process

## Unit 5. Rancidity in oils, Fats and oil bearing substances

CO5.1 To Introduce autooxidation

CO 5.2.to understand theories of Autooxidation

CO 5.3 To understand tests for Rancidity

CO5.4.To understand Factors Affecting Stability

CO 5.5 To define Induction Period

CO 5.6.To understand prooxidants and antioxidants

CO 5.7.To differentiate Types of Oils - Drying, Semi-Drying, and Non-Drying

# **UNIT - 6 ANALYSIS AND FATS AND OILS**

CO 1: To understand various testing methods for oils and fats to analyse the physical properties.

CO 2: To understand various testing methods for oils and fats to analyse the chemical properties

CO 3: To understand the adulterations in oils and fats.

## Unit 7: Waxes and Fatty alcohols (9 Hrs)

CO7a	To define waxes and explore their occurrence in nature, emphasizing their diversity in plant and animal sources.
CO7b	To classify waxes based on their origin and chemical structure, and analyze their physical and chemical properties.
CO7c	To investigate the molecular composition of waxes, focusing on the roles of esters, hydrocarbons, and other components in determining wax properties.
CO7d	To examine the methods employed in the synthesis of artificial or synthetic waxes, including chemical processes and industrial applications.
CO7e	To compare the properties of synthetic waxes with natural waxes, evaluating their advantages, disadvantages, and potential applications.
CO7f	To introduce analytical techniques used for the characterization and quality assessment of synthetic waxes.
CO7g	To explore analytical methods for the qualitative and quantitative analysis of waxes, including chromatography and spectroscopy.

CO7h	To investigate the industrial applications of waxes, such as in cosmetics, pharmaceuticals, food, and manufacturing, and assess their functional roles.
CO7i	To discuss sustainable practices in the extraction, processing, and use of waxes, considering environmental and ethical considerations.
CO7j	To examine methods for the production of naturally occurring fatty alcohols, including extraction and synthesis processes.
CO7k	To analyze the industrial applications of naturally occurring fatty alcohols, with a focus on their roles in personal care products, detergents, and pharmaceuticals.
CO71	To explore the synthesis methods and properties of alcohol ethers, considering their chemical structure and applications.
CO7m	To investigate the diverse industrial applications of alcohol ethers, such as solvents, fuel additives, and as intermediates in the synthesis of other chemicals.

### CH 84 04 02 BIOCHEMISTRY OF FATTY ACIDS Credit : 4 Contact Lecture Hours: 90

## **Unit 1.Lipids**

- CO1.1 To understand the classification of lipids
- CO 1.2. To understand sources and classification of oils and fats
- CO 1.3.To evaluate nutritional functions of fats and oils
- CO1.4.To investigate Caloric and non caloric functions

## Unit 2: Glyceride structure (9 Hrs)

- CO 2a To define and describe the glyceride composition of natural fats, exploring the molecular structure of triglycerides, diglycerides, and monoglycerides.
- CO 2b To examine the diversity of glycerides found in various natural fats, including the role of fatty acids in determining the properties of different lipid species
- CO 2c To analyze the functional roles of glycerides in biological systems, such as energy storage, insulation, and cellular structure.
- CO 2d To introduce and explain analytical methods used in investigating glycerides, including chromatography, spectroscopy, and mass spectrometry.
- CO 2e To demonstrate proficiency in sample preparation techniques required for the analysis of glyceride composition in natural fats.
- CO 2f To develop skills in interpreting data obtained from analytical techniques to characterize and quantify glycerides in different lipid samples
- CO 2g To explore the historical development of theories regarding the structure of glycerides, from early models to contemporary understanding.
- CO 2h To explain and critically evaluate modern theories of glyceride structure, considering evidence from experimental studies and molecular simulations.
- CO 2i To discuss how the proposed structures of glycerides influence their functionality in biological systems and industrial applications.

### Unit 3: Nonglyceride constituents of fats and oils

- CO 1 Understand the chemical structure and properties of carotenes.
- CO 2 Analyze the role of carotenes as precursors of vitamin A.
- CO 3 Understand the essential functions of various vitamins in the human body.
- CO 4 Understand the chemical structure and properties of tocopherols.:
- CO 5 Explore the role of tocopherols as antioxidants.
- CO 6 Analyze the protective function of tocopherols in biological systems.
- CO 7 Define steroids and discuss their structural characteristics.
- CO 8 Explore the natural occurrence of steroids.
- CO 9 Understand the diverse biological functions of steroids.
- CO 10 Analyze the roles of steroids in hormone regulation and cellular processes.
- CO 11 Define phospholipids and discuss their structural features.
- CO 12 Explore the occurrence of phospholipids in biological membranes.
- CO 13 Understand the functions of phospholipids in cellular structure and signaling.
- CO 14 Analyze the role of phospholipids in lipid metabolism.
- CO 15 Define sphingolipids and discuss their structural diversity.
- CO 16 Explore the occurrence of sphingolipids in biological membranes.
- CO 17 Understand the diverse functions of sphingolipids in cell signaling.
- CO 18 Analyze the roles of sphingolipids in cellular processes.
- CO 19 Define antioxidants and discuss their importance in biological systems.
- CO 20 Explore the mechanisms by which antioxidants protect cells from oxidative stress.
- CO 21 Explore the chemical constituents responsible for flavor and odor in foods.
- CO 22 Understand the sensory impact of different compounds contributing to flavor and odor.

### **Unit 4: Isolation and Characterization of Fatty Acids**

- CO 1 Learn various methods of crystallization and their applications in isolating pure compounds.
- CO 2 Demonstrate the ability to obtain high-purity crystals using selected techniques.
- CO 3 Apply the nomenclature rules to identify and name fatty acids.
- CO 4 Explore the diverse uses of fatty acids in textiles, leather, pharmaceuticals, and petroleum processing.
- CO 5 Analyze the role of fatty acids in different industrial processes.
- CO 6 Characterization of fatty acids using various spectroscopic techniques

## **Unit 5: Fatty Acids Occurring in Nature**

- CO 5a Identify important sources of saturated fatty acids in nature.
- CO 5b Explain the synthesis pathways of these saturated fatty acids.
- CO 5c Analyze the occurrence of monoethenoid fatty acids in nature.
- CO 5d Explore the diversity of polyunsaturated fatty acids in nature.
- CO 5e Examine artificially produced fatty acids and their relevance.
- CO 5f Understand the synthetic pathways leading to the formation of various types of fatty acids.
- CO 5g Relate the structural features of fatty acids to their functions in biological systems.
- CO 5h Analyze the chemical properties and reactivity of different types of fatty acids.
- CO 5i Relate the reactivity of fatty acids to their roles in metabolic pathways.
- CO 5j Explore the functional significance of various fatty acids in living organisms.

- CO 5k Examine the health implications of consuming different types of fatty acids.
- CO 51 Evaluate the impact of fatty acid composition on human health.
- CO 5m Introduce analytical techniques used for the qualitative and quantitative analysis of fatty acids.
- CO 5n Demonstrate proficiency in interpreting analytical data related to fatty acid composition.

### **Unit 6: Physical properties of Fatty Acids**

- CO 1 Explore the crystal structures of fatty acids in the liquid state.
- CO 2 Analyze the factors influencing the crystalline properties of fatty acids.
- CO 3 Learn techniques for crystallographic analysis of fatty acids.
- CO 4 Explore the thermal behavior of fatty acids, including melting points and solidification.
- CO 5 Understand the factors influencing the thermal properties of fatty acids in the liquid state.
- CO 6 Analyze the heat capacity and thermal conductivity of fatty acids.
- CO 7 Explore the IR spectra of fatty acids in the liquid state.
- CO 8 Analyze NMR spectra to deduce structural information about fatty acids.
- CO 9 Investigate the UV-Vis spectra of fatty acids.
- CO 10 Explore the solubility of fatty acids in various solvents in the liquid state.
- CO 11 Understand the solution properties of fatty acids, including viscosity and conductivity.
- CO 12 Explore the influence of temperature and concentration on solution behavior.

## **Unit 7: Chemical properties of Fatty Acids**

- CO 1 Define salt formation and understand the principles involved.
- CO 2 Explore various methods and conditions for the formation of salts.
- CO 3 Analyze the practical applications of salt formation in different chemical processes.
- CO 4 Understand the mechanism of esterification reactions.
- CO 5 Analyze the factors influencing the rate and equilibrium of esterification.
- CO 6 Explore the diverse applications of esterification in organic synthesis.
- CO 7 Apply esterification reactions in the preparation of specific compounds.
- CO 8 Define halogenation and discuss the conditions under which it occurs.
- CO 9 Explore the different halogenation reactions.
- CO 10 Analyze the applications of halogenation in the synthesis of organic compounds.
- CO 11 Understand the selectivity and regiochemistry in halogenation reactions.Define oxidation reactions and understand their importance.
- CO 12 Explore the role of oxidizing agents in various chemical transformations. Analyze the uses of oxidizing agents such as chromic acid, ozone, peroxides, potassium
- CO 13 permanganate, periodic acid, and lead tetraacetate. Apply the appropriate oxidizing agent in specific oxidation reactions.
- CO 14 Understand the mechanism of hydrogenation reactions.
- CO 15 Analyze the conditions and factors influencing the rate of hydrogenation.
- CO 16 Explore the applications of hydrogenation in the food industry, pharmaceuticals, and organic

- CO 17 synthesis.Apply hydrogenation reactions to selectively modify functional groups.:
- CO 18 Understand the mechanism of dehydration reactions.
- CO 19 Analyze the factors affecting the rate and selectivity of dehydration.
- CO 20 Explore the applications of dehydration reactions in the synthesis of alkenes, ethers, and other
- CO 21 compounds.
- CO 22 Apply dehydration reactions in organic transformations.
- CO 23 Define pyrolysis and understand the conditions under which it occurs.
- CO 24 Analyze the products and applications of pyrolysis reactions.
- CO 25 Understand the principles of polymerization reactions.
- CO 26 Explore different types of polymerization and their applications.
- CO 27 Discuss the mechanisms of addition reactions to double bonds.

CO 28 Analyze the regiochemistry and stereochemistry in addition reactions

### **Unit 8: Biochemistry and Metabolism of Fats**

CO 8a	To explain the biochemical processes involved in the
	transformation of fats in the human body, covering lipolysis, beta-
	oxidation, and fatty acid synthesis.
CO 8b	To explore the regulatory mechanisms that control fat
	metabolism, including hormonal influences and enzymatic reactions.
CO 8c	To analyze the role of fat metabolism in maintaining energy
	homeostasis and the utilization of fatty acids as a fuel source during
	various physiological conditions.
CO 8d	To describe the biosynthesis of fats in plants, emphasizing the
	role of photosynthesis and pathways leading to the formation of plant
	lipids.
CO 8e	To Compare and contrast lipid biosynthesis in animals with a
	focus on the liver and adipose tissue, highlighting key enzymatic
	reactions and regulatory steps.
CO 8f	To investigate how dietary factors influence the biosynthesis of
	fats in both plants and animals.
CO 8g	To define prostaglandins and their role as bioactive lipid
	compounds, emphasizing their diverse functions in various physiological
	processes.
CO 8h	To explain the biosynthetic pathways leading to the formation of
	prostaglandins, with a focus on the enzymatic reactions involved.
CO 8i	To analyze the signaling functions of prostaglandins in the
	body, including their roles in inflammation, pain modulation, and
	regulation of blood pressure.
CO 8j	To explore the pharmaceutical applications of prostaglandins,
	including their use as drugs in the management of conditions such as
	inflammation, cardiovascular diseases, and reproductive health.
CO 8k	To discuss the clinical relevance of understanding the
	biochemical transformation of fats and the role of prostaglandins in the
	development of therapeutic interventions.

To consider the ethical implications of utilizing prostaglandins as drugs, discussing issues related to safety, side effects, and potential societal impacts.

### CH 84 04 03 ADVANCED APPLIED CHEMISTRY **Credit 4 Contact Lecture Hours: 90**

#### **Unit 1: Soaps and Detergents**

- CO 1aUnderstand the molecular principles underlying the interaction between surfaces and cleaning agents.
- CO 1bIdentify the raw materials used in soap manufacturing.
- CO 1c Explain the characteristics and steps involved in the cold process of soap manufacturing.
- CO 1dAnalyze the advantages and limitations of the cold process.
- CO 1eDescribe the characteristics and steps involved in the semi-boiled process.
- CO 1f Compare and contrast the semi-boiled process with other soap manufacturing methods.
- CO 1gExplain the characteristics and steps involved in the boiled process of soap manufacturing.
- CO 1hDefine additives used in soap manufacturing.
- CO 1i Explore different types of additives used in soap formulations.
- CO 1j Understand the detergent action of soap on surfaces.
- CO 1kExplore the influence of fatty acid composition of oils on the properties of soap.
- CO 11 Describe the specific requirements and characteristics of laundry soaps.
- CO 1mDefine the unique features and requirements of toilet soaps.
- CO 1nExplore the manufacturing processes and characteristics of various specialized soaps.
- CO 10Understand the determination and control of T.F.M values in soap formulations.
- CO 1pUnderstand the specific requirements for effective hair cleaning and conditioning.
- CO 1qDefine and classify anionic, cationic, amphoteric, and nonionic detergents based on their chemical
- CO 1r structures and properties.
- CO 1s Analyze the diverse industrial and household applications of each type of detergent.
- CO 1t Define agglomeration in the context of detergent technology.
- CO 1uAnalyze the advantages of synthetic detergents (syndets) over traditional soaps.
- CO 1vDiscuss the limitations and challenges associated with the use of syndets.
- CO 1w Discuss the environmental impact of detergents and the importance of biodegradability.
- CO 1xExplore regulations and standards related to the biodegradability of detergents.
- CO 1yExplain the role of surfactants in the synthesis of nanoparticles.
- CO 1z Explore applications of surfactant-assisted nanoparticle synthesis in various industries.
- CO 1aa Define enzyme detergents and their role in stain removal and fabric care.
- CO 1bb Explain the mechanism by which enzymes enhance the cleaning efficacy of detergents.

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- CO 1cc Define green detergents and their principles of sustainability.
- CO 1dd Analyze the use of eco-friendly ingredients in the formulation of green detergents.
- CO 1ee Define compact detergents and their role in reducing packaging waste.
- CO 1ff Analyze the benefits of compact detergents for consumers, including convenience and reduced
- CO 1gg environmental footprint.

### **Unit 2: Paints and Varnishes**

- CO 2a To Recognize the importance of paints as protective coatings for various surfaces.
- CO 2b To Identify the materials used in paint manufacture, including unmodified oils, modified drying oils, resins, and copolymers.
- CO 2c To Evaluate the properties and suitability of different materials for specific paint formulations.
- CO 2d To Differentiate between unmodified oils and their pretreatment and modified drying oils used in paint formulations.
- CO 2e To Identify various types of resins used in paints, including natural resins, phenolic resins, alkyd resins, urethane resins, and epoxy resins.
- CO 2f To Understand the role of copolymers and additives in enhancing the performance of paints.
- CO 2g To Explore the impact of each additive on the properties of the final paint product.
- CO 2h To Explain the mechanism of polymerization and drying of oils in the context of paint formulations.
- CO 2i To Describe the composition and uses of varnishes and lacquers.
- CO 2j To Explore the composition and characteristics of oleoresinous varnishes.
- CO 2k To Apply the knowledge of paints and varnishes to practical scenarios, considering specific applications and requirements.

### **Unit 3: Flavour and Perfume Chemistry**

- CO 3a To Recognize the key characteristics that differentiate flavor and perfume chemistry.
- CO 3b To Differentiate between descriptive and discriminant sensory analysis in evaluating flavors.
- CO 3c To analyze the flavor profiles of coffee, tea, cocoa, onion, and garlic.
- CO 3d To Identify synthetic ingredients commonly used in food flavorings.
- CO 3e To classify odors and discuss the general physiology of olfaction.
- CO 3f To describe the raw materials used in perfume raw materials.
- CO 3g To understand the source and chemical nature of commercially important gums, balsams, and resins.
- CO 3h To identify the source and chemical nature of gums, balsams and resins
- CO 3i To Understand the principles and practices in aerosol spray perfumes.
- CO 3j To Apply knowledge of perfume raw materials and technology in the blending and formulation of perfumes.

## **Unit 4: Drug Chemistry and Phytochemicals**

CO-1: Demonstrate a comprehensive understanding of drug design principles, including the relationship between molecular structure and biological activity.

- CO-2: Analyze various drug targets, including receptors, enzymes, and ion channels, and understand the mechanisms of drug action at the molecular level.
- CO-3: Study pharmacokinetics and pharmacodynamics, including drug absorption, distribution, metabolism, and excretion, as well as the time course of drug effects.
- CO-4: Evaluate medicinal chemistry strategies for the design and optimization of drug candidates, considering factors such as bioavailability, selectivity, and toxicity.
- CO-5: Explore the principles underlying the design and mechanism of action of antibiotics and antiviral drugs, including the study of resistance mechanisms.
- CO-6: Analyze the role of natural products in drug discovery, including the isolation, structural elucidation, and bioactivity assessment of phytochemicals.
- CO-7: Study the application of bioinformatics tools in drug discovery, including molecular docking, virtual screening, and structure-activity relationship (SAR) analysis.
- CO-8: Investigate synthetic methods used in medicinal chemistry for the preparation of drug candidates, including asymmetric synthesis and combinatorial chemistry.

#### **Unit 5: Dairy Chemistry**

- CO 5a Identify the major constituents of milk, including lipids, proteins, carbohydrates, vitamins, and minerals.
- CO 5b Analyze the factors influencing the composition of milk.
- CO 5c Demonstrate techniques for the estimation of fat, acidity, and total solids in milk.
- CO 5d Explain the methods for the destruction of microorganisms in milk.
- CO 5e Explore the physico-chemical changes occurring in milk during processing, including boiling and pasteurization.
- CO 5f Explain the chemistry of the creaming process.
- CO 5g Demonstrate the estimation of fat in cream.
- CO 5h Discuss the theory of churning in butter production.
- CO 5i Demonstrate the estimation of acidity and moisture content in butter.
- CO 5j Identify the major constituents of ghee.
- CO 5k Discuss common adulterants added to ghee and methods for their detection.
- CO 51 Apply quality control measures to ensure the purity and safety of milk and dairy products.
- CO 5mDevelop skills in using analytical techniques for the evaluation of dairy products.
- CO 5n Apply the knowledge of dairy chemistry in the development and improvement of dairy products.
- CO 50 Discuss the economic and nutritional significance of various dairy products.
- CO 5p Analyze the impact of processing on the sensory and nutritional qualities of dairy products.

### **Unit 6: Green Chemistry**

- CO-1: Demonstrate a thorough understanding of the principles of green chemistry, including the 12 principles of green chemistry proposed by Anastas and Warner.
- CO-2: Analyze and apply sustainable synthetic methods, including the use of alternative reaction conditions, catalysis, and renewable feedstocks.
- CO-3: Evaluate and design solvent-free reactions and low-impact solvent systems, considering the environmental and health implications.
- CO-4: Explore the use of green solvents in organic synthesis, such as water, supercritical fluids, and ionic liquids, for environmentally friendly reactions.
- CO-5: Assess and implement energy-efficient processes, including microwave and ultrasound-assisted reactions, to minimize energy consumption in chemical transformations.
- CO-6: Study green analytical techniques, including green chromatography, green spectroscopy, and other environmentally friendly methods for chemical analysis.
- CO-7: Analyze the environmental impact of chemical processes using life cycle assessment (LCA) and other sustainability metrics.
- CO-8: Explore green polymer chemistry, including the use of renewable resources, biodegradable polymers, and sustainable production processes.
- CO-9: Evaluate the use of biocatalysis and enzyme-mediated reactions in green chemistry, emphasizing sustainable and selective transformations.

### **Unit 7: Nanotechnology**

- CO-1: Demonstrate an advanced understanding of the principles and theories underlying nanotechnology, including quantum effects, nanoscale materials, and their unique properties.
- CO-2: Utilize and critically evaluate advanced nanomaterial characterization techniques, such as high-resolution microscopy, spectroscopy, and advanced imaging methods.
- CO-3: Design and evaluate advanced strategies for the synthesis of nanoparticles, considering size control, shape engineering, and surface modifications for specific applications.
- CO-4: Apply nanotechnology concepts to multidisciplinary areas, particularly in nanomedicine, by designing nanocarriers for drug delivery, theranostic systems, and bioimaging applications.
- CO-5: Analyze advanced nanoelectronics and photonics principles, including the design and fabrication of nanoscale electronic devices, sensors, and optical systems.
- CO-6: Evaluate advanced principles of nanocatalysis and green nanotechnology, exploring sustainable and eco-friendly approaches to chemical transformations and environmental applications.
- CO-7: Assess the advanced principles of nanotoxicology, conduct safety assessments, and critically evaluate the potential risks associated with nanomaterials in biological and environmental contexts.

CO-8: Explore and apply advanced nanofabrication techniques, including top-down and bottom-up approaches, and analyze the properties and applications of cutting-edge nanomaterials.

### **SEMESTERS 3 AND 4**

# CH 03 04 05 INDUSTRIAL OILS AND FAT PRODUCTS - PRACTICAL I Credit: 3 Lab Hours: 54+54=108

- CO 1 To prepare refined and bleached oils, soaps, detergent powders, shampoo and vanishing cream
- CO 2 To Establish the quality specifications and do the complete analysis of vansapati, soap, glycerine and detergent powder.

# CH 03 04 06 ESSENTIAL OILS AND AROMATICS - PRACTICAL II Credit: 3 Lab Hours: 54+54=108

- CO 1 To prepare essential oils, aromatics and perfumery compounds
- CO 2 To prepare isolates from essential oils
- CO 3 To detect and estimate common adulterants in essential oils.
- CO 4 To Determine the assay of essential oils and perfumery materials

# CH 03 04 07 ADVANCED APPLIED CHEMISTRY - PRACTICAL III Credit: 3 Lab Hours: 72+72=144

- CO 1 Determine the physical and chemical constants of common oils and fats
- CO 2 Detect common adulterants in oils and fats
- CO 3 Separate and estimate saturated acid in mixtures and in oils
- CO 4 Investigate of the fatty acid composition of the oils and fats
- CO 5 Establish the quality specifications of fats and oils