Enclosure- OA-IIIB

Yogi Divine Society inspired,

Sarvodaya Kelavani Samaj managed,

Shree Manibhai Virani and Smt. Navalben Virani Science College, Rajkot

(Affiliated to Saurashtra University, Rajkot)

Re-Accredited at 'A' Level by NAAC

STAR college Scheme & Status by MST-DBT

UGC- College with Potential for Excellence (CPE)

UGC-DDU KAUSHAL Kendra

GAAA – Highest Grade A-1 by KCG, Government of Gujarat

GPCB-Government of Gujarat approved Environment Audit Center

UGC-Autonomous College

DEPARTMENT OF CHEMISTRY

M.Sc. Chemistry

(With Specialization in Organic /Analytical Chemistry)

SEMESTER I

16PCECC01	Core 1: Inorganic Chemistry	4 hrs./Wk	4 Credits

Objectives:

At the successful completion of the course, students will be able to:

- Understand Molecular Orbital & Valance Bond theories of bonding.
- Describe Huckel's theory & its applications to Ethylene, Butadiene and Benzene.
- Understand the basic principle, theory and instrumentation of Mössbauer Spectroscopy
- Identify the possible inorganic complexes/salt which can be analyzed and Interpret the Mössbauer Spectra for structure determination
- Understand preparation, chemical and physical properties and applications of organic and inorganic Reagents in inorganic analysis.
- State the principle, draw instrumentation and describe theory and applications of ESR
- Illustrate Zeeman levels & Calculate the energies of Zeeman levels
- Describe bonding, synthesis and application of σ- & π–bonded organometallic compounds.

Unit 1. Quantum Mechanics and its Applications: (10 Hrs.)

- MO-VB Theory: Born-Oppenheimer approximation, Hydrogen Molecule ion. LCAO-MO and VB treatments of hydrogen molecule.
- Electron Density, forces and their role in chemical bonding.
- Hybridization and valence MO's of H_2O, NH_3 and CH_4.
- Hückel pi-electron theory and its applications to Ethylene, Butadiene and Benzene.
- Idea of Self-consistent field method.

Unit 2. Mössbauer Spectroscopy: (09 Hrs.)

- Introduction of Mössbauer effect, Isomer- Shift,
- Magnetic hyperfine interactions.
- Quadrupole moment. Electric field gradient, Quadrupole splitting,
- Applications in Structure determination.

Unit 3. Electron Spin Resonance: (09 Hrs.)

- Introduction to Electron Spin Resonance,

- Technique of electron spin resonance, interaction between nuclear spin and electron spin:- hyper fine splitting,
- Calculation and energies of Zeeman levels, calculations of energies, frequency and the ESR spectrum when one electron influenced by a single proton and one electron delocalize over two equivalent protons.

Unit 4. Uses of Organic and Inorganic Reagents in Inorganic Analysis: (11 Hrs.)

- Cupferron, Dithiozone, Aluminon, Oxine, Dithiooxamide,
- α-Benzoinoxime, α-Nitro-β-naphthol, α-Nitroso-β-naphthol,
- Diphenyl carbazone, Diphenyl carbazide,
- Pyrogallol, Benzidine, Salicylaldoxime, *o*-Phenanthroline,
- Potassium bromate ($KBrO_3$), Potassium iodate (KIO_3),
- Ammonium vanadate (NH_4VO_3), Ceric suphate [$Ce(SO_4)_2$], Ethylenediaminetetraacetic acid (EDTA).

Unit 5. Organometallic Complexes: **(09 Hrs.)**

- Introduction, bonding and structure & Classification,
- Synthesis and application of:
  - σ-bonded Organ transition metal compounds
  - π–bonded (alkenes, alkynes, allyl, cyclopentadiene and arene) Organometallic compounds.

Reference Books

1. Prasad, R. K. (2004, Second edition) *Quantum Chemistry*. New Delhi: New Age International (P) Ltd. (ISBN: 81-224-1264-5).
2. Chandra, A. K. (2008, Fourth edition) *Introductory Quantum Chemistry*, New Delhi: Tata McGraw-Hill. (ISBN: 0-07-462054-1).
3. Drago, R. S. (1977) *Physical Method in Chemistr*y. Philadelphia: Saunders College Publishing. (ISBN: 0721631843).
4. Singh, A.; Singh, R. (2005) *Textbook of Inorganic Chemistry Vol. I & II*. New Delhi: Campus Books International (ISBN: 8180300714).
5. Jeffery, G. H.; Bassett, J.; Mendham, J.; Denny, R. C. (1989, Fifth edition) *Vogel's Textbook of Quantitative Chemical Analysis*. Hoboken: John Willey & Sons (ISBN: 0-582-44693-7).
6. Crabtree, R. H. (2005, Fourth edition) *The Organometallic Chemistry of the Transition Metals*. Hoboken: John Willey & Sons (ISBN: 0-471-66256-9).
7. Mehrotra, R. C. and Singh, A. (2004, Second edition) *Organometalic Chemistry A Unified Approach*, New Delhi: New Age International (P) Ltd. (ISBN: 81-224-1258-05).

SEMESTER I

16PCECC02	Core 2: Organic Chemistry	4 hrs./Wk	4 Credits

Objectives:

To enable the students to

- Understand concept and types of reaction mechanism, draw arrow notation, categorize bond cleavages, and determine the stability of reactive intermediates applying inductive, resonance and mesomeric effect.
- Understand Interaction between orbitals over many bonds, effect of delocalization and conjugation on acidity, basicity and pK_a.
- Identify types of enols and enolates, reaction of enols and enolates.
- Explain criteria of aromaticity, Understand concept of electrophilic aromatic substitution.
- Understand concept of radicals, stability of radical, radical chain reactions.

Unit 1. Reaction path Way & Reactive Intermediates: (06 Hrs.)

Reactivity of organic molecule, collision, charge interaction, orbital overlap, Homolytic and Heterolytic fission, Different types of arrow notation, Electrophile and Nucleophile, Carbocation, Carbanion, Free radical, Carbene, Nitrene, Ylides, Dithioketene acetal and Enamines.

Unit 2. Delocalization and Conjugation: **(12 Hrs.)**

Introduction, non cyclic polynes, conjugation, the allyl system, allyl-like system, conjugation of two pi bond, electrophilic & nucleophilic conjugate addition, Conjugate addition of carbonyl with ammonia and alcohol and organo-copper reagent, effect of delocalization and conjugation on acidity, basicity and Pka.

Unit 3. Chemistry of Enols and enolates: **(10 Hrs.)**

Introduction, Acid & base catalyzed enolization, types of enols and enolates, stabilization of enol, reaction with enols and enolates as intermediates, stable enol equivalents, reaction of enol ethers, alkylation of enolates, alkylation of β-dicarbonyl compounds, reaction of enolates with aldehyde and ketones, acylation of enolates and ketones.

Unit 4. Aromaticity and aromatic substitution reaction: (10 Hrs.)

Introduction, criteria of aromaticity, Huckels rule, aromaticity and anti-aromaticity, aromatic hydrocarbon & heterocycles. Electrophilic aromatic substitution; activation & deactivation, position of substitution, phenols as

aromatic enols, reaction with one carbon electrophile, electrohilic addition to alkene.

Unit 5. Radical Reaction: (10 Hrs.)

Formation of radicals, structure and stability of radical, radical chain reaction, selectivity in radical chain reaction, radical reaction initiator AIBN, electrophilic and nucleophilic radicals.

Reference Books

1. Ahluwalia, V. K. (2011, Fourth edition) *Organic Reaction Mechanism*. New Delhi: Narosa (ISBN: 978-81-8487-115-9).
2. Clayden Jonathan; Greeves Nick, Warren Stuart (2012, Second edition) *Organic Chemistry*. Oxford: Oxford University Press (ISBN: 0199270295).
3. Morrison & Boyd (2009, Sixth edition) *Organic Chemistry*. New Jersey: Pearson Education (ISBN: 978-81-7758-169-0).
4. McMurry, John E. (2011, Eight edition) *Organic Chemistry*. Boston: Cengage Learning (ISBN: 0840054440).
5. Smith, Michael B.; March, Jerry (2013, Seventh edition) *March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure*. Hoboken: Wiley-Blackwell (ISBN: 978-0-470-46259-1).
6. Bansal, Raj K. (2009, Fifth) *A Textbook of Organic Chemistry*. New Delhi: New Age International (ISBN: 978-81-224-2025-8).
7. T. W. Graham Solomons (2011, 10th edition) *Organic Chemistry*. Hoboken: John Willey & Sons (ISBN: 978-0-470-55659-7).

SEMESTER I

16PCECC03	Core 3: Physical Chemistry	4 hrs./Wk	4 Credits

Objectives:

At the successful completion of the course, students will be able to:

- Understand concepts & theories of statistical thermodynamics and related statistical methods with its applications.
- Understand the ideal properties & behaviour of solutions and various equillibria
- Determine of Molecular weight from freezing and boiling point.
- Understand the Chemical equilibrium in homogeneous & heterogeneous systems & catalysis. Free energy change in chemical reactions and their applications.
- Understand structure and chemical & thermal properties of Polymers.
- Understand spectroscopic & thermal methods of polymer analysis and apply the same for the identification of polymers.

Unit 1. Statistical Thermodynamics: **(11 Hrs.)**

Basic Terms: probability, cell, phase space, micro and macro states, thermodynamic probability, statistical weight factor, assembly, ensemble and its classification and statistical equilibrium. Derivation of Boltzmann-Maxwell, Bose-Einstein and Fermi- Dirac statistics, Partition function and derivations of translational, rotational, vibrational and electronic partition functions and thermodynamic functions such as internal energy, heat capacity, entropy, work function, pressure, heat content, etc. Partition function & third law of thermodynamics. Applications of partition function to monoatomic gases, diatomic molecules, equilibrium constant and equilibrium constants of metathetic reactions. Problems

Unit 2. The Properties of Solutions: **(09 Hrs.)**

Ideal solutions: Properties, the Duhem-Margules equation, vapour pressure curves. Composition of liquid and vapour in equilibrium influence of temperature on gas solubility and solid-liquid equillibria. Non ideal solutions: Deviation from ideal behaviour, vapour pressure curves, liquid and vapour compositions. General equations for liquid mixtures, partially miscible liquids

Dilute solutions: Henry's law. Determination of molecular weights from freezing and boiling points. Problems.

Unit 3. Free Energy and Chemical Reactions: **(09 Hrs.)**

Chemical equilibrium and the equilibrium constant: Equilibrium in homogeneous gaseous systems. Homogeneous reactions in liquid solutions. Homogeneous reactions in dilute solutions. Chemical equillibria in heterogeneous systems. Free energy change in chemical reactions: The reaction isotherm, standard free energy of reaction, the direction of chemical variation of equilibrium constant with pressure and temperature. Influence of temperature on heterogeneous reactions. Integration of the Van 't Hoff equation. Variation of standard free energy with temperature. Simultaneous equillibria. Formation of standard free energies and entropy changes and their applications, problems

Unit 4. Homogeneous & Heterogeneous Catalysis: **(08 Hrs.)**

Introduction, types of catalysis (Homogeneous & heterogeneous) & their characteristics. Theory of catalysis, autocatalysis, promoters or activators, types of acid base catalysis. Mechanism of acid-base catalysis & catalytic coefficients, Enzyme catalysis.

Unit 5. Polymer Chemistry: **(11 Hrs.)**

Introduction & classification of polymers, chemical analysis, spectroscopic methods, X-ray diffraction and microscopic methods, thermal methods (DSC, DTA, TGA), differential and integral methods of kinetics, analysis, effect of various operating parameters, thermal stability index, physical methods of testing: mechanical properties like stress, strain, modulus and compliance; fatigue tests, impact test, tear resistance, hardness, abrasion resistance, thermal properties: softening temperature and flammability, optical properties: transmittance and reflection, colour, glass transparency, electrical properties: dialectical constant and loss factor, resistivity, dielectric strength and arc strength, effect of temperature on structure of polymers, Chemical properties: resistance to solvents, vapour permeability and weathering.

Reference Books

1. Glasstone, Samuel. (2007) *Thermodynamics for Chemists*: Narahari Press (ISBN: 1406773220).
2. Nash, L. K. (2006, Second edition) *Elements of Statistical Thermodynamics*. America: Dover Publications (ISBN: 0486449785).
3. Gurdeep Raj (2014, Third edition) *Thermodynamics*. Meerut: GOEL publishing House (ISBN: 8187224886).
4. Gurtu, J. N. Gurtu, A. (2014, Twelfth edition) *Advanced Physical Chemistry*. Meerut: Pragati Prakashan (ISBN: 9350060191).
5. Barrow, Gordon M. (1996, Sixth edition) *Physical Chemistry*. New York: McGraw-Hill International. (ISBN: 0070051119).

SEMESTER I

16PCECC04	Core 4: Analytical Chemistry	4 hrs./Wk	4 Credits

Objectives:

To enable the students to

- Understand different analytical methods, laboratory operations and safety.
- Describe various errors in Chemical Analysis.
- State various methods for the treatment of water and air pollutants, and various treatment for pollution control.
- Describe Opto-analytical, Electro-analytical Instruments and Analytical Separation by Solvent Extraction.
- Understand criteria of Intellectual property rights (IPR).

Unit 1. Introduction of Analytical Chemistry: (10 Hrs.)

Classification of analytical methods-classical and instrumental, Types of instrumental analysis. Selecting an analytical method, Neatness and cleanliness, Laboratory operations and practices, Analytical balance, Techniques weighing, errors, volumetric glassware-cleaning and calibration of glassware, samples preparation, dissolution and decompositions, gravimetric techniques, selecting and handling reagents, laboratory notebooks, safety in the analytical laboratory.

Unit 2. Errors in Chemical Analysis: (10 Hrs.)

Statistical Data Analysis: Data processing, Types of errors, Hypothesis, Test of significance, Confidence interval, t-test (mean, paired t-test) & F-test (Ratio analysis), Control charts, Least square analysis (linear), Examples.

Unit 3. Environmental Chemistry: (12 Hrs.)

Introduction, classification and causes of Air, Water and soil pollution, Definitions of pollution, Particulates Types Classifications, Organic Particulates, Air pollution control methods, Photolytic cycle, Photochemical smog chemistry. Water analysis and treatment methods, various parameters, Sampling and preservation techniques, Volume reduction, Neutralization, Sedimentation, Chemical coagulation, Oxidation Ports, Aerators, Various other methods involving

Screening, Sedimentation, Floatation, Activated Sludge Treatment, Trickling Filter, Oxidation Pond, Aerated Lagoons, In Hoff's Tanks. Classification of primary, secondary and tertiary treatments.

Unit 4. Analytical Separation by Solvent Extraction: (08 Hrs.)

Introduction, types of extraction, extraction methods, application of extraction procedure, and separation of constituents present in trace amount, ion exchange separation.

Unit 5. Intellectual property rights (IPR): (08 Hrs.)

Introduction, various Technical Terms, Legislation, IPA, Criteria for Patent, introduction and criteria for USP.

Reference Books

1. Skoog, D. A., West D. M., Holler, F. J., Crouch, Stanley R. (2013, Ninth edition) *Fundamentals of Analytical Chemistry*. Boston: Cengage Learning. (ISBN: 0495558281).
2. Svehla, G. (1996, Seventh edition) *Vogel's Qualitative Inorganic Analysis*. New Jersey: Pearson Education. (ISBN: 0582218667).
3. De, Anil Kumar. (2007, Seventh edition) *Environmental Chemistry*. New Delhi: New Age International Publishers (P) Ltd. (ISBN: 8122426174).
4. Kenneth Wark, Cecil F. Warner, Wayne T. Davis. (1997, Third edition) *Air Pollution: Its Origin and Control*. New Jersey: Pearson Education. (ISBN: 0673994163).
5. Mido, Y., Satake, M. (2003) *Chemicals In The Environment*. New Delhi: Discovery Publishing House. (ISBN: 9788171412679).
6. Sharma, B. K. (2014) *Instrumental Method of Chemical Analysis*. Meerut: GOEL publishing House (ISBN: 978-81-8283-099-8).

SEMESTER I

16PCECC05	**Core Practical -1:** **Inorganic, Organic, Physical, Analytical Chemistry, Practical & Viva Voce**	**12 hrs./Wk**	**6 Credits**

Objectives:
To enable the students to

- Demonstrate Inorganic Qualitative Analysis of a mixture containing six radicals including one rare metal ion.
- Perform Electrophilic aromatic substitution reactions, Functional group interconversion.
- Show Calibration & Instrumentation of Conductometry, pH metry, Refractometry, Potentiometry, and Ultrasonic instruments.
- Perform Partition Co-efficient, First and second order reactions-order determination, energy of activation, Heat of vaporization, Partial molar volume.
- Prepare and standardize the solutions.
- Perform Calibration of glassware and apparatus.
- Perform Assay & % Purity of fine chemicals.
- Demonstrate water and soil analysis.

1. **Inorganic Chemistry:**

   Qualitative Analysis: Analysis of a mixture containing six radicals including one less common / rare metal ion.

2. **Organic Chemistry:**

   Organic preparation: Electrophilic aromatic substitution reactions, Functional group interconversion.

3. **Physical Chemistry:**

   Calibration & Instrumentation:

   - **Conductometry:** Mono and biprotic acids, mixtures of acids against strong/weak bases, hydrolysis constant, verification of Onsagar's equation
   - **pH metry**: Quantitative drug analysis, Hemmet constant, hydrolysis constant of electrolytes, acid-base titration, pKa of acids and E^0_{QH2}.
   - **Refractometry**: Molar refraction, refractive index, composition of Binary mixtures.

- **Spectrophotometry:** Maximum absorption, Lambert-Beers Law, drug estimation, indicator constant.
- **Adsorption:** adsorption isotherm
- **Potentiometry**: Acid-base, normality and dissociation constant, Redox and Argentometric titrations.
- **Ultrasonic**: Acoustical parameters of liquids, compressibility of binary mixture.

Physicochemical Exercises:

- **Partition Co-efficient**: Distribution of Benzoic acid in organic solvent & aqueous phase, equilibrium constant by distribution method.
- **Reaction Kinetics**: First and second order reactions-order determination, energy of activation.
- **Thermodynamics**: Heat of vaporization, Partial molar volume, etc.

4. Analytical Chemistry:

- Preparation and Standardization solution
- Calibration of glassware and apparatus,
- Assay & % Purity of fine chemicals
- **Environmental Analysis:** Water parameter determination (anionic, cationic, DO, COD etc.), Soil analysis, pH, alkalinity and acidity, macro nutrients, Air pollution control apparatus.

SEMESTER I

16PCECE01	IT Tools for Chemist	1 hr./Wk	1 Credit

Objectives:

At the successful completion of the course, students will be able to understand:

- Draw and develop chemical reaction mechanism & assemblies.
- Predict and correlate physicochemical & spectral properties and characteristics of chemical / materials
- Study spatial arrangement of molecules and energy minimization.
- Search & retrieve authenticated scientific reference materials using NLIST, ScienceDirect and SciFinder.

Unit 1. ChemDraw Ultra Software: **(06 Hrs.)**

Introduction of ChemDraw, Chem Sketch, Drawing chemical reaction, Structure drawing using templates, Structure to name and name to structure, Drawing mechanism of reaction, Diagram of Distillation Assembly, Chiral Structure Draw. Drawing apparatus used in laboratory. Reproducing reaction scheme from given research paper.

Introduction of 3D ChemDraw Ultra, export chemical structure from 2D to 3D, run energy minimization of given molecule, predicting log P value & other physicochemical parameters for given set of molecules.

Unit 2. NLIST: **(02 Hrs.)**

Introduction of NLIST website, available e-resources, access of e-books and research articles, e-learning through NPTEL

Unit 3. ScienceDirect: **(02 Hrs.)**

Introduction to publishing house, various journals formats, various search option, recent publication, citation index, impact factor, h-index.

Unit 4. SciFinder: **(02 Hrs.)**

Introduction, accessing SciFinder, keyword search, reaction search and data mining, patent search and referencing.

SEMESTER I

16PVE01	Value Education	1 hr./Wk	1 Credit

- **Value Education**

SEMESTER II

16PCECC06	Core 5: Separation Techniques	5 hrs./Wk	5 Credits

Objectives:

To enable the students to

- Describe Principle, Basic theory, Technique & Applications of Adsorption & Partition Chromatography, Column Chromatography, Planar Chromatography, Gas Chromatography and Liquid Chromatography.
- Discuss Instrumentation, Working and Applications of GC & GC-MS, HPLC & LC-MS.

Unit 1. Adsorption & Partition Chromatography: (08 Hrs.)

Classification, Definition of terms; Principle, Basic theory, Technique & Applications

Unit 2. Column Chromatography: **(10 Hrs.)**

Principle, Basic theory, Technique & Applications of: Column, Ion-exchange and Affinity chromatography.

Unit 3. Planar Chromatography: **(10 Hrs.)**

Principle, Basic theory, Technique & Applications of:

Paper Chromatography: AC, DC, CC, 2D-AC

Thin Layer chromatography: TLC, 2D-TLC & HP-TLC

Unit 4. Gas Chromatography: **(08 Hrs.)**

Instrumentation, Working and Applications of GC & GC-MS

Unit 5. Liquid Chromatography: **(12 Hrs.)**

Instrumentation, Working and Applications of HPLC & LC-MS.

Band broadening & Column efficiency: Definition of terms, Factors affecting, Plate theory & Rate theory of chromatography, Limitations of theory.

Reference Books

1. Sethi, P. D. (2013) *Sethi HPTLC: High Performance Thin Layer Chromatography: Quantitative Analysis of Pharmaceutical Formulations 3 Volume Set*. New Delhi: CBS Publishers & Distributors Pvt. Ltd. (ISBN: 9788123922799).
2. Stahl, E. (1969, Second edition) *Thin-Layer Chromatography: A Laboratory Handbook*. New Berlin: Springer. (ISBN: 978-3-642-88488-7).
3. Heftmann, E. (2004, Sixth edition) *Fundamentals and applications of chromatography and related differential migration methods - Part A (Journal of Chromatography Library)*. Philadelphia: Elsevier Publishing Company. (ISBN: 0444511075).
4. Skoog, D. A., West D. M., Holler, F. J., Crouch, Stanley R. (2013, Ninth edition) *Fundamentals of Analytical Chemistry*. Boston: Cengage Learning. (ISBN: 0495558281).
5. Skoog, D. A., Holler, F. J., Crouch, Stanley R. (2006, Sixth edition) *Principles of Instrumental Analysis*. Boston: Cengage Learning. (ISBN: 0495012017).

SEMESTER II

16PCECC07	Core 6: Stereochemistry	4 hrs./Wk	4 Credits

Objectives:

To enable the students to

- Understand and Describe Fundamental of Stereochemistry.
- Discuss Prochirality and Asymmetric Synthesis.
- Describe Conformational Analysis & Reactivity.
- Describe Stereochemistry of Substitution, Elimination Reactions and addition reactions.

Unit 1. Fundamental of Stereochemistry: (14 Hrs.)

Chirality, Isomers, Classification of stereoisomerism, Optical isomerism, Conventions for D, L and R, S- system, Inter-conversion between Fischer and Three-dimensional formulas with one stereo center, Stereoisomerism for more than one stereogenic unit, Threo & Erythro, Geometrical isomerism, Cis/Trans, E-Z isomerism resulting from double bonds, Oximes, Racemic mixtures and Racemization, Resolution of racemic mixtures, Optical purity & Enantiomeric excess, Formation of diasteromers, Stereoselective and stereospecific reactions, Stereoisomerism without a stereogenic carbon (axial chirality), Planar chirality, Helicity and Molecular stereoisomerism.

Unit 2. Prochirality and Asymmetric Synthesis: (06 Hrs.)

Introduction, Homotopic & Heterotopic ligands and faces, Enantiotopic ligands & faces, Asymmetric synthesis.

Unit 3. Conformational Analysis & Reactivity: (12 Hrs.)

Restricted rotation around single bonds-confirmations of ethane & butane, Origin of conformational energy, Conformations and chemical reactivity of acyclic system, Cycloalkane ring other than cyclohexane, Conformations of substituted cyclohexane, Stereoisomerism in di-substituted cyclohexane, Effect of confirmations on reactivity-cyclic system, Conformation of heterocycles, Conformation of sugars (Fisher, haworth and chair), Epimers, Anomers, Epimerization and Anomeric effect.

Unit 4. Stereochemistry of Substitution & Elimination Reactions: (08 Hrs.)

- **Aliphatic Nucleophilic Substitution Reactions**: Introduction, stereochemistry of S_N1 & S_N2 reaction mechanism, The S_Ni mechanism, Mixed S_N^1 & S_N^2 reaction, ambient nucleophile, Regioselectivity, Neighboring group participation.
- **Stereochemistry of Elimination Reactions:** Introduction, Mechanism E^1, E^2 and E^1cB, Stereochemistry of E^2-anti-ellimination reaction, E2-syn-elimination, Orientation of the double bond, Pyrolytic elimination.

Unit 5. Stereochemistry of Addition Reactions to Carbon-Hetero multiple bonds: (08 Hrs.)

Introduction, Stereo chemical aspects of addition to carbonyl compounds, Stereochemistry of metal hydride reduction, Cannizzaro reaction, Meerwein-Ponndorf reduction, Addition of organometallic compounds, Conjugate addition of organocopper reagents.

Reference Books

1. Kalsi, P. S. (2012, Fourth edition) *Organic Reactions Stereochemistry and Mechanism (Through Solved Problems)*. New Delhi: New Age International (P) Limited. (ISBN: 9788122417661).
2. Kalsi, P. S. (2011, Seventh edition) *Stereochemistry Confirmation and Mechanism*. New Delhi: New Age International (P) Limited. (ISBN: 81-224-2356-6).
3. Finar, I. L. (1989, Fifth edition) *Organic Chemistry: Vol -2: Stereochemistry and the Chemistry of Natural Products*. Harlow: Longman. (ISBN: 0-582-05916-X).
4. Nasipuri, D. (2011, Third edition) *Stereochemistry of Organic Compounds: Principles and Applications*. New Delhi: New Age International (P) Limited. (ISBN: 978-81-224-3029-5).
5. Clayden Jonathan; Greeves Nick, Warren Stuart (2012, Second edition) *Organic Chemistry*. Oxford: Oxford University Press (ISBN: 0199270295).
6. Eliel, Ernest L., Wilen, Samuel H. (1994) *Stereochemistry of Organic Compounds*. Hoboken: Wiley-Blackwell (ISBN: 0471016705).
7. Nogradi, M. (2008, Second revised and updated edition) *Stereoselective synthesis: A practical approach*. Weinheim: Wiley VCH. (ISBN: 978-3-527-61568-1).

SEMESTER II

16PCECC08	Core 7: Interpretative Molecular Spectroscopy (Self Study Course)	1 hrs./Wk	4 Credits

Objectives:

To enable the students to

- Understand, discuss and describe Interpretation and case study of UV spectrum, IR spectrum, Mass spectrum, PMR & CMR of organic compounds (single or mixed).
  - ❖ Interpretation and case study (characteristic absorption, Simple chromophoric groups, conjugated and aromatic systems, effect of acid and base) of UV spectrum of organic compounds.
  - ❖ Interpretation and case study (characteristic frequency, functional group identification) of IR spectrum of organic compounds.
  - ❖ Interpretation and case study (base peak, molecular ion peak, isotopic abundance, rearrangement) of Mass spectrum of organic compounds.
  - ❖ Interpretation and case study (characteristic chemical shift, spin-spin coupling, exchangeable proton, cis-trans isomer, o/m/p substitution pattern, saturated & unsaturated system) of NMR spectrum (PMR & CMR) of organic compounds.
  - ❖ Mixed Examples: Structure determination using combination of UV, IR, Mass & NMR spectroscopy**.**

Reference Books

1. Martin, M. L., Delpuech, J. J. and Martin, G. J. (1980) *Martin *Practical* Nmr Spectroscopy*. Weinheim: John Wiley & Sons Ltd. (ISBN: 0471258652).
2. Silverstein, Robert M., Webster, Francis X., Kiemle, David J., Bryce, David L. (2014, Eighth edition) *Spectrometric identification of Organic Compounds*. Weinheim: John Wiley & Sons Ltd. (ISBN: 978-0-470-91401-4).
3. Abraham, R. J., Fisher, J. and Loftus, P. (1988) *Introduction to NMR Spectroscopy*. Weinheim: John Wiley & Sons Ltd. (ISBN: 0471918946).

4. Dyer, J. R. (1965) *Application of absorption Spectroscopy of Organic Compounds*. Upper Saddle River: Prentice Hall.
5. Williams, D. H., Fleming, I. (2007, Sixth edition) *Spectroscopic Methods in Organic Chemistry*. New Delhi: Tata McGraw-Hill. (ISBN: 007711812X).
6. Kalsi, P. S. (2006, Sixth edition) *Spectroscopy of Organic Compounds*. New Delhi: New Age International Pvt. Ltd. (ISBN: 8122415431).
7. Breitmaier E. (2002, Third edition) *Structure elucidation by NMR in Organic Chemistry-A Practical approach.* Weinheim: John Wiley & Sons Ltd. (ISBN: 978-0-470-85007-7).

SEMESTER II

16PCECC09	Core 8: Modern Analytical Techniques	4 hrs./Wk	4 Credits

Objectives:

To enable the students to

- Describe Types of Analytical techniques, Overview of spectroscopic methods.
- Understand Principle & Theory of Infrared absorption spectrometry, Instrumentation and Interpretation of IR spectra.
- Describe Introduction, Principle, Theory and components of mass spectrometers and Applications of Mass spectrometry.
- Discuss Atomic emission spectroscopy, ^{1}H NMR (PNR), ^{13}C NMR, Polarimetry and Spectropolarimetry.

Unit 1. Introduction to Spectroscopic Techniques: (10 Hrs.)

Types of Analytical techniques, Introduction of Instrumental methods and its classification, Overview of spectroscopic methods based on wave length regions of Electromagnetic radiation, Properties of Electromagnetic radiation.

Infrared Spectroscopy: Introduction to IR and FTIR, Principle & Theory of Infrared absorption spectrometry, Infrared sources and transducers, Sample handling, Instrumentation, Interpretation of IR spectra, Applications and limitations of IR spectroscopy.

Unit 2. Mass Spectroscopy: (10 Hrs.)

Introduction, Principle, Theory and components of mass spectrometers, Different ionization and detection techniques, recording and resolution of mass spectrometer, Types of ions produced in mass spectrometer, Interpretation of Mass spectra of selected compounds /API, Applications of Mass spectrometry, Introduction to ICP-MS.

Unit 3. Emission Spectroscopy: (08 Hrs.)

Atomic emission spectroscopy, Principle, theory and Instrumentation, Atomization techniques, Flame atomizer, Electro thermal atomizer and Inductively coupled plasma atomizer (ICPA).

Flame emission spectroscopy: Principle, Instrumentation and applications.

Fluorimetry: Principle, Instrumentation and applications.

Unit 4. Nuclear Magnetic Resonance Spectroscopy: (10 Hrs.)

Introduction, NMR active nuclei, Basic Theory, NMR Spectrometer, internal Standard & solvent

^{1}H NMR (PNR): Principle, Chemical shift, Magnetic anisotropy, spin-spin coupling (multiplicity), applications & problems of Nuclear magnetic resonance spectroscopy.

^{13}C NMR: Introduction, Principle, Chemical shift, Application and Problems of ^{13}C – NMR, Introduction to 2D NMR.

Structure Elucidation: Structure determination and distinction of various isomeric compounds through spectroscopic techniques (UV, IR, Mass & NMR)**.**

Unit 5. Polarimetry and Spectropolarimetry: (10 Hrs.)

Introduction, Polarized light, Optical activity, Specific rotation measurement of rotatory power, Optical rotatory dispersion and circulardichroism, Instrumentation and applications, Saccharimetry.

Reference Books

1. Martin, M. L., Delpuech, J. J. and Martin, G. J. (1980) *Martin *Practical* Nmr Spectroscopy*. Weinheim: John Wiley & Sons Ltd. (ISBN: 0471258652).
2. Silverstein, Robert M., Webster, Francis X., Kiemle, David J., Bryce, David L. (2014, Eighth edition) *Spectrometric identification of Organic Compounds*. Weinheim: John Wiley & Sons Ltd. (ISBN: 978-0-470-91401-4).
3. Abraham, R. J., Fisher, J. and Loftus, P. (1988) *Introduction to NMR Spectroscopy*. Weinheim: John Wiley & Sons Ltd. (ISBN: 0471918946).
4. Dyer, J. R. (1965) *Application of absorption Spectroscopy of Organic Compounds*. Upper Saddle River: Prentice Hall.
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SEMESTER II

16PCECC10	**Core Practical -2:** **Separation Techniques and Stereochemistry, Modern Analytical Techniques practical & Viva Voce**	**15 hrs./Wk**	**6 Credits**

Objectives:
To enable the students to

- Demonstrate Ternary Mixture Separation & Qualitative Analysis of each component from Organic Mixtures.
- Perform Polarimetric analysis of Racemic mixture and determination of enantiomeric excess.
- Understand techniques of separation using HPLC and GC-Mass spectrometer.

1. **Organic Mixture Separation Techniques:**
   - Ternary Mixture Separation & Qualitative Analysis of each component
2. **Stereo Chemistry:**
   - **Polarimetry**: Specific and molecular rotation, % composition of optically active compounds, Racemic mixture, determination of enantiomeric excess, optical activity of Enantiomer, Diastereomer.
3. **Separation Techniques Demonstrative Practical**:
   - HPLC analysis of Active Pharmaceutical Ingredients
   - GC-Mass spectral study of selected APIs/intermediates
4. **Modern Analytical Techniques**
   - **UV-VIZ. Spectroscopy:** scanning, shifts, transitions, linearity.
   - **IR Spectroscopy**: spectral study of selected APIs

SEMESTER II

16PCECE02	Scientific Writing (Research)	1 hrs./Wk	1 Credits

Objectives:

At the successful completion of the course, students will be able to:

- Learn searching & retrieving scientific literature and patent search using E-resources.
- Understand and write different international scientific publications (research article, review, proposal, patent and book)
- Prepare & present scientific article / proposal.

Unit 1. Literature search & retrieval: scientific peer reviewed research articles, review, patent etc. **(02 Hrs.)**

Unit 2. Full article, letters, note, communication, mini review and review with case study. **(02 Hrs.)**

Unit 3. Writing Research article & Review article preparation (Introduction, Objectives, Methodology, Result & discussion, Chemistry, Experimental section, Acknowledgement & References) **(04 Hrs.)**

Unit 4. Research Proposal for given topic (Introduction, Objectives, Chemistry, Methodology, Plan of Work, Resources required, References) & IP**.** **(04 Hrs.)**

Unit 5. Presentation (ppt) of recent research paper (full article, letters or review) published in the chemistry journals.