# Indrashil University



# Department of Chemistry School of Science

M.Sc. 2025-2027 Sem I-IV

Analytical Chemistry

Course Profile

Academic Year 2025-2026

Course Structure M.Sc. Analytical Chemistry Semesters I to IV

| SEMESTER: I | MINIMUM SEMESTER CREDIT REQUIRED: 20<br>CUMULATIVE SEMESTER CREDITS REQUIRED: 20 |         |         |  |  |
|-------------|--|---------|---------|--|--|
| SUBJECT NO. | SUBJECT NAME   | L-T-P   | CREDITS |  |  |
| CH4 101     | ORGANIC CHEMISTRY – I:<br>LOGICS IN ORGANIC REACTION AND<br>MECHANISM            | 3-0-0   | 3       |  |  |
| CH4 102     | INORGANIC CHEMISTRY – I:<br>COORDINATION CHEMISTRY                               | 3-0-0   | 3       |  |  |
| CH4 103     | PHYSICAL CHEMISTRY – I: MOLECULAR<br>THERMODYNAMICS AND SOLID STATE              | 3-0-0   | 3       |  |  |
| CH4 104     | ANALYTICAL CHEMISTRY – I: INSTRUMENTAL METHODS OF ANALYSIS                       | 3-0-0   | 3       |  |  |
| CH4 105     | QUANTUM MECHANICS FOR CHEMISTS   | 3-0-0   | 3       |  |  |
| CH4 106     | BASIC ORGANIC CHEMISTRY LABORATORY   | 0-0-8   | 4       |  |  |
| CH4 107     | INORGANIC CHEMISTRY LABORATORY   | 0-0-8   | 4       |  |  |
|             | Total  | 15L-16P | 23      |  |  |

| SEMESTER: II  | MINIMUM SEMESTER CREDIT REQUIRED: 43 CUMULATIVE SEMESTER CREDITS REQUIRED: 23 |         |         |  |  |
|---------------|---|---------|---------|--|--|
| SUBJECT CODES | SUBJECT NAME  | L-T-P   | CREDITS |  |  |
| CH4 201       | ORGANIC CHEMISTRY – II: REACTIONS,<br>REAGENTS AND REARRANGEMENTS             | 3-0-0   | 3       |  |  |
| CH4 202       | INORGANIC CHEMISTRY – II: MAIN GROUP AND ORGANOMETALLIC COMPOUNDS             | 3-0-0   | 3       |  |  |
| CH4 203       | PHYSICAL CHEMISTRY – II: SURFACE AND INTERFACIAL CHEMISTRY                    | 3-0-0   | 3       |  |  |
| CH4 204       | BIOORGANIC CHEMISTRY:   | 3-0-0   | 3       |  |  |
| CH4 205       | SPECTROSCOPY – I: MOLECULAR STRUCTURE DETERMINATION                           | 3-0-0   | 3       |  |  |
| CH4 206       | ANALYTICAL TECHNIQUES LABORATORY  | 0-0-8   | 4       |  |  |
| CH4 207       | PHYSICAL CHEMISTRY LABORATORY   | 0-0-8   | 4       |  |  |
|               | Total   | 15L-16P | 23      |  |  |

| SEMESTER: III | MINIMUM SEMESTER CREDIT REQUIRED: 24 CUMULATIVE                     |                               |         |  |  |  |  |
|---------------|---|-------------------------------|---------|--|--|--|--|
|               | SEMESTER CREDITS REQUIRE  | SEMESTER CREDITS REQUIRED: 67 |         |  |  |  |  |
| SUBJECT CODES | SUBJECT NAMES   | L-T-P                         | CREDITS |  |  |  |  |
| CH5 AN101     | ANALYTICAL CHEMISTRY - II: PHARMACEUTICAL ANALYSIS AND MEASUREMENTS | 3-0-0                         | 3       |  |  |  |  |
| CH5 AN102     | ANALYTICAL CHEMISTRY - III:<br>ELECTROANALYTICAL TECHNIQUES         | 3-0-0                         | 3       |  |  |  |  |
| CH5 AN103     | ANALYTICAL CHEMISTRY-IV: QUALITY MEASUREMENTS IN ANALYSIS           | 3-0-0                         | 3       |  |  |  |  |
| CH5 104       | SPECTROSCOPY-II   | 3-0-0                         | 3       |  |  |  |  |
| CH5 105       | SPECTROSCOPIC ANALYSIS AND DATA INTERPRETATION LABORATORY           | 0-0-8                         | 4       |  |  |  |  |
| CH5 AN106     | ANALYTICAL CHEMISTRY LABORATORY                                     | 0-0-8                         | 4       |  |  |  |  |
|               | ELECTIVE-I  | 2-0-0                         | 2       |  |  |  |  |
|               | <u>ELECTIVE-II</u>  | 2-0-0                         | 2       |  |  |  |  |
|               | Total   | 19L-16P                       | 24      |  |  |  |  |

| SEMESTER: IV  | MINIMUM SEMESTER CREDIT REQUIRED: 15 CUMULATIVE SEMESTER CREDITS REQUIRED: 82 |        |         |  |
|---------------|---|--------|---------|--|
| SUBJECT CODES | SUBJECT NAMES   | L-T-P  | CREDITS |  |
| CH5 AN201     | RESEARCH OR INDUSTRIAL PROJECT  | 0-0-20 | 10      |  |
| CH5 AN202     | PROJECT REPORT  | 3-0-0  | 3       |  |
| CH5 AN203     | PROJECT PRESENTATION  | 2-0-0  | 2       |  |
|               | Total   |        |         |  |

#### Semester III: LIST OF AVAILABLE SUBJECTS FOR ELECTIVE I, II

| SUBJECT CODES | SUBJECT NAMES                         | L-T-P | CREDIT |
|---------------|---------------------------------------|-------|--------|
| CH5 EAN1      | SEPARATION METHODS                    | 2-0-0 | 2      |
| CH5 EAN2      | APPLICATIONS OF COMPUTER IN           | 2-0-0 | 2      |
|               | CHEMISTRY                             |       |        |
| CH5 EAN3      | SUPRAMOLECULAR CHEMISTRY              | 2-0-0 | 2      |
| CH5 EAN4      | APPLIED ANALYSIS AND GREEN ANALYTICAL | 2-0-0 | 2      |
|               | CHEMISTRY                             |       |        |

## SEMESTER I SYLLABUS WITH COURSE LEARNING OUTCOME (CLO)

#### CH4 101: ORGANIC CHEMISTRY-I: LOGICS IN ORGANIC REACTION AND MECHANISM (L-T-P-C: 3-0-0-3)

| Program: M. Sc. Chemistry | Semester: I   |
|---------------------------|---|
| Course code: CH4 101      | Course name: ORGANIC CHEMISTRY-I: LOGICS IN ORGANIC |
|                           | REACTION AND MECHANISM                              |

| Locture            | Practical Gradita |                    | Total | Evaluation Scheme |          |            |           |
|--------------------|-------------------|--------------------|-------|-------------------|----------|------------|-----------|
| Lecture<br>(Hours) | (Haure)           | Hours) Credits Hou |       | Component         | Exam     | Max. Marks | Passing % |
| 3 per week         | -                 | 3                  | 45    | Lecture           | CCE, ESE | 100        | 35        |

#### **Course Objectives:**

- Understand and apply the fundamental principles of structure and reactivity
- Analyze and compare reaction mechanisms
- Develop proficiency in stereochemical concepts and conformational analysis

#### **Course Learning Outcome:** At the end of this course, the students will be able to

CLO1: Familiarize with types of reactions, their mechanisms, and reactivity of organic reactive intermediates

**CLO2:** Understand the Hammett equation, Hammond's postulate, Curtin-Hammett principle, and HSAB Principle.

CLO3: Get an idea about SNAr, SRN1, and benzyne mechanism, the NGP, and anchimeric assistance.

**CLO4:** Be able to understand Classical and non-classical carbocations. Aromatic electrophilic substitution reactions, arenium ion mechanism, the ortho/para ratio, ipso attack,

**CLO5:** Knowledge of Basic principles of Stereochemistry, chirality, Prochiral relationship, and optical activity in biphenyls, spiranes, allenes, and helical structures. Stereochemistry of compounds containing Nitrogen, Sulphur, and Phosphorus.

| Units      | Contents   | Hours |
|------------|--|-------|
| Unit I:    | Basic principles of Structure and Reactivity: Chemical bonding; Hybridization;       | 15    |
| Structure  | Molecular Geometry, Bond Polarity and Dipole Moment, Resonance and                   |       |
| and        | Delocalization, Inductive, Mesomeric Effects and Tautomerism, Hyperconjugation       |       |
| Reactivity | and its Role in Stability; Steric Effects; Electron Donating and Withdrawing Groups; |       |
|            | Concept of Aromaticity; Hard and Soft Acids and Bases (HSAB Principle); Frontier     |       |
|            | Molecular Orbital Theory (HOMO-LUMO Concepts); Thermodynamic vs. Kinetic             |       |
|            | Control; Hammond's Postulates; Stability and Reactivity of Reactive Intermediates:   |       |
|            | Carbocations, Carbanions, Free Radicals, Carbenes and Nitrenes; Transition State     |       |
|            | Theory and Curtin-Hammett Principle; Energy profiles and reaction coordinate,        |       |
|            | diagrams for Exothermic and Endothermic Reactions; Energy profiles and reaction      |       |
|            | Coordinate Diagrams for Catalysed and Uncatalysed Reactions; Effect of Solvent       |       |
|            | Polarity and Proticity; Substituent Effects on Reactivity; Molecular Strain and      |       |
|            | reactivity; Ring Strain and Bredt's Rule; Baeyer Strain Theory                       |       |
| Unit II:   | <b>Organic Reaction Mechanism:</b> Arrow pushing formalism (curved arrow notation);  | 15    |
| Organic    | Types of electron movement: homolytic vs. heterolytic cleavage                       |       |
| Reaction   | Types of Reactions and their mechanism:  |       |
| Mechanism  | Nucleophilic Substitution Reactions: SN1 and SN2 mechanisms (Stereoelectronic        |       |
|            | Control in SN1/SN2): kinetics, stereochemistry, and energy diagrams; Neighboring     |       |
|            | group participation (NGP); Ambident nucleophiles                                     |       |
|            | Elimination Reactions: E1, E2, and E1cb mechanisms; Hofmann vs. Zaitsev              |       |
|            | elimination; Base strength and solvent effects; Stereoelectronic requirements and    |       |
|            | Antiperiplanar geometry  |       |

|   | Addition Reactions: Electrophilic, nucleophilic, and radical additions; Markovnikov vs. anti-Markovnikov additions; Stereochemistry in syn/anti additions; Addition to carbon–heteroatom multiple bonds (e.g., C=0, C=N)  Aromatic Substitution Mechanisms: Electrophilic aromatic substitution (EAS); Nucleophilic aromatic substitution (NAS): SNAr, benzyne mechanism; Diazonium coupling and related transformations  Radical Reactions: Generation and stability of radicals; Chain initiation, propagation, termination  |    |
|---|--|----|
| Unit III: Stereoch emistry and Conform ational Analysis | Fundamental Concepts in Stereochemistry: Isomerism; Constitutional vs. Stereoisomerism; Types of Stereoisomers: Enantiomers, Diastereomers, Meso Compounds; Optical Activity: Chirality, Specific Rotation, Optical Purity; Absolute and Relative Configuration: CIP Rule for R/S Nomenclature; Stereoselective vs. Stereospecific Reactions Projection Formulas and Interconversion Define Fischer, Sawhorse, Newman, and Wedge-Dash Representations; Interconversion of different projections; Stereochemical correlation and configuration assignment Conformational Analysis of Acyclic and Cyclic Systems Conformations of ethane, butane: eclipsed, staggered, gauche, anti; Cyclohexane conformations: chair, boat, twist-boat; Axial/equatorial positions; conformational preference; Energy barriers and conformational equilibrium; Effect of substituents on conformational stability | 15 |

- 1. E. L. Eliel. *Stereochemistry of Carbon Compounds*. TATA McGraw-Hill Publishing Company Ltd., New Delhi. 1962, 1st Ed.
- 2. D. Nasipuri. *Stereochemistry of Organic Compounds*. New Age International (P) Ltd., Publishers, New Delhi. 1994, 2nd Ed.
- 3. P. S. Kalsi. *Stereochemistry: Conformation and Mechanism*. New Age International (P) Ltd., Publishers, New Delhi. 2019, 10th Ed.
- 4. J. March. *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*. Wiley-Interscience, A John Wiley & Sons, Inc., New York. 2006, 6th Ed.
- 5. P. Sykes. *A Guidebook to Reaction Mechanisms in Organic Chemistry*. Longman Scientific & Technical, Essex. 1986, 6th Ed.
- 6. S. M. Mukherji; S. P. Singh. *Reaction Mechanism in Organic Chemistry*. Macmillan India Ltd., New Delhi. 1976, Revised
- 7. L. G. Wade Jr. *Organic Chemistry*. Pearson Education, New Delhi. 2011, 8th Ed.
- 8. F. A. Carey; R. J. Sundberg. *Advanced Organic Chemistry, Part A and Part B: Structure and Mechanisms*. Springer, New York. 2007, 5th Ed.
- 9. J. Clayden; N. Greeves; S. Warren; P. Wothers. Organic Chemistry. Oxford University Press, Oxford. 2014, 2nd Ed.

### CH4 102: INORGANIC CHEMISTRY-I: COORDINATION CHEMISTRY & MAGNETIC MATERIALS (L-T-P-C: 3-0-0-3)

| Program: M. Sc. Chemistry | Semester: I                                 |
|---------------------------|---|
| Course code: CH4 102      | Course name: INORGANIC CHEMISTRY-I:         |
|                           | COORDINATION CHEMISTRY & MAGNETIC MATERIALS |

| Practical          |         | Cradita | Total |           | Evaluation Scheme |            |           |
|--------------------|---------|---------|-------|-----------|-------------------|------------|-----------|
| Lecture<br>(Hours) | (Hours) | Credits | Hours | Component | Exam              | Max. Marks | Passing % |
| 3 per week         | -       | 3       | 45    | Lecture   | CCE, ESE          | 100        | 35        |

#### **Course Objectives:**

- Learn about different types of isomers, coordination polyhedra and molecular symmetry.
- Understand redox reactions, the Nernst equation
- Comprehend inorganic reaction mechanisms
- Have a concept of magnetic materials, calculation of magnetic moment

Course Learning Outcomes: At the end of this course, students will be able to

**CL01:** Identify different coordination isomers.

**CLO2:** Compare different strengths of acids and bases.

**CLO3:** Classify the molecular symmetry by using the group theory concept.

**CLO4:** Develop the concept of a redox reaction, the Nernst equation, and Inorganic reaction mechanisms.

| Units   | Content  | Hours |
|---|--|-------|
| <b>Unit I:</b><br>Isomerism                                       | <b>Principles of Inorganic Chemistry</b> : Isomerism, Structural and stereoisomerism of tetrahedral, square planar and octahedral complexes, facial and meridional isomers, methods to distinguish cis and trans isomers, the concept of ligand- ambidentate, chelating, innocent, non-innocent and bridging ligand, flexidentate behavior of polydentate ligand, Chelate complex, EDTA, Coordination polyhedra - Enumeration of geometrical and optical isomers.  | 15    |
| UNIT-II<br>Molecular<br>Symmetry,<br>Structure, and<br>Reactivity | Symmetry and Group Theory: Definitions and theorems of group theory, subgroups, Classes Molecular symmetry and symmetry groups – symmetry elements and operations. Symmetry planes, reflections, inversion centre, proper/improper axes of rotation, products of symmetry operations, equivalent symmetry elements and atoms, symmetry elements and optical isomerism, symmetry point groups, classes of symmetry operations.  Inorganic Reaction Mechanisms: Substitution reactions - Dissociative and associative interchange - trans-effect: polarization theory, pi-complexing theory, cis effect, and -redox reactions, concept of oxidant and reductant, disproportionation and comproportionation reaction, std electrode potential and electrochemical series, formulation of Nernst equation, calculation of k value for given inorganic reaction, Latimer diagram, redox indicator, Z-R solutions. | 15    |
| III  Magnetism and  Inorganic  Compounds                          | Magnetic Properties: Classification of magnetic materials; Cooperative phenomena – Diamagnetism, Paramagnetism, ferro, anti-ferro and ferrimagnetism, Magnetic permeability, molar susceptibility, Magnetic moment, quenching of magnetic moment: 1. By super exchange process, 2) by metal-metal direct bond formation(compounds of Cr and Cu), Curie equation, effect of orbital contribution to spin magnetic moment in oct. and tet-field for dn ion and calculation of effective magnetic moment.   | 15    |

- 1. P. Atkins; T. Overton; J. Rourke; M. Weller; F. Armstrong. *Shriver and Atkins' Inorganic Chemistry*. W. H. Freeman and Company, New York. 2009, 5th Ed.
  - or
- D. F. Shriver; P. W. Atkins. *Inorganic Chemistry*. W. H. Freeman and Company, New York. 1999, 3rd Ed.
- 2. C. Housecroft; A. G. Sharpe. *Inorganic Chemistry*. Prentice Hall/Pearson Education, Harlow. 2008, 3rd Ed. or
  - C. Housecroft; A. G. Sharpe. *Inorganic Chemistry*. Prentice Hall/Pearson Education, Harlow. 2012, 4th Ed.
- 3. F. A. Cotton; G. Wilkinson. *Advanced Inorganic Chemistry*. John Wiley & Sons, New York. 1988, 5th Ed. or
  - F. A. Cotton; C. A. Murillo; M. Bochmann; R. N. Grimes. *Advanced Inorganic Chemistry*. John Wiley & Sons, New York. 1999, 6th Ed.
- 4. J. E. Huheey; E. A. Keiter; R. L. Keiter. *Inorganic Chemistry: Principles of Structure and Reactivity*. Prentice Hall, New Jersey. 1997, 4th Ed.
- 5. G. L. Miessler; D. A. Tarr. *Inorganic Chemistry*. Pearson Education, New Delhi. 2004, 3rd Ed.
- 6. G. Wulfsberg. *Inorganic Chemistry*. University Science Books, Sausalito. 2000, 2nd Ed.

## CH4 103: PHYSICAL CHEMISTRY-I: MOLECULAR THERMODYNAMICS AND SOLID-STATE PROPERTIES (L-T-P-C: 3-0-0-3)

| <b>Program:</b> M. Sc. Chemistry | Semester: I                                  |
|----------------------------------|--|
| Course code: CH4 103             | Course name: PHYSICAL CHEMISTRY-I: MOLECULAR |
|                                  | THERMODYNAMICS AND SOLID-STATE PROPERTIES    |

| Lastura            | Practical | Cradita | Total |           | Evaluatio | n Scheme   |           |
|--------------------|-----------|---------|-------|-----------|-----------|------------|-----------|
| Lecture<br>(Hours) | (Houre)   | Credits | Hours | Component | Exam      | Max. Marks | Passing % |
| 3 per week         | -         | 3       | 45    | Lecture   | CCE, ESE  | 100        | 35        |

#### **Course Objectives:**

- Understand and apply the principles of statistical thermodynamics to explain macroscopic thermodynamic behaviour.
- Analyze complex chemical reaction mechanisms through kinetic models, including steady-state and transition state theories, and explore experimental techniques.
- Explore the structural and dynamic properties of solids, including crystal symmetry, defects, and polymorphism, with relevance to materials and pharmaceutical sciences.
- Examine the thermal and electronic properties of solid-state materials.

#### Course Learning Outcomes: In brief, through this course, the students will be able to

**CLO1:** Connect statistics and thermodynamics. Build the fundamental understanding of the computational world.

CLO2: Understand the rate laws of complex reactions.

**CLO3:** Analyze the scientific insights of chemical kinetics of complex reactions.

**CLO4:** Demonstrate the ability to identify different bonding contributions in the solid state.

**CLO5:** Acquire the knowledge of polymorphism which will help the students in the pharma industry.

| Units  | Content  | Hours |
|--|--|-------|
| Unit I: Statistical Thermodynamics and Applications in Chemistry | <b>Statistical Thermodynamics:</b> Limitations of classical thermodynamics. Introduction to terms like ensemble, population, equipartition of energy, degeneracy. Boltzmann's distribution law, partition function, Distinguishable and indistinguishable particles, molar partition function, Electronic, Translational, Rotational, and Vibrational partition functions. Fermi-Dirac statistics and Bose-Einstein statistics distribution law, and their application. Applications of statistical thermodynamics- Heat capacity behavior of solid and calculation of equilibrium constant, variation in equilibrium constant with temperature and pressure, Le Chatelier's Principle.  | 15    |
| Unit II:<br>Chemical Kinetics<br>and Dynamics                    | Chemical Kinetics: Revision and basics of simple chemical kinetics. Reactions approaching equilibrium, steady state approximation, Complex Reactions: Rate laws for consecutive, opposing, parallel reactions, explosive reactions, chain reactions. Comparison between gas phase and solution reactions, factors determining rates in solution. Reaction between ions, reactions involving dipoles, reactions in solution, and the solvent reorganization energy. Fast reactions: Relaxation, stop flow, and flash photolysis. Introduction to ultrafast spectroscopy and femtochemistry. Kinetics of enzyme-catalyzed reactions: Michaelis-Menten mechanism, Lineweaver-Burk plot, Harpoon mechanism and its study using molecular beam techniques, Applications of kinetic isotope effects in reaction mechanism studies. Basics of simple collision theory. Activated complex theory: Reaction coordinate and the transition state theory, potential energy surface, rate constant derivation. experimental evidence on transition state and activated complex. Theories of uni-molecular reactions: | 15    |
| Unit III:  | Solid State Chemistry: Crystallography- Recapitulation, diffraction properties   | 15    |

#### Crystalline Materials: From Lattice to Device

of crystals. Symmetry elements, space groups. Concept of crystal planes, Miller indices. Ionic crystals. Determination of crystal structure. Imperfection in crystalspoint defects (Thermodynamic treatment) and line defects. Crystal growth, engineering, polymorphism, and drug polymorphism regulatory issues.

**Thermal Properties:** Lattice vibrations - phonon spectrum; Lattice heat capacity; Thermal expansion; Thermal conductivity.

**Electrical Properties:** Free electron theory (Drude model, limitations)- electrical conductivity and Ohm's law - Hall effect; Band theory - band gap - metals and semiconductors - intrinsic and extrinsic semiconductors; Temperature dependence on conductivity. Hopping semiconductors and disordered semiconductors; Semiconductor/metal transition; p-n junctions; Organic semiconductors and perovskites. Superconductors - Meissner effect - type I and II superconductors - isotope effect - basic concepts of BCS theory - manifestations of the energy gap - Josephson devices. High-temperature superconductors and cuprates.

- 1. M. C. Gupta. Statistical Thermodynamics. New Age International Publishers, New Delhi. 1998, Revised Printing.
- 2. T. L. Hill. An Introduction to Statistical Thermodynamics. Dover Publications, New York. 1986, 1st Ed.
- 3. B. N. Roy. Fundamentals of Classical and Statistical Thermodynamics. Wiley, New Delhi. 2002, 1st Ed.
- 4. K. J. Laidler. *Chemical Kinetics*. Pearson Education, Noida. 1987, 3rd Ed.
- 5. R. D. Levine. *Molecular Reaction Dynamics*. Cambridge University Press, New York. 2009, Paperback Ed.
- 6. Raja Ram; J. C. Kuriacose. *Kinetics and Mechanism of Chemical Transformations*. Macmillan India Ltd., New Delhi. 1993, 1st Ed.
- 7. S. Glasstone. Textbook of Physical Chemistry. Macmillan Publishers, London. 1942, 2nd Ed.
- 8. P. Atkins. *Physical Chemistry*. Oxford University Press, Oxford. 2018, 8th Ed.
- 9. M. M. Woolfson. *An Introduction to X-ray Crystallography*. Cambridge University Press–Vikas Publishing House, New Delhi. 1980, 2nd Ed.
- 10. W. Cochran. *Dynamics of Atoms in Crystals*. Edward Arnold, London. 1973. (pp. 24–37).
- 11. P. M. A. Sherwood. Vibrational Spectroscopy of Solids. Cambridge University Press, Cambridge. 1972. (pp. 1-45).
- 12. C. N. R. Rao; K. J. Rao. Phase Transitions. Cambridge University Press, Cambridge. 1st Ed.
- 13. G. H. Stout; L. H. Jenson. *X-ray Structure Determination: A Practical Guide*. Macmillan Publishing Co. Inc. and Collier Macmillan Publishers, New York. 1989, 2nd Ed.
- 14. Gurdeep Raj. Advanced Physical Chemistry. Krishna Prakashan Media Pvt. Ltd., Meerut. 2022, 1st Ed.

#### CH4 104: ANALYTICAL CHEMISTRY-I: INSTRUMENTAL METHODS OF ANALYSIS (L-T-P-C: 3-0-0-3)

| Program: M. Sc. Chemistry | Semester: I                          |
|---------------------------|--------------------------------------|
| Course code: CH4 104      | Course name: ANALYTICAL CHEMISTRY-I: |
|                           | INSTRUMENTAL METHODS OF ANALYSIS     |

| Practical          |         | Cuadita | Total | Evaluation Scheme |          |            |           |
|--------------------|---------|---------|-------|-------------------|----------|------------|-----------|
| Lecture<br>(Hours) | (Hours) | Credits | Hours | Component         | Exam     | Max. Marks | Passing % |
| 3 per week         | -       | 3       | 45    | Lecture           | CCE, ESE | 100        | 35        |

#### **Course Objectives:**

- This course covers the basics of Analytical Chemistry.
- They will understand the importance of analytical science in real-world applications.
- Learn fundamental knowledge of spectrophotometric techniques
- This course enhances scientific understanding and prepares students for industry roles.
- Students will also learn most of the chromatographic techniques and their principles

Course Learning Outcomes: At the end of this course, students will be able to

**CLO1:** Know the importance of Analytical science in the Research & Development of an industry.

CLO2: Operate several analytical instruments within a very short period.

**CLO3:** Understand several analytical data representation techniques.

**CLO4:** Learn the techniques to analyze unknown samples.

**CLO5:** Be familiar with several computer-based data plots.

#### **Syllabus**

| Unit  | Content   | Hours |
|---|---|-------|
| Unit I:<br>Principles, Errors,<br>and Quality<br>Assurance                      | Scope of analytical chemistry, Qualitative and quantitative analysis, Accuracy and precision, Types of errors and their causes; Significant figures, Control charts, Confidence limit, Mean deviation, Standard deviation, Coefficient of variance, Rejection of a result- the Q-test. Good Laboratory Practice (GLP), Standard operating procedures, Quality assurance and quality control, Finding the best straight line-least square regression, correlation coefficient; Calibration curves, Concept of reference material internal standards, | 15    |
| Unit II: Spectrophotometric Methods and Optical Techniques in Chemical Analysis | Properties of light, absorption of light, interaction of light with matter and origin of spectra. The spectrophotometer- calibration, sources of light, monochromators and detectors. Beer's law in chemical analysis, optical rotatory dispersion and circular dichroism, Stoichiometry-method of continuous variation-the Jobs plot, Photometric titrations. Atomic absorption spectroscopy.  | 15    |
| Unit-III: Chromatographic Techniques: Principles, Methods, and Instrumentation  | Principles of chromatography, Classification and mechanism of different chromatographic methods, Paper chromatography, Thin layer chromatography, Column chromatography, High-performance thin-layer chromatography, Fast protein liquid chromatography. High performance liquid chromatography, Gas chromatography, Detectors.   | 15    |

#### **Self-learning topics:**

Unit-I Scope of analytical science and its literature, ways to express accuracy and precision

**Unit-II** sources of light.

**Unit-III** Basic Chromatographic Principles

#### **Reading references:**

- 1. D. A. Skoog; D. M. West; F. J. Holler; S. R. Crouch. *Fundamentals of Analytical Chemistry*. Brooks/Cole Publishing, Belmont. 2013, 9th Ed.
- 2. E. Prichard; V. Barwick. *Analytical Chemistry by Open Learning (Set of 34 Titles)*. Wiley India, New Delhi. 2008, 1st Ed.
- 3. D. A. Ray; Underwood. Quantitative Analysis. Prentice-Hall International Ltd., New Delhi. 1991, 6th Ed.
- 4. G. H. Jeffery; J. Bassett; J. Mendham; R. C. Denny. *Vogel's Textbook of Quantitative Inorganic Analysis*. Longman Scientific & Technical, Essex. 1989, 5th Ed.
- 5. G. D. Christian. *Analytical Chemistry*. John Wiley & Sons Inc., New York. 1994, 6th Ed.
- 6. G. R. Chatwal; S. K. Anand. *Instrumental Methods of Chemical Analysis*. Himalaya Publishing House, Mumbai. 2016, 5th Revised and Enlarged Ed.
- 7. H. H. Willard; L. L. Merritt; J. A. Dean. *Instrumental Methods of Analysis*. Van Nostrand Reinhold, New York. 1974, 5th Ed.

#### and

- H. H. Willard; L. L. Merritt; J. A. Dean. *Instrumental Methods of Analysis*. CBS Publishers, New Delhi. 1986, 6th Ed.
- 8. H. Kaur. Analytical Chemistry. Pragati Prakashan, Meerut. 2021, Paperback Ed.
- 9. D. C. Harris. Quantitative Chemical Analysis. W. H. Freeman and Company, New York. 1998, 5th Ed.
- 10. G. D. Christian. Analytical Chemistry. John Wiley & Sons Inc., New Jersey. 2004, 6th Ed.
- 11. D. A. Skoog. Principles of Instrumental Analysis. Holt Saunders International Edition, New York. 2016, 7th Ed.
- 12. G. W. Ewing. Instrumental Methods of Chemical Analysis. International Student Edition, New York. 1975, 4th Ed.

#### CH4 105: QUANTUM MECHANICS FOR CHEMISTS (L-T-P-C: 3-0-0-3)

| Program: M. Sc. Chemistry | Semester: I                        |
|---------------------------|------------------------------------|
| Course code: CH4 105      | Course name: QUANTUM MECHANICS FOR |
| Course code: CH4 105      | CHEMISTS                           |

| Loctumo    | Practical | Cuadita         | Total | Evaluation Scheme |          |            |           |
|------------|-----------|-----------------|-------|-------------------|----------|------------|-----------|
| Lecture (H | (Hours)   | (Hours) Credits | Hours | Component         | Exam     | Max. Marks | Passing % |
| 3 per week | -         | 3               | 45    | Lecture           | CCE, ESE | 100        | 35        |

#### **Course Objective:** The students will learn

- The different types of mathematical tools can be understood and their applications.
- Postulates of quantum mechanics, Schrödinger equation and its application, Heisenberg Uncertainty principle to understand the basics for quantum chemistry.
- Qualitative treatment of simple harmonic oscillator model of vibrational motion: Vibrational energy of diatomic molecules and zero-point energy to understand the various types of motions and energy in atoms or molecules.
- Chemical bonding to understand the concept about the different kind of chemical bonding and molecular orbital.

**Course Learning Outcomes:** At the end of this course students will be able to

**CLO1:** Remember the concept of different mathematical tools and their applications.

**CLO2:** Understand the concept of postulates of quantum, Schrodinger equation and its application, Heisenberg Uncertainty principle, Pauli exclusion principle to understand the basics.

**CLO3:** Apply the concept on different types of problems such as 1D box, harmonic oscillator, hydrogen atom, etc.

**CLO4:** Analyze the concept to evaluate the eigenvalues and eigenfunction of different molecular structures.

#### **Syllabus**

| Unit   | Content   | Hours |
|--|---|-------|
| Unit I:<br>Linear Vector                             | Linear vector space, Matrix representation of Observables and states, Determination of eigenvalues and eigenstate for observables using matrix representations, rules of  |       |
| Space and<br>Structure of<br>Quantum                 | differentiation, applications of differential calculus, application of integral calculus, Dirac notations of Bra - Ket notation, the postulates of quantum mechanics Operators and observables, operators as matrices, significance of eigenvalues and  | 15    |
| Chemistry  | eigenfunctions, Commutation relations, Uncertainty principle.   |       |
| <b>Unit II:</b> Schrödinger Equation and 1D Problems | The Schrodinger equation to some model system- particle in a box, the Harmonic oscillator, the rigid rotator, the hydrogen atom, Angular momentum: ordinary angular momentum, generalized angular momentum, Eigen functions for angular momentum, eigenvalues of angular momentum, operator using ladder operators.   | 15    |
| <b>Unit-III:</b> Spherically Symmetric Potentials    | Pauli matrices and spinors, Identical particles: Indistinguishability, symmetric and antisymmetric wave functions, incorporation of spin, Pauli exclusion principle. Born-Oppenheimer approximation, VB and MO theory, H <sub>2</sub> +, H <sub>2</sub> molecule problem, Hückel molecular orbital theory and its application to ethylene, butadiene and benzene. Hybridisation and valence MOs of H <sub>2</sub> O, NH <sub>3</sub> and CH <sub>4</sub> . Introduction to the SCF. | 15    |

- 1. P. Tebbutt. *Basic Mathematics for Chemists*. Wiley, New York. 1998, 2nd Ed.
- 2. B. Singh. Mathematics for Chemists. Pragati Prakashan, Meerut. 2015, 1st Ed.
- 3. I. N. Levine. *Quantum Chemistry*. Tata McGraw-Hill Publishing Company Ltd., New Delhi. 2002, 5th Ed.
- 4. A. K. Chandra. Introductory Quantum Chemistry. Tata McGraw-Hill Publishing Company Ltd., New Delhi. 1995, 4th Ed.
- 5. H. C. Verma. *Quantum Physics*. Surva Publications, Ghaziabad. 2009, 2nd Ed.
- 6. P. W. Atkins. *Molecular Quantum Mechanics: An Introduction to Quantum Chemistry*. Clarendon Press, Oxford. 1970, 1st Ed.
- 7. D. A. McQuarrie. Quantum Chemistry. University Science Books, Sausalito. 2007, 2nd Ed.

#### CH4 106: BASIC ORGANIC CHEMISTRY LABORATORY (L-T-P-C: 0-0-8-4)

| Program: M. Sc. Chemistry | Semester: I                          |
|---------------------------|--------------------------------------|
| Course code: CH4 106      | Course name: BASIC ORGANIC CHEMISTRY |
| Course code: Ch4 100      | LABORATORY                           |

| Practical       |            | Cradita | Total | Evaluation Scheme |            |           |    |
|-----------------|------------|---------|-------|-------------------|------------|-----------|----|
| Lecture (Hours) | (Houre)    | Credits | Hours | Component         | Max. Marks | Passing % |    |
| -               | 8 per week | 4       | 120   | Lab               | CCE, ESE   | 100       | 35 |

#### **Course Objectives:**

- To separate and purify mixture of organic acids and bases.
- To understand and apply synthetic planning and experimental execution of one or two step synthesis.
- To characterize the organic compounds by use of various analytical techniques like IR, NMR and mass.

#### **Course Learning Outcomes:** At the end of this course, students will be able to

- **CLO1:** Describe the separation and purification techniques used in organic synthesis.
- **CLO2:** Illustrate the experimental techniques for one or two step synthesis.
- **CLO3:** Apply chromatographic techniques in monitoring and analyzing reaction progress.
- **CLO4:** Evaluate the analytical techniques line IR and NMR for characterization of products.

#### **Syllabus**

| Sr. No. | Name of the Experiment  | Hours |
|---------|---|-------|
| 1       | To Separate components mixtures (nitrophenols, amines, carboxylic acids, and watersoluble substances) | 12    |
| 2       | To synthesize and characterize of m-dinitrobenzene by nitration method                                | 12    |
| 3       | To synthesize and characterize Benzanilide by benzoylation process                                    | 12    |
| 4       | To preparation and characterize pyridinium salt   | 12    |
| 5       | To prepare and characterize Methyl orange by Diazotization  | 12    |
| 6       | To prepare and characterize aldol condensation product by reaction with benzaldehyde and acetophenone | 12    |
| 7       | To prepare and characterize dibenzalacetone   | 12    |
| 8       | To prepare and characterize benzyl alcohol from benzaldehyde by sodium borohydride                    | 12    |
| 9       | To synthesize and characterize phenylacetic acid by hydrolysis of Benzyl cyanide                      | 12    |
| 10      | To prepare and characterize benzoic acid by oxidation of benzaldehyde                                 | 12    |

- 1. I. Vogel; B. S. Furniss. *Vogel's Textbook of Practical Organic Chemistry*. Longman Scientific & Technical, Essex. 1989, 5th Ed.
- 2. F. G. Mann; B. C. Saunders. Practical Organic Chemistry. Longman Scientific & Technical, London. 1960, 4th Ed.
- 3. N. K. Vishnoi. Advanced Practical Organic Chemistry. Vikas Publishing House, New Delhi. 2010, 3rd Ed.
- 4. R. K. Bansal. Laboratory Manual of Organic Chemistry. New Age International Publishers, New Delhi. 1983, 5th Ed.

#### CH4 107: INORGANIC CHEMISTRY LABORATORY (L-T-P-C: 0-0-8-4)

| Program: M. Sc. Chemistry | Semester: I                                 |
|---------------------------|---|
| Course code: CH4 107      | Course name: INORGANIC CHEMISTRY LABORATORY |

| Lastuma            | Practical  | Cuadita | Total |           | Evaluation |            |           |
|--------------------|------------|---------|-------|-----------|------------|------------|-----------|
| Lecture<br>(Hours) | (Hours)    | Credits | Hours | Component | Exam       | Max. Marks | Passing % |
| -                  | 8 per week | 4       | 120   | Lab       | CCE, ESE   | 100        | 35        |

#### Course Objectives: The laboratory course focuses on

- Quantitative analysis by gravimetric method
- Emphasize the principles of different redox titrimetric analyses like a) mermanganometry, b) dichrometry, c) iodometry

#### Course Learning Outcomes: At the end of this course students will be able to

**CLO1:** Demonstrate practical execution of redox titrimetric estimations of different metal ions based on a)

Permanganometry, b) Dichoromatometry, c) Iodometry

**CLO2:** Estimation of different ions based on complexometric EDTA titration.

**CLO3:** Determination of different metal ions quantitively by Gravimetric estimation.

**CLO4:** Separation of different ions in a mixture like brass or Dolomite by volumetric estimation

#### **Syllabus**

| Sr. No. | Name of the Experiment   | Hours |
|---------|--|-------|
| 1.      | Estimation of Fe(II) in a given solution (Permanganometry). Estimation of Fe(II) with K <sub>2</sub> Cr <sub>2</sub> O(dichromatometry/dichrometry).                             | 15    |
| 2.      | Estimation of Cu(II) in a solution (Iodometry). Estimation of total hardness of water using EDTA by complexometric method  | 15    |
| 3.      | Estimate the amount of magnesium present per liter of the given solution of magnesium sulfate  To determine the percentage of iron in hematite ore                               | 15    |
| 4.      | To estimate the mass of nickel in the whole of the given nickel ammonium sulfate solution  | 15    |
| 5.      | Synthesis and analysis of 3d metal complexes. Synthesis and analysis of rare earth metal complexes   | 15    |
| 6.      | Gravimetric estimation of Cu from a mixture of Cu and Fe solution. Gravimetric determination of Fe in Fe and Cr solution. Gravimetric determination of Ni in Cu and Ni solution. | 15    |
| 7.      | Volumetric estimation of Cu in Cu and Ni (German silver). Volumetric estimation of Ca and Mg in Dolomite solution.   | 15    |
| 8.      | Volumetric estimation of Fe in Cu and Fe solution. Volumetric estimation of Zn in Brass Volumetric estimation of Ni in Ni and Zn solution.                                       | 15    |

- 1. G. H. Jeffery; J. Bassett; J. Mendham; R. C. Denny. *Vogel's Textbook of Quantitative Chemical Analysis*. Longman Scientific & Technical, Essex. 1989, 5th Ed.
- 2. G. Svehla. *Vogel's Textbook of Macro and Semimicro Qualitative Inorganic Analysis*. Orient Longman, Hyderabad. 1982, 5th Ed.

## SEMESTER II SYLLABUS WITH COURSE LEARNING OUTCOME (CLO)

#### CH4 204: ORGANIC CHEMISTRY-II REACTIONS, REAGENTS AND REARRANGEMENTS (L-T-P-C: 3-0-0-3)

| Program: M. Sc. Chemistry | Semester: II                            |
|---------------------------|---|
| Course code: CH4 201      | Course name: ORGANIC CHEMISTRY-II       |
|                           | REACTIONS, REAGENTS, AND REARRANGEMENTS |

| Locture            | Practical | Cwadita | Total |           | Evaluation | n Scheme   |           |
|--------------------|-----------|---------|-------|-----------|------------|------------|-----------|
| Lecture<br>(Hours) | (Hours)   | Credits | Hours | Component | Exam       | Max. Marks | Passing % |
| 3 per week         | -         | 3       | 45    | Lecture   | CCE, ESE   | 100        | 35        |

#### **Course Objectives:**

- Develop a mechanistic understanding of redox processes
- Explore the reactivity and synthetic utility of organometallic and selective reagents
- Analyze diverse organic rearrangements and reaction pathways

#### **Course Learning Outcomes:** At the end of this course, students will be able to:

**CLO1**: Explain the mechanisms and stereochemical aspects of organic reactions, including addition, elimination, oxidation, and reduction.

**CLO2:** Analyze molecular rearrangements and their significance in synthetic organic chemistry.

**CLO3**: Identify and describe the synthesis, chemical reactions, and properties of heterocyclic compounds.

**CLO4**: Apply knowledge of reaction mechanisms and heterocyclic chemistry to solve complex problems in organic synthesis.

**CLO5**: Evaluate the applications of heterocyclic compounds in pharmaceuticals, agrochemicals, and materials science.

| Unit                         | Content  | Hours |
|------------------------------|--|-------|
| Unit I:                      | Fundamentals of Redox Reactions in Organic Chemistry: Electron transfer vs.                                  | 15    |
| Organic                      | hydride transfer vs. atom transfer; Redox potential and selectivity; <b>Mechanistic</b>                      |       |
| Reaction                     | Insights: Electron flow (arrow-pushing); Stereoselectivity and   |       |
| Mechanisms                   | chemo/regioselectivity; Transition states, intermediates, catalytic cycles                                   |       |
| <ul><li>Oxidations</li></ul> | Oxidation Mechanisms:  |       |
| and                          | <b>Alcohols</b> → <b>Aldehydes/Ketones/Acids</b> : PCC, PDC, Dess-Martin, Swern, Jones,                      |       |
| Reductions                   | KMnO <sub>4</sub> , TEMPO; <b>Alkenes and Alkynes</b> : Epoxidation (m-CPBA, peracids),                      |       |
|                              | Dihydroxylation (OsO <sub>4</sub> , KMnO <sub>4</sub> ), Oxidative cleavage (ozonolysis, KMnO <sub>4</sub> ) |       |
|                              | Reduction Mechanisms:  |       |
|                              | Carbonyl compounds: NaBH <sub>4</sub> , LiAlH <sub>4</sub> , DIBAL-H; Reductive amination, Birch             |       |
|                              | reduction, Clemmensen, Wolff-Kishner; <b>Selective reductions</b> : Rosenmund,                               |       |
|                              | Lindlar, Meerwein Ponndorf-Verley  |       |
|                              | Asymmetric Oxidations and Reductions (Brief Introduction):   |       |
|                              | Sharpless epoxidation, Corey–Bakshi–Shibata (CBS) reduction  |       |
| Unit II:                     | Classification of reagents; about air and moisture sensitive reagents; handling,                             | 15    |
| Reagents in                  | storage and precaution. Reagent role in stepwise mechanism; Stereocontrol and                                |       |
| Organic                      | functional group compatibility; Concept of functional group interconversion                                  |       |
| Synthesis                    | (FGI); Chemoselectivity, regioselectivity, and protecting group strategies                                   |       |
|                              | Organometallic Reagents: Grignard, organolithium, organocuprates, Gilman                                     |       |
|                              | reagents Applications in C-C bond formation; Transition-metal catalysts (Pd, Ru,                             |       |
|                              | Rh) and other cross-coupling reagents  |       |
|                              | <b>Hypervalent iodine reagents-</b> Various types of hypervalent iodine reagents and                         |       |
|                              | their preparation; application in organic transformation, selectivity, sensitivity                           |       |
|                              | and reactivity; Peptide couplingreagents and their applications. Functional                                  |       |

|                | <b>group protecting agents</b> – Different types of protecting/masking agents;        |    |  |  |  |
|----------------|---|----|--|--|--|
|                | Selective and Protective Reagents: Silyl protecting groups (TBDMS, TMS),              |    |  |  |  |
|                | Acetals, Carbamates, PMP protection and their deprotection after completion of        |    |  |  |  |
|                | reaction; <b>Electrophilic halogenating agents</b> (NBS, NCS), sulfonation, acylation |    |  |  |  |
|                | reagents.   |    |  |  |  |
|                | Phase-transfer Catalysts  |    |  |  |  |
| Unit III:      | Intramolecular vs. Intermolecular; Pericyclic, ionic, and radical pathways;           | 15 |  |  |  |
| Molecular      | Rearrangement vs. Isomerization; Importance of Rearrangements in installation         |    |  |  |  |
| Rearrangements | of Stereocenters and importance of conformational aspects in this regard              |    |  |  |  |
|                | Rearrangements Involving Carbocations:  |    |  |  |  |
|                | Wagner-Meerwein, Pinacol-Pinacolone, Tiffeneau-Demjanov                               |    |  |  |  |
|                | Benzilic acid and related 1,2-shifts  |    |  |  |  |
|                | Rearrangements Involving Carbanions and Ylides:                                       |    |  |  |  |
|                | Favorskii, Wittig, Stevens, Sommelet-Hauser, Ireland-Claisen                          |    |  |  |  |
|                | Rearrangements Involving Nitrenes:  |    |  |  |  |
|                | Curtius, Hofmann, Lossen, Schmidt, Beckmann   |    |  |  |  |
|                | Pericyclic Rearrangements (Concerted):  |    |  |  |  |
|                | Cope and Claisen rearrangements; Aza–Claisen, Oxy–Cope, Sigmatropic shifts            |    |  |  |  |
|                | Oxidative Rearrangements:   |    |  |  |  |
|                | Baeyer-Villiger, Dienone-Phenol rearrangement   |    |  |  |  |

- 1. R. K. Mackie; D. M. Smith; R. A. Aitken. *Guidebook to Organic Synthesis*. Addison-Wesley Longman Ltd., Harlow. 1990, 2nd Ed.
- 2. H. O. House. *Modern Synthetic Reactions*. W. A. Benjamin, Menlo Park. 1972, 2nd Ed.
- 3. M. B. Smith. *Organic Synthesis*. Editorial Staff, Boca Raton. 2016, 4th Ed.
- 4. S. N. Sanyal. Reactions, Rearrangements, and Reagents. Bharti Bhawan Publishers, Patna. 2020, 4th Ed.
- 5. F. A. Carey; R. J. Sundberg. *Advanced Organic Chemistry: Part A Structure & Mechanism*. Springer, New York. 2007, 5th Ed.
- 6. R. K. Bansal. *Heterocycles*. New Age International Publishers, New Delhi. 2022, 7th Ed.
- 7. I. L. Finar. Organic Chemistry Vol. I & II. ELBS Publication, London. 2002, 5th Ed.
- 8. M. C. Ray. Reaction Mechanisms in Organic Chemistry. MTG Learning Media, New Delhi. 2021, Revised Ed.
- 9. J. J. Li. Name Reactions. Springer, New York. 2018, 4th Ed.
- 10. C. M. Rojas. Molecular Rearrangements in Organic Synthesis. Wiley, Hoboken. 2015, 1st Ed.
- 11. R. K. Bansal. Organic Reaction Mechanisms. New Age International, New Delhi. 2012, 4th Ed.
- 12. J. March. Advanced Organic Chemistry. Wiley India Pvt. Ltd., New Delhi. 2007, 6th Ed.
- 13. L. M. Harwood. Advanced Organic Chemistry. Oxford University Press, Oxford. 1992, 1st Ed.
- 14. P. S. Kalsi. Organic Reactions and Their Mechanisms. New Age International, New Delhi. 2020, 3rd Ed.
- 15. R. M. Acheson. *An Introduction to the Chemistry of Heterocyclic Compounds*. Wiley Student Edition, New York. 2008, 3rd Ed.
- 16. J. A. Joule; K. Mills. *Heterocyclic Chemistry*. Wiley, Chichester. 2010, 5th Ed.
- 17. T. L. Gilchrist. Heterocyclic Chemistry. Pearson Education, Harlow. 2005, 3rd Ed.
- 18. R. R. Gupta; M. Kumar; V. Gupta. Heterocyclic Chemistry. Springer, Berlin. 1998, 1st Ed.

## CH4 202: INORGANIC CHEMISTRY-II MAIN GROUP AND ORGANOMETALLIC COMPOUNDS (L-T-P-C: 3-0-0-3)

| Program: M. Sc. Chemistry | Semester: II                            |
|---------------------------|---|
| Course code: CH4 202      | Course name: INORGANIC CHEMISTRY-II     |
|                           | MAIN GROUP AND ORGANOMETALLIC COMPOUNDS |

| Lockwa             | Practical | Cuadita | Total |           | Evaluation | n Scheme   |           |
|--------------------|-----------|---------|-------|-----------|------------|------------|-----------|
| Lecture<br>(Hours) | (Houre)   | Credits | Hours | Component | Exam       | Max. Marks | Passing % |
| 3 per week         | -         | 3       | 45    | Lecture   | CCE, ESE   | 100        | 35        |

#### **Course Description:**

- This course deals with the understanding of different periodic properties and periodic anomalies.
- This course provides a detailed study of s- and p-block group elements. This course also focuses on EAN rule and various Carbonyl, nitrosyl metal complexes.

Course Learning Outcomes: At the end of this course students will be able to

**CL01:** Define periodic properties and anomalies

**CLO2:** Elaborate discussion of s &p-block group (1-2 &13-18) elements **CLO3:** Calculate the EAN value of different organometallic compounds

CLO4: Summarize bonding, structure and property of different carbonyl-nitrosyl compounds

| Units                                       | Content   | Hours |
|---|---|-------|
| Unit I: Periodic trends, structure, bonding | Periodic Trend: Radius, Ionization enthalpy, electron gain enthalpy, electronegativity. Relativistic effects on chemical properties. Hydrogen and its compounds: H-bond and its influence on the structure and properties of crystals Hydrides, classification: electron deficient, electron precise and electron rich hydrides. Concept of ortho and para hydrogen, Alkali and alkaline earth metals: Solutions in liquid ammonia - Synthesis, properties, uses and structures of crown ether complexes, <b>Group 13 elements:</b> Borides, borates, boron halides, boranes, carboranes and metallocarboranes, BN compounds, transition-metal stabilized borylene and boryllithium, organoaluminum compounds, Lewis Base adducts of AlR3 compounds, Subvalent organo-Al compounds, Organo-gallium, -indium, and -thallium compounds. <b>Group 14 elements:</b> Allotropes of Carbon- C60 and its compounds (fullerenes) - carbon nanotubes: synthesis and properties - Intercalation compounds of graphite - Pure Silicon, silica and silicates, Silicones - Low coordinated and hypervalent Silicon compounds - Brief survey of Ge, Sn, and Pb chemistry- Organo-germanium, -tin, and -lead compounds <b>Group 15 elements:</b> P(V) compounds (structure, bonding, reactivity)-P(III) compounds: diphosphenes, phosphaalkenes, iminophosphanes - P-containing ring systems (phosphabenzene, phosphole), phosphazenes, Oxo-acids of Phosphrous. Comparison of basicity, reducing property of oxoacids. <b>Group 16 elements:</b> Sulfurpolycationic and anionic species - SN compounds. | 15    |
| Unit II:                                    | Group 17 elements: Charge-transfer complexes of halogens, inter-halogen   | 15    |
| Halogens and                                | compounds, halogen oxides and oxygen fluorides, pseudo halogens. <b>Group 18</b>  |       |
| Nobel gases                                 | <b>elements:</b> Physical properties and reactivity, Xenon compounds: preparation,  |       |
|   | bonding and structure, noble gas clathrates   |       |

| Unit III:      | Organometallic Chemistry: Complexes with pi-acceptor and sigma-donor             | 15 |
|----------------|--|----|
| Metal carbonyl | ligands - 16 electron and 18 electron rules- Stability and Reactivity - Isolobal |    |
| and nitrosyl   | analogy, synergic effect, preparation, Structure, and property and bonding of    |    |
| complexes      | carbonyl and nitrosyl compounds, evidence for multiple bonds in Carbonyl         |    |
| •              | compounds, nature of bonding, stretching frequency and ligand effect, Roussin's  |    |
|                | salt- Metal carbenes and metal carbynes, Ferrocene.                              |    |

#### **Reading references:**

- 1. A. G. Massey. Main Group Chemistry. Wiley, Chichester. 2000, 2nd Ed.
- 2. N. N. Greenwood; A. Earnshaw. Chemistry of the Elements. Pergamon Press, Oxford. 1989, 1st Ed.
- 3. P. Atkins; T. Overton; J. Rourke; M. Weller; F. Armstrong. *Shriver and Atkins' Inorganic Chemistry*. W. H. Freeman and Company, New York. 2009, 5th Ed.

or

- D. F. Shriver; P. W. Atkins. Inorganic Chemistry. W. H. Freeman and Company, New York. 1999, 3rd Ed.
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- 5. F. A. Cotton; G. Wilkinson. *Advanced Inorganic Chemistry*. John Wiley & Sons, New York. 1988, 5th Ed.
  - F. A. Cotton; C. A. Murillo; M. Bochmann; R. N. Grimes. *Advanced Inorganic Chemistry*. John Wiley & Sons, New York. 1999, 6th Ed.
- 6. J. E. Huheey; E. A. Keiter; R. L. Keiter. *Inorganic Chemistry: Principles of Structure and Reactivity*. Prentice Hall, New Jersey. 1997, 4th Ed.

#### CH4 203: PHYSICAL CHEMISTRY-II: SURFACE AND INTERFACIAL CHEMISTRY (L-T-P-C: 3-0-0-3)

| Program: M.Sc. Chemistry | Semester: II                       |
|--------------------------|------------------------------------|
| Course code: CH4 203     | Course name: PHYSICAL CHEMISTRY-II |
|                          | SURFACE AND INTERFACIAL CHEMISTRY  |

| Lostuno            | Practical Cradita |         | Total | Evaluation Scheme |          |            |           |
|--------------------|-------------------|---------|-------|-------------------|----------|------------|-----------|
| Lecture<br>(Hours) | (Hours)           | Credits | Hours | Component         | Exam     | Max. Marks | Passing % |
| 3 per week         | -                 | 3       | 45    | Lecture           | CCE, ESE | 100        | 35        |

#### **Course Objectives:**

- Understand the principles of surface and interfacial phenomena.
- · Apply electrochemical theories and models,
- Evaluate the mechanisms of heterogeneous surface reactions.
- Gain familiarity with modern characterization techniques

#### Course Learning Outcomes: At the end of this course students will be able to

**CLO1**: Explain the fundamental principles of surface interactions, including adsorption, surface energy, and surface phenomena, and their role in chemical and physical processes.

**CLO2**: Apply surface science concepts to analyze and solve problems in catalysis, material design, and energy systems.

**CLO3:** Apply electrochemical concepts to analyze and solve problems related to energy storage systems, corrosion, and industrial electrochemical applications.

**CLO4:** Explain the fundamental principles of catalysis, including reaction mechanisms, catalyst types, and factors influencing catalytic efficiency.

| Units  | Content  | Hours |
|--|--|-------|
| Unit I:<br>Surface Sciences                          | Adsorption – surface tension, capillary action pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, Langmuir and Freundlich Adsorption Isotherms, estimation of surface area (BET equation), surface films on liquids (Electro-kinetic phenomenon), Catalytic activity at surfaces. Micelles- Surface active agents, classification of surface-active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC),  | 15    |
|  | factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization-phase separation, solubilisation, micro emulsion, reverse micelles. Industrial relevance in cosmetics, food science, and detergents.  |       |
| Unit II: Electrochemical Interfaces and Applications | Electrochemistry of solutions. Debye-Hückel-Onsager treatment and its extension, ion-solvent interactions, Debye-Hückel-Jerum model. Thermodynamics of electrified interface equations, derivation of electro-capillarity, Lippmann equations (surface excess), methods of determination. Structure of electrified interfaces- Guoy-Chappman, Stern, Graham-Devanathan-Mottwatts models. Polarography theory- Ilkovic equation, half-wave potential, and its significance. Introduction to corrosion, homogeneous theory, forms of corrosion monitoring, and prevention methods. Introduction to Electrochemical Sensors and Biosensors, concepts of amperometric, potentiometric, and voltammetric sensors. | 15    |
| Unit III:<br>Heterogeneous<br>Catalysis              | Mechanism of surface reactions. Surface heterogeneity, activity and selectivity, deactivation, and regeneration. Theories of promotion and poisoning of catalysts. Zeolites and zeolite-like materials, Common synthesis. Characterization of catalysts: Surface area, pore size distribution (mercury porosimetry) Thermal methods (DTA, TG, TPD, and TPR), Surface acidity, DRIFTS, Photoelectron spectroscopy (XPS, AES, XRF, LEED, Mossbauer spectroscopy, SIMS, Scanning Tunnelling Microscopy (STM), Atomic  | 15    |

| Force Microscopy (AFM). Catalysis in Green Chemistry and Sustainability. Nano- |  |
|--|--|
| catalysis: Role of Particle Size, Shape, and Support Effects at the Nanoscale  |  |

- 1. M. J. Schick. *Non-ionic Surfactants*. Surfactant Science Series, Marcel Dekker, New York. 1985, Vol. 72.
- 2. P. Ghosh. *Colloids and Interface Science*. PHI Learning Pvt. Ltd., New Delhi. 2009, 1st Ed.
- 3. M. J. Rosen. Surfactants and Interfacial Phenomena. John Wiley & Sons, New Jersey. 2004, 3rd Ed.
- 4. M. R. Porter. Handbook of Surfactants. Chapman and Hall, London. 1994, 2nd Ed.
- 5. A. W. Adamson. *Physical Chemistry of Surfaces*. John Wiley & Sons, New York. 1997, 6th Ed.
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- 7. A. Tager. *Physical Chemistry of Polymers*. Mir Publishers, Moscow. 1978, 1st Ed.
- 8. H. S. Harned; B. B. Owen. The Physical Chemistry of Electrolytic Solutions. Reinhold Publishing, New York. 1950, 1st Ed.
- 9. S. Glasstone. *Textbook of Physical Chemistry*. Macmillan Publishers, London. 1948, 2nd Ed.

#### CH4 204: BIOORGANIC CHEMISTRY (L-T-P-C: 3-0-0-3)

| Program: M. Sc. Chemistry | Semester: II                      |
|---------------------------|-----------------------------------|
| Course Code: CH4 204      | Course name: BIOORGANIC CHEMISTRY |

| Locture            | Practical Cradita |         | Total | Evaluation Scheme |          |            |           |
|--------------------|-------------------|---------|-------|-------------------|----------|------------|-----------|
| Lecture<br>(Hours) | (Hours)           | Credits | Hours | Component         | Exam     | Max. Marks | Passing % |
| 3 per week         | -                 | 3       | 45    | Lecture           | CCE, ESE | 100        | 35        |

#### **Course Objectives:**

- To understanding the role of biological molecules used in daily life.
- To know and analyze the structure and function of proteins and carbohydrates.
- To discuss the structure, synthesis and application of nucleic acids, lipids and enzymes.

#### Course Learning Outcomes: At the end of this course, students will be able to

**CLO1:** Understand the structure and classification of proteins, lipids, carbohydrates and nucleic acid.

**CLO2:** Learn various structural determination techniques of biomolecules.

**CLO3:** Apply the knowledge of biomolecules in the progression of diseases.

**CLO4:** Demonstrate the role of biomolecules in drug discovery and development.

| Units                                   | Content  | Hours |
|---|--|-------|
| Unit I:<br>Protein and<br>Carbohydrates | Peptides and Proteins: Building blocks to the Quaternary structure of proteins, structure-stabilizing interactions in secondary structures. $\alpha$ -helix, $\beta$ -sheets, secondary structures, triple helix structure of collagen. Tertiary structure of protein-folding and domain structure, Peptidomimetics, Carbohydrates: Classification and structure of simple and complex carbohydrates. Structure and function of the most important carbohydrates Structural polysaccharides-cellulose and chitin. Storage polysaccharides-starch and glycogen. Structure and biological function of glucosaminoglycans or mucopolysaccharides.   | 15    |
| Unit II:<br>Nucleic Acids and<br>Lipids | <b>Nucleic Acids:</b> Detailed Structure of nucleic acids, Different types of DNA, the double helix model of DNA, and forces responsible for holding it. Chemical and enzymatic hydrolysis of nucleic acids. Chemical synthesis of mono and trinucleosides. The chemical basis for heredity, an overview of replication of DNA, transcription, translation, and genetic code, Nucleic Acids as Therapeutic Targets. <b>Lipids:</b> Classification, chemical structure, and biological functions of lipids, glycerol phospholipids, sphingolipids, cholesterol, bile acids, prostaglandins, Lipoproteins-composition and function, role in atherosclerosis. Properties of lipid aggregates-micelles, bilayers, liposomes, and their possible biological function. | 15    |
| Unit III: Enzymes                       | Enzymes, Coenzymes, enzyme-kinetics, metalloenzymes, applications of enzymes in organic synthesis, enzyme-models and applications. Enzyme-catalyzed carboxylation and decarboxylation reactions. Enzyme inhibition and drug design, Molecular recognition, chiral recognition, crown ethers, cryptands, host-guest chemistry.  | 15    |

#### **Reading references:**

Indrashil University

- 1. L. Lehninger. *Principles of Biochemistry*. Worth Publishers, New York. 2007, 7th Ed.
- 2. L. Stryer. Biochemistry. W. H. Freeman and Company, New York. 2019, 5th Ed.
- 3. D. Voet; J. G. Voet. Biochemistry. John Wiley & Sons, New York. 2010, 3rd Ed.
- 4. J. L. David; J. Rawn. Biochemistry. Neil Patterson Publishers, North Carolina. 1989, International Ed.
- 5. E. E. Conn; P. K. Stumpf. Outlines of Biochemistry. John Wiley & Sons, New York. 2006, 5th Ed.
- 6. T. Palmer. *Understanding Enzymes*. Prentice Hall, London. 1995, 2nd Ed.
- 7. C. H. Collins; J. Suckling. Enzyme Chemistry: Impact and Applications. Chapman and Hall, London. 1990, 2nd Ed.
- 8. U. Satyanarayana; U. Chakrapani. Essentials of Biochemistry. Elsevier Health Sciences, New Delhi. 2021, 3rd Ed.
- 9. R. K. Murray; V. W. Rodwell; D. Bender; K. M. Botham; P. A. Weil; P. J. Kennelly. *Harper's Illustrated Biochemistry*. McGraw Hill Professional, New York. 2009, 28th Ed.

#### CH4 205: SPECTROSCOPY-I: MOLECULAR STRUCTURE ELUCIDATION (L-T-P-C: 3-0-0-3)

| <b>Program:</b> M. Sc. Chemistry | Semester: II                           |
|----------------------------------|--|
| Course Code: CH4 205             | Course name: SPECTROSCOPY-I: MOLECULAR |
|                                  | STRUCTURE ELUCIDATION                  |

| Locture            | Practical Cradita |         | Total | Evaluation Scheme |          |            |           |
|--------------------|-------------------|---------|-------|-------------------|----------|------------|-----------|
| Lecture<br>(Hours) | (Hours)           | Credits | Hours | Component         | Exam     | Max. Marks | Passing % |
| 3 per week         | -                 | 3       | 45    | Lecture           | CCE, ESE | 100        | 35        |

#### **Course Description:**

**Understand the principles, instrumentation, and interpretive strategies** of UV-Vis, IR, NMR (<sup>1</sup>H and <sup>13</sup>C), and mass spectrometry

Correlate spectral data with molecular structure and functional groups

Apply spectroscopic techniques to differentiate isomers, elucidate structures, and analyze mixtures

Course Learning Outcomes: At the end of this course students will be able to

CLO1: Remember the basic concept of Vibrational, UV, IR, 1H and Mass spectroscopy

**CLO2:** Understand the concept of vibrational frequency in IR, chemical shift in NMR, fragmentation pattern in Mass spectrometry

**CLO3:** Apply the knowledge for structure elucidation of organic compounds.

**CLO4:** Analyze the UV, IR, 1H NMR and Mass spectra

| Units        | Content   | Hours |
|--------------|---|-------|
| Unit I:      | UV, and IR Spectroscopy -   | 15    |
| UV and IR    | UV Spectroscopy: Origin of electronic spectra, Lambert-Beer's absorption law,   |       |
| Spectroscopy | Types of electronic transitions. Principle of UV spectroscopy and instrumentation.  |       |
|              | Effect of solvent, substituent, and conjugation on electronic transitions. Factors  |       |
|              | affecting the position and intensity of bands and $\lambda$ max, Chromophores and   |       |
|              | auxochromes, Benzene and its substituted derivatives. Applications of UV-visible  |       |
|              | spectroscopy in analysis (qualitative/quantitative) of polyenes/aromatic (hetero &  |       |
|              | homo) systems, geometrical isomers, keto-enol tautomer's, components of a   |       |
|              | mixture. Woodward-Fieser rules for calculating absorption maximum in dienes, trienes, α, β-unsaturated carbonyl compounds and aromatic compounds. |       |
|              | Application of UV spectroscopy  |       |
|              | IR Spectroscopy: Instrumentation–sources-sampling techniques. Factors   |       |
|              | influencing IR spectroscopy, Characteristic vibrational frequencies of alkanes,   |       |
|              | alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines.   |       |
|              | Detailed study of vibrational frequencies of carbonyl compounds (ketones,   |       |
|              | aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated  |       |
|              | carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational   |       |
|              | frequencies, overtones, combination bands and Fermi resonance. Differentiation of   |       |
|              | compounds/isomers by IR. Application of IR spectroscopy and limitations.  |       |
| Unit II:     | IH NMR Spectroscopy: Introduction, Definition, Chemical shift and factor affecting  | 15    |
| NMR          | chemical shift, spin-spin interaction, shielding and deshielding mechanism,   |       |
| Spectroscopy | mechanism of measurement, chemical shift values and correlation for protons   |       |
|              | bonded to carbon (aliphatic, olefinic, carbonyl and aromatic) and other nuclei  |       |
|              | (alcohols, phenols, enols, carboxylic acids, amines, amides & mercapto), coupling   |       |
|              | constants – vicinal, geminal, long range and virtual couplings, Intensity of signal   |       |
|              | (Peak area or integration) the effect of deuteration, complex spin-spin interaction   |       |
|              | between two, three nuclei. Stereochemistry, hindered rotation, Karplus curve  |       |
|              | variation of coupling constant with dihedral angle.   |       |

|              | <sup>13</sup> C NMR Spectroscopy: <sup>13</sup> C NMR, introduction to FT technique, relaxation phenomena, NOE effects, <sup>1</sup> H and <sup>13</sup> C chemical shifts to structure correlations. Chemical shift and (Aliphatic, olefinic, Alkyne, Aromatic, Heteroaromatic and carbonyl carbon), Coupling constants. To identify structure from <sup>13</sup> C NMR data; Use of <sup>13</sup> C spectra in differentiating compounds/isomers. Difference between <sup>1</sup> H NMR and <sup>13</sup> C NMR |    |
|--------------|---|----|
| Unit III:    | Mass Spectrometry - Origin of mass spectrum, principles of EI mass spectrometer-  | 15 |
| Mass         | Instrumentation. Preliminary account of chemical ionization, Types of fragments:  |    |
| Spectrometry | odd electron and even electron containing neutral and charged species (even   |    |
|              | electron rule, Nitrogen rule, isotopic peaks, metastable ion peaks, determination of  |    |
|              | molecular formula and High-resolution mass spectrometry. Salient features of the  |    |
|              | fragmentation pattern of organic compounds- α-cleavage, β cleavage, McLafferty  |    |
|              | rearrangement, the Fragmentation pattern of individual heterocyclic systems viz.,   |    |
|              | Furan, Pyrrole, Thiophene and Pyridine.   |    |

- 1. C. N. Banwell; E. M. McCash. *Fundamentals of Molecular Spectroscopy*. McGraw-Hill Education, New Delhi. 2011, 4th Ed.
- 2. G. Aruldhas. Molecular Structure and Spectroscopy. Prentice Hall of India, New Delhi. 2004, 2nd Ed.
- 3. R. M. Silverstein; F. X. Webster; D. J. Kiemle; D. L. Bryce. *Spectroscopic Identification of Organic Compounds*. John Wiley & Sons, New York. 2014, 8th Ed.
- 4. Y. R. Sharma. Elementary Organic Spectroscopy. S. Chand & Company Ltd., New Delhi. 2007, Revised Ed.
- 5. R. Kakkar. Atomic and Molecular Spectroscopy. Cambridge University Press, Cambridge. 2015, 1st Ed.
- 6. W. Kemp. *Organic Spectroscopy*. Macmillan, London. 1994, 3rd Ed.
- 7. D. H. Williams; I. Fleming. Spectroscopic Methods in Organic Chemistry. McGraw-Hill Education, London. 1995, 5th Ed.
- 8. A. B. Derome. Modern NMR Techniques for Chemistry Research. Pergamon Press, Oxford. 1987, Reprinted Ed.
- 9. D. L. Pavia. Introduction to Organic Spectroscopy. Cengage India Pvt. Ltd., New Delhi. 2015, 5th Ed.
- 10. G. C. Levy; O. L. Nelson. Carbon-13 NMR for Organic Chemists. Wiley, New York. 1980, 2nd Ed.
  - Atta-ur-Rahman. Nuclear Magnetic Resonance: Basic Principles. Springer-Verlag, New York. 2011, 1st Ed.
- 11. P. S. Kalsi. *Spectroscopy of Organic Compounds*. New Age International Pvt. Ltd., New Delhi. 2020, 8th Ed.

#### CH4 206: ANALYTICAL TECHNIQUES LABORATORY (L-T-P-C: 0-0-8-4)

| Program: M. Sc. Chemistry | Semester: II                                  |
|---------------------------|---|
| Course code: CH4 206      | Course name: ANALYTICAL TECHNIQUES LABORATORY |

| Lecture<br>(Hours) | Practical  | Cuadita | Total | Evaluation Scheme |          |            |           |
|--------------------|------------|---------|-------|-------------------|----------|------------|-----------|
|                    | (Haure)    | Credits | Hours | Component         | Exam     | Max. Marks | Passing % |
| -                  | 8 per week | 4       | 120   | Lab               | CCE, ESE | 100        | 35        |

#### **Course Objectives:**

- To understand and learn analytical techniques in biochemical studies.
- To separate and identify biomolecules such as amino acids, carbohydrates, and proteins.
- To determine the iodine value of lipids
- To determine the concentration of biomolecules in tea and coffee

#### **Course Learning Outcomes:** At the end of this course students will be able to

**CLO1:** Demonstrate proficiency in techniques for the separation and identification of biomolecules, including amino acids and sugars.

CLO2: Quantify biomolecules using standard methods like Anthrone and Lowry's techniques.

**CLO3:** Evaluate lipid properties through determination of iodine and acetyl numbers.

**CLO4:** Analyze organic compounds using spectroscopic methods, including UV-visible and IR spectroscopy.

**CLO5:** Compare and interpret shifts in electronic absorption spectra under varying chemical conditions.

| Sr. No. | Name of the Experiment  | Hours |
|---------|---|-------|
| 1       | Determination of Isoelectronic point (PI) of Amino acid by titration method.  | 8     |
| 2       | Characterize mono- and disaccharides by recrystallization, solubility, melting points, and crystal morphology.  | 8     |
| 3       | Estimation of total sugar in biological samples using the Anthrone method involving spectrophotometric detection.   | 8     |
| 4       | Estimation of amino acids using Ninhydrin-Anthrone method involving colorimetric analysis.  | 8     |
| 5       | Estimation of protein by Lowery's method  | 8     |
| 6       | Determination of Iodine number and acetyl number of Lipid molecules.  | 8     |
| 7       | Separation of amino acids by paper chromatography   | 8     |
| 8       | Study the bathochromic shift of p-nitrophenol in UV-Vis spectra under alkaline vs. neutral conditions to assess pH-dependent resonance effects.                           | 8     |
| 9       | Study the hypsochromic shift in aniline by comparing its UV-Vis spectra in neutral and acidic media.  | 8     |
| 10      | Compare IR spectra of acetone and benzophenone to distinguish aliphatic and aromatic ketones based on key vibrations.   | 8     |
| 11      | Comparative IR Analysis of Aromatic and aliphatic Nitro compounds, Amines, Nitriles and Amides  | 8     |
| 12      | Analyze unknown organic samples to identify alcohols, acids, amines, or esters based on diagnostic IR bands   | 8     |
| 13      | UV-Vis Spectrophotometric Analysis of caffeine and benzoic acid in soft drinks via Beer's Law.  | 8     |
| 14      | Assign $^{1}\mathrm{H}$ NMR peaks of common compounds using chemical shift, splitting, and integration with software or spectra.  | 8     |
| 15      | Record and analyze spectra of complexes like [Cu(NH <sub>3</sub> ) <sub>4</sub> ] <sup>2+</sup> or [Fe(SCN)] <sup>2+</sup> to observe d-d transitions and ligand effects. | 8     |

- 1. R. Katoch. Analytical Techniques in Biochemistry and Molecular Biology. Springer, New York. 2011, 1st Ed.
- 2. H. Martin. Basic Methods for the Biochemical Lab. Springer, Berlin. 2007, 1st Ed.
- 3. K. Wilson; J. Walker. *Principles and Techniques in Biochemistry and Molecular Biology*. Cambridge University Press, Cambridge. 2010, 7th Ed.
- 4. J. A. A. Chambers; D. Rickwood. Biochemistry Lab Fax. Blackwell Science, Oxford. 1993, 1st Ed.
- 5. T. S. Work; E. Work. *Laboratory Techniques in Biochemistry and Molecular Biology, Vol. I & II.* North-Holland Publishing Company, Amsterdam. 1970, 1st Ed.
- 6. R. K. Bansal. Practical Organic Chemistry. New Age International Pvt. Ltd., New Delhi. 2008, 5th Ed.
- 7. D. Field; S. Sternhell; J. R. Kalman. Organic Structures from Spectra. John Wiley & Sons Ltd., Chichester. 2008, 4th Ed.
- 8. F. G. Mann; B. C. Saunders. Practical Organic Chemistry. Pearson Education India, New Delhi. 2009, 4th Ed.
- 9. W. Kemp. *Organic Spectroscopy*. Macmillan, London. 1994, 3rd Ed.
- 10. P. S. Kalsi. Spectroscopy of Organic Compounds. New Age International Publishers, New Delhi. 2007, 6th Ed.
- 11. Y. R. Sharma. *Elementary Organic Spectroscopy Principles and Chemical Applications*. S. Chand & Company Ltd., New Delhi. 1992, 5th Ed.

#### CH4 207: PHYSICAL CHEMISTRY LABORATORY (L-T-P-C: 0-0-8-4)

| Program: M. Sc. Chemistry | Semester: II                               |
|---------------------------|--|
| Course code: CH4 207      | Course name: PHYSICAL CHEMISTRY LABORATORY |

| Lastures           | Practical  | Credite Total |       | Evaluation Scheme |          |            |           |
|--------------------|------------|---------------|-------|-------------------|----------|------------|-----------|
| Lecture<br>(Hours) | [ [Houre)  | Credits       | Hours | Component         | Exam     | Max. Marks | Passing % |
| -                  | 8 per week | 4             | 120   | Lab               | CCE, ESE | 100        | 35        |

#### **Course Objectives:**

- **Develop proficiency in measurement techniques**, including conductometry, potentiometry, viscometry, polarimetry, and pH-metry,
- Apply experimental methods to determine key physical and chemical constants, such as rate constants, activation energies, dissociation constants, solubility products, redox potentials, and molecular weights.
- **Analyze thermodynamic and kinetic behavior** of systems involving acid-base equilibria, micellization, protein denaturation, complex formation, and polymer solutions through laboratory investigations.
- **Interpret experimental data using modern instrumental techniques** and relate them to theoretical models in physical chemistry.

**Course Learning Outcomes:** At the end of this course, students will be able to

**CLO1:** Learn the science of buffer preparation, highlighting the theories of ionic equilibrium

**CLO2:** Perform experiments to determine reaction rates and rate constants for chemical reactions using appropriate laboratory techniques.

**CLO3:** Conduct equilibrium experiments to determine equilibrium constants and verify Le Chatelier's principle

**CLO4:** Learn graph plotting and data interpretation.

**CLO5:** Demonstrate proficiency in laboratory practices, including accurate measurements, data recording, and safety protocols

| Sr. No. | Name of the Experiment   | Hours |  |  |  |
|---------|--|-------|--|--|--|
| 1       | Conductometric Determination of the Percentage Composition of Strong and Weak Acids in a Mixture   |       |  |  |  |
| 2       | Conductometric Determination of the Rate Constant and Activation Energy for the Hydrolysis of Methyl Acetate   | 8     |  |  |  |
| 3       | To determine the relative strengths of the given strong acids by studying the kinetics of inversion of cane sugar using the polarimetric method.   | 8     |  |  |  |
| 4       | Determination of the Viscosity Average Molecular Weight of a Polymer Using Ostwald's Viscometer  | 8     |  |  |  |
| 5       | To determine the Redox potential of Fe2+/Fe3+ system by potentiometric method. (pH metry) Or, Potentiometric Determination of KCl and KI Concentrations in a Mixture Using Standard AgNO <sub>3</sub> Solution | 8     |  |  |  |
| 6       | Potentiometric Determination of the Strength of an Unknown Silver Nitrate (AgNO <sub>3</sub> ) Solution  | 8     |  |  |  |
| 7       | pH-Metric Determination of the Dissociation Constants (pK <sub>1</sub> and pK <sub>2</sub> ) of a Dibasic Acid   | 8     |  |  |  |
| 8       | Conductometric Determination of the Solubility Product (Ksp) of Barium Sulfate and Silver Chloride.  |       |  |  |  |
| 9       | Potentiometric Determination of the Dissociation Constants of Monobasic Acids: Acetic Acid, Benzoic Acid, and Salicylic Acid   | 8     |  |  |  |
| 10      | Kinetic study of the esterification of an alcohol by NMR Spectroscopy. (Chemical kinetics)   | 8     |  |  |  |

| 11 | Determination of Critical Micelle Concentration (CMC) and Thermodynamics of              | 8 |
|----|--|---|
|    | Micellization  |   |
| 12 | Thermodynamic Study of Protein Denaturation  | 8 |
| 13 | Determination of the equilibrium constant for the formation of tri-iodide ion. (Chemical | 8 |
|    | equilibrium)   |   |
| 14 | Determination of the Thermodynamic Parameters and Equilibrium Constant of a Complex      | 8 |
|    | Formation Reaction   |   |
| 15 | Conductometric Determination of the Critical Micelle Concentration (CMC) of Sodium       | 8 |
|    | Dodecyl Sulfate (SDS)  |   |

- 1. B. D. Khosla; V. C. Garg. Senior Practical Physical Chemistry. R. Chand & Co., New Delhi. 2018, 18th Ed.
- 2. B. Viswanathan; P. S. Raghavan. *Practical Physical Chemistry*. Viva Books Pvt. Ltd., Navi Mumbai. 2017, 1st Ed.
- 3. A. K. Nad; B. Mahapatra; A. Ghoshal. *An Advanced Course in Practical Chemistry*. New Central Book Agency Pvt. Ltd., Kolkata. 2012, 3rd Ed.
- 4. J. N. Gurtu; A. Gurtu. Advanced Physical Chemistry Experiments. Pragati Prakashan, Meerut. 2008, 1st Ed.

#### **SEMESTER III**

## SYLLABUS WITH COURSE LEARNING OUTCOME (CLO) CH5 AN101: ANALYTICAL CHEMISTRY II: PHARMACEUTICAL ANALYSIS AND MEASUREMENTS (L- T-P-C: 3-0-0-3)

| Program: M. Sc. Chemistry (Analytical) | Semester: III                            |
|--|--|
| Course code: CH5 AN101                 | Course name: ANALYTICAL CHEMISTRY II:    |
|  | PHARMACEUTICAL ANALYSIS AND MEASUREMENTS |

| Lockwas            | Practical Credite |         | Total | Evaluation Scheme |          |            |           |
|--------------------|-------------------|---------|-------|-------------------|----------|------------|-----------|
| Lecture<br>(Hours) | (Hours)           | Credits | Hours | Component         | Exam     | Max. Marks | Passing % |
| 3 per week         | -                 | 3       | 45    | Lecture           | CCE, ESE | 100        | 35        |

#### **Course Objectives:**

- Introduction to the basics of Analytical Chemistry.
- Understanding the importance and applications of analytical science.
- In-depth study of fundamental spectrophotometric techniques.
- Enhancement of scientific knowledge relevant to industrial applications.
- Introduction to and understanding of major Chromatographic techniques.

**Course Learning Outcomes:** At the end of this course, students will be able to

**CLO1:** Know the importance of Analytical science in the Research & Development of an industry.

**CLO2:** Operate several analytical instruments within a very short period.

CLO3: Understand several analytical data representation techniques.

**CLO4:** Unknown sample determination techniques.

**CLO5:** Be familiar with several computer-based data plots.

| Units   | Content   | Hours |
|---|---|-------|
| Unit I:<br>Automation in<br>Measurements                      | Principles of automation, automatic and automated devices, Process control: off-line, at-line, and on-line analysis. Continuous and discrete analyzer's, feedback mechanism. Flow injection analysis, principles, dispersion coefficient, factors affecting peak height-sample volume, channel length, flow rate, and channel geometry. Applications of FIA, stopped-flow measurements, and gradient FIA.   | 15    |
| Unit II:<br>Food Analysis and<br>Pharmaceutical<br>Analysis   | Introduction to food analysis, regulations and international standards related to food analysis, nutritional labelling, sample and sample preparation. Compositional analysis of foods for moisture, proteins, fat, fibres, ash, vitamins and minerals. Adulteration of fats and oils; milk and milk products. Heavy metal ion analysis in pharmaceuticals. Importance of UV-Visible spectrophotometry, IR spectroscopy and HPLC with UV, fluorescence and photodiode array detection in pharmaceutical industry. | 15    |
| Unit III: Analysis of Pesticides, Detergents, and Fertilizers | Analysis of pesticides, soaps and detergents, fertilizers: Classification of pesticides. Analysis of different pesticides by classical and instrumental methods. Classification of soaps and detergents with suitable examples. Characterization of soaps and detergents. Types of fertilizers and analysis of different elements like, nitrogen, phosphates, calcium, sodium, potassium, and ammonia.  | 15    |

#### **Self-learning topics:**

**Unit I:** Several instrumental detail with their working principle

Unit II: Heavy metal ion analysis in pharmaceuticals

**Unit III:** Soap and Detergents

#### **Reference Books:**

- 1. G. D. Christian. Analytical Chemistry. John Wiley & Sons Inc., New Jersey. 2007, 6th Ed.
- 2. D. A. Skoog. Principles of Instrumental Analysis. Holt-Saunders International Edition, New York. 2016, 7th Ed.
- 3. J. Martinez Calatayud. *Flow Injection Analysis of Pharmaceuticals: Automation in the Laboratory*. Taylor & Francis, London. 1996, 1st Ed.
- 4. S. S. Nielsen. Food Analysis. Springer, New York. 2003, 3rd Ed.
- 5. S. S. Nielsen. *Food Analysis Laboratory Manual*. Springer, New York. 2003, 3rd Ed.
- 6. P. D. Sethi. Quantitative Analysis of Drugs in Pharmaceutical Formulation. CBS Publishers, New Delhi. 2008, 3rd Ed.
- 7. S. Ahuja; S. Scypinski. *Handbook of Modern Pharmaceutical Analysis*. Academic Press, San Diego. 2001, Vol. 3.
- 8. F. J. Welcher. *Standard Methods of Chemical Analysis, Vols. 1, 2 & 3, Part Two*. Van Nostrand Reinhold Company, New York. 1917, 6th Ed.

#### CH5 102: ANALYTICAL CHEMISTRY III: ELECTROANALYTICAL TECHNIQUES (L-T-P-C: 3-0-0-3)

| Program: M. Sc. Chemistry | Semester: III  |
|---------------------------|--|
| Course code: CH5 AN102    | Course name: ANALYTICAL CHEMISTRY-III: ELECTROANALYTICAL |
|                           | TECHNIQUES   |

| Lockwas            | Practical Credite |         | Total | Evaluation Scheme |          |            |           |
|--------------------|-------------------|---------|-------|-------------------|----------|------------|-----------|
| Lecture<br>(Hours) | (Hours)           | Credits | Hours | Component         | Exam     | Max. Marks | Passing % |
| 3 per week         | -                 | 3       | 45    | Lecture           | CCE, ESE | 100        | 35        |

#### **Course Objectives:**

- Understanding of different electrogravimetric analyses.
- Explains the principles of potentiometry, voltammetry, Polarography, and Cyclic Voltammetry.
- Delivers the idea about different kinds of electrodes used in different techniques

Course Learning Outcomes: At the end of this course students will be able to

**CLO1:** State different techniques used for electrogravimetry analysis

**CLO2:** Summarize the working principle of different techniques.

CLO3: Identify the different types of electrodes used in different techniques

**CLO4:** Analyze different electroanalytical titration used for the separation method.

#### **Syllabus**

| Units           | Content   | Hours |
|-----------------|---|-------|
| Unit I:         | Basic revision of electrochemistry, Idea about electrode, working principal of different      | 15    |
| Electrochemical | electrode: SHE, reference electrode, glass electrode, type-I/II electrode, saturated          |       |
| measurements    | calomel electrode, advantages and disadvantages of different electrode, gravimetric           |       |
|                 | analysis, classification: precipitation, volatilization, electroanalytical, extraction and    |       |
|                 | chromatographic method, determination of ions by gravimetric method, Faraday's law of         |       |
|                 | electrolysis, electrogravimetry: principle and instrumentation, method: constant current      |       |
|                 | electrolysis, constant potential electrolysis, determination of Cu ion by electrogravimetry.  |       |
| Unit II:        | Fundamentals, indicator and ion-selective electrodes, Instrumentation, types of               | 15    |
| Potentiometry,  | potentiometric titration: acid-base, redox, complexometric and precipitation                  |       |
| Voltammetry,    | titration, determination of end point. Voltammetry: principle, instrumentation,               |       |
| Polarography    | voltammogram, Randles-Sevick equation, modified voltammetry, cyclic voltammetry,              |       |
|                 | quantitative applications of voltammetry. Polarography: introduction, principle,              |       |
|                 | ILKOVIC Equation & instrumentation, construction and working of dropping mercury              |       |
|                 | electrode, application of polarography  |       |
| Unit III:       | Coulometry: Introduction: principles, instrumentation, coulometry at constant                 | 15    |
| Coulometry      | current and controlled potential, coulometric titration, advantages of coulometric titration, |       |
|                 | applications.   |       |

- 1. P. T. Kissinger; W. R. Heineman. *Laboratory Techniques in Electroanalytical Chemistry*. Marcel Dekker Inc., New York. 1996, 2nd Ed.
- 2. B. H. Vassos; G. W. Ewing. Electroanalytical Chemistry. John Wiley & Sons, New York. 1983, 1st Ed.
- 3. A. J. Bard; L. R. Faulkner. *Electrochemical Methods Fundamentals and Applications*. John Wiley & Sons, New York. 2001, 2nd Ed.
- 4. D. C. Harris. Quantitative Chemical Analysis. W. H. Freeman and Company, New York. 2015, 9th Ed.
- 5. I. M. Kolthoff; P. J. Elving. Treatise on Analytical Chemistry. Wiley-Interscience, New York. 1968, 1st Ed.
- 6. B. R. Eggins. Chemical Sensors and Biosensors. John Wiley & Sons, New York. 2002, 1st Ed.

#### CH5 AN103: ANALYTICAL CHEMISTRY IV: QA QC VALIDATION (L-T-P-C: 3-0-0-3)

| Program: M. Sc. Chemistry | Semester: III  |
|---------------------------|--|
| Course code: CH5 AN103    | Course name: ANALYTICAL CHEMISTRY-IV: QUALITY MEASUREMENTS IN ANALYSIS |

| Lecture<br>(Hours) | Practical |         | Total | Evaluation Scheme |          |            |           |
|--------------------|-----------|---------|-------|-------------------|----------|------------|-----------|
|                    | (Haure)   | Credits | Hours | Component         | Exam     | Max. Marks | Passing % |
| 3 per week         | -         | 3       | 45    | Lecture           | CCE, ESE | 100        | 35        |

#### **Course Objectives:**

- Detailed understanding of Quality Assurance (QA) and Quality Control (QC) in Analytical Chemistry.
- Gaining insight into the importance of accuracy, precision, and quality control in analytical science.
- Understanding the importance and use of reference materials.
- Introduction to the basics of analytical method development and validation.
- Preparation for roles in the analytical division of industries, especially pharmaceutical companies.

Course Learning Outcomes: At the end of this course, students will be able to

**CLO1:** Explain the significance of quality control and assurance.

**CLO2:** Understand the operating procedures of analytical

**CLO3:** Analyze analytical data and their interpretation.

**CLO4:** Demonstrate quantitative determination of the given sample using various techniques.

| Units  | Content  | Hours |
|--|--|-------|
| Unit I: Quality Assurance and Quality Control              | Quality Assurance and Quality Control: Industrial Analysis: Quality characteristics of chemical analysis, errors occurring at the start, during or by the end of the analysis, Shewhart Chart, CUSUM chart and EWMA chart; Batch and process evaluation, QA schemes, experimental designs for optimization studies and ruggedness testing, system management.  Clinical Analysis: Introduction, analytical responsibilities, Managerial responsibilities, practical approaches to QA, characterization of a method, Results, and preparation of reports. Internal QC, Accuracy and external quality assessment, near-patient testing, and QC.  Water Industry: Water quality field sampling QA/QC program, QA/QC documentation, QA project plan, designing a water quality monitoring plan, Site selection, sampling frequency and sample size, cost considerations, training of field personnel, field trip preparations, Water quality sampling, toxic chemicals in bottom sampling and biota, bacterial sample collection, sequential triplicate sampling, sample handling, preservation, storage and transport, chain of custody, field safety, field audit program. | 15    |
| <b>Unit II:</b><br>Reference<br>Materials                  | <b>Reference Materials:</b> Analytical standards, primary and secondary standards, high purity substances, reference materials, use of RMs in statistical control schemes and in intercomparisons, the role of certified reference materials (CRMs), production and requirements, obtaining reference value and certified value.   | 15    |
| Unit III: Development and validation of Analytical Methods | <b>Development and validation of Analytical Methods:</b> Analytical method development: Theory and factors affecting resolution separation factor (selectivity), retention factor (capacity factor), and column efficiency). Selecting the HPLC separation mode (reversed phase, normal phase etc.) Selecting the most appropriate detector Gradient/isocratic operation, selecting the column for analysis, Selecting   | 15    |

| and optimizing the mobile phase, the effect of pH, considering pKa of the analytic |  |
|--|--|
| Requirements for a stability-indicating analytical method                          |  |

#### **Self-learning topics:**

Unit-I Shewhart Chart, CUSUM chart, and EWMA chart

**Unit-II** High-purity substances

Unit-III Introduction to ICH guidelines: ICH Q2(R1)

- 1. D. A. Skoog; D. M. West; F. J. Holler. *Fundamentals of Analytical Chemistry*. Saunders College Publishing, Philadelphia. 1991, 2nd Ed.
- 2. R. A. Day; A. L. Underwood. Quantitative Analysis. Prentice-Hall of India Pvt. Ltd., New Delhi. 1993, 6th Ed.
- 3. I. A. Fowlis. Gas Chromatography. Analytical Chemistry Series, Open Book Learning, Oxford. 1995, 2nd Ed.
- 4. L. Hargis. *Analytical Chemistry: Principles and Techniques*. Pearson Education, New Delhi. 1988, Facsimile Ed.
- 5. S. Ahuja; S. Scypinski. *Handbook of Modern Pharmaceutical Analysis, Vol. 3.* Academic Press, San Diego. 2001, 1st Ed.
- 6. F. J. Welcher. *Standard Methods of Chemical Analysis, Vols. 1, 2 & 3.* Van Nostrand Reinhold Company, New York. 1963, 6th Ed.

#### CH5 104: SPECTROSCOPY II: ADVANCED NMR AND MOLECULAR SPECTROSCOPY (L-T-P-C: 3-0-0-3)

| Program: M. Sc. Chemistry | Semester: III                           |
|---------------------------|---|
| Course code: CH5 104      | Course name: SPECTROSCOPY II            |
|                           | ADVANCED NMR AND MOLECULAR SPECTROSCOPY |

| Locture            | Practical Cradita |         | Total | Evaluation Scheme |          |            |           |
|--------------------|-------------------|---------|-------|-------------------|----------|------------|-----------|
| Lecture<br>(Hours) | (Hours)           | Credits | Hours | Component         | Exam     | Max. Marks | Passing % |
| 3 per week         | -                 | 3       | 45    | Lecture           | CCE, ESE | 100        | 35        |

#### **Course Objectives:**

- Students will learn the basic Principles of NMR, <sup>13</sup>C NMR, Raman, and Mössbauer spectroscopy.
- Student will learn the Interpretation of first-order and second-order NMR spectra and methods for their simplification.
- The course will cover the analysis and structure elucidation of organic compounds using 2D NMR techniques.
- Students will learn the fundamentals and applications of rotational and vibrational Raman spectra and mössbauer spectroscopy in chemical analysis.

Course Learning Outcomes: At the end of this course, students will be able to

**CLO1:** Remember the basic concept of  ${}^{1}$ H and  ${}^{13}$ C, Raman and Mossbauer spectroscopy

**CLO2:** Understand the concept of first and second-order spectra

**CLO3:** Apply the knowledge for the structure elucidation of an organic compound.

**CLO4:** Analyze the <sup>1</sup>H, <sup>13</sup>C NMR, and IR spectra of organic compounds

| Units   | Content  | Hours |
|---|--|-------|
| Unit I:<br>Proton NMR<br>Spectroscopy               | IH NMR Spectroscopy -Pople notation and spin assignments; chemical shift equivalence and magnetic equivalence; Differences between first order and Second order effects, examples of AB, AX, A2X2, AX2, AA'XX', AMC and ABX systems,  Simplification of second order spectrum: selective decoupling, use of chemical shift reagents for stereochemical assignments, Proton exchange, Deuterium exchange, Nuclear Overhauser Effect (NOE); Differentiation of compounds/ isomers by PMR; To identify structure from PMR data, Study of dynamic processes by VT NMR, restricted rotation (DMF, DMA, biphenyls, annulenes), cyclohexane ring inversion, degenerate rearrangements (bullvalene and related systems).   | 15    |
| Unit II:<br>Carbon NMR<br>Spectroscopy              | <sup>13</sup> C NMR Spectroscopy- To identify structure from <sup>13</sup> C NMR data; Use of <sup>13</sup> C spectra in differentiating compounds/isomers; 2D NMR Spectroscopy: Theory and Principles of 2D NMR Spectroscopy (COSY); two-dimensional NMR spectroscopy. COSY, HMBC, HMQC, NOESY.  Editing techniques: INEPT and DEPT methods, Time scale- Multinuclear, Introduction to NMR of nuclei other than proton and carbon   | 15    |
| Unit III:<br>Raman and<br>Mossbauer<br>Spectroscopy | Raman spectroscopy- Quantum theory of Raman effect, Classical theory of Raman effect, Pure rotational Raman spectra, Raman activity of vibrations, Vibrational Raman spectra, polarization of light and Raman effect, applications., Mutual exclusion principle Mossbauer Spectroscopy: Basic principles, spectral parameters and spectrum display. Application of the technique to the studies of (1) bonding and structures of Fe+2 and Fe+3 compounds including those of intermediate spin, (2) Sn+2 and Sn+4 compounds- nature of M-L bond, coordination number, structure and detection of oxidation state and in equivalent MB atoms.  Raman spectroscopy- Quantum theory of Raman effect, Classical theory of Raman effect, Pure rotational Raman spectra, Raman activity of vibrations, Vibrational Raman spectra, | 15    |

polarisation of light and Raman effect, applications., Mutual exclusion principle **Mossbauer Spectroscopy:** Basic principles, spectral parameters and spectrum display. Application of the technique to the studies of (1) bonding and structures of Fe<sup>+2</sup> and Fe<sup>+3</sup> compounds, including those of intermediate spin, (2) Sn<sup>+2</sup> and Sn<sup>+4</sup> compounds- nature of M-L bond, coordination number, structure and detection of oxidation state and in equivalent MB atoms.

- 1. R. M. Silverstein; G. C. Bassler; T. C. Morrill. *Spectrometric Identification of Organic Compounds*. John Wiley & Sons, New York. 1991, 5th Ed.
- 2. R. J. Abraham; J. Fisher; P. Loftus. Introduction to NMR Spectroscopy. Wiley, Chichester. 1992, 1st Ed.
- 3. J. R. Dyer. Application of Spectroscopy of Organic Compounds. Prentice Hall, Englewood Cliffs, N.J. 1965, 1st Ed.
- 4. D. H. Williams; I. Fleming. *Spectroscopic Methods in Organic Chemistry*. Tata McGraw-Hill, New Delhi. 1968, 7th Ed.
- 5. J. L. McHale. *Molecular Spectroscopy*. CRC Press, Boca Raton. 2017, 2nd Ed.
- 6. D. L. Pavia. Introduction to Organic Spectroscopy. Cengage India Pvt. Ltd., New Delhi. 2015, 5th Ed.
- 7. D. N. S. Narayana. *Handbook of Molecular Spectroscopy*. J. K. International Publishers, New Delhi. 2015, 1st Ed.
- 8. Y. R. Sharma. Elementary Organic Spectroscopy. S. Chand & Company Ltd., New Delhi. 2007, Revised Ed.
- 9. D. A. Skoog. Principles of Instrumental Analysis. Holt Saunders International Edition, New York. 2016, 7th Ed.
- 10. R. Kakkar. *Atomic and Molecular Spectroscopy*. Cambridge University Press, Cambridge. 2015, 1st Ed.

#### CH5 105: SPECTROSCOPY ANALYSIS & DATA INTERPRETATION LABORATORY (L-T-P-C: 0-0-8-4)

| Program: M. Sc. Chemistry (Analytical) | Semester: III   |
|--|---|
| Course code: CH5 105                   | Course name: SPECTROSCOPY ANALYSIS & DATA INTERPRETATION LABORATORY |

| Loctura            | Practical  | Con dita Total |       | Evaluation Scheme |          |            |           |
|--------------------|------------|----------------|-------|-------------------|----------|------------|-----------|
| Lecture<br>(Hours) | (Hours)    | Credits        | Hours | Component         | Exam     | Max. Marks | Passing % |
| -                  | 8 per week | 4              | 120   | Lab               | CCE, ESE | 100        | 35        |

#### **Course Objectives:**

- The objective of the practical course is to make students understand the spectral analysis of various organic compounds which are synthesized in laboratory and chemical industries.
- Students will also learn various software used in analysis of data in NMR and IR spectroscopy.
- Students will learn structural prediction and confirmation of compounds through their spectral analysis.

Course Learning Outcomes: At the end of this course students will be able to

**CLO1:** Understand the analysis of  ${}^{1}\text{H}$  and  ${}^{13}\text{C-NMR}$  spectra with analysis

**CLO2:** Explain the IR spectra analysis for functional group determination

**CLO3:** Apply the knowledge of spectral analysis in structural characterization

**CLO4:** Demonstrate the application of software for NMR analysis

| Sr. No. | Name of the Experiment  | Hours |
|---------|---|-------|
| 1       | Solving structure elucidation problems using multiple spectroscopic data sheets (NMR, MS, IR, and UV-Vis) on at least 20 examples. The elucidation of the chemical structure based on the given spectroscopic data. Students will first calculate the Double bond equivalence based on the given chemical formula. Then, the structural prediction will be made using the provided spectroscopic data (UV, IR, PMR, CMR, and Mass spectra). | 40    |
| 2       | Determination of the Effect of alkaline and acidic media on the organic compound using UV-Vis spectroscopy. For example, Determination Bathochromic shift in Alkaline medium of p-Nitrophenol Compared to p-Nitrophenol. Determination of Hypsochromic shift in acidic medium of Aniline compared to Aniline.   | 20    |
| 3       | Recording the I.R. Spectrum of Different Organic Compounds  (i) Aliphatic and aromatic alcohols.  (ii) Aliphatic and aromatic carbonyl compounds (aldehydes, ketones, esters, and acids, etc.)  Aromatic and aliphatic Nitro, Amines, Nitriles, alkenes, alkynes, and Amides.   | 30    |
| 4       | Use of computer techniques  (i) Chem Draw, Chemsketch, ISIS Draw, Pymol calculations, and MestrecSoftwares operations.  (ii) Draw the Structure of Simple aliphatic, aromatic, and heterocyclic compounds in ChemDraw with different substituents. Get the correct IUPAC Name and predict the <sup>1</sup> H-NMR Spectra.   | 30    |

- 1. R. K. Bansal. Practical Organic Chemistry. New Age International Pvt. Ltd., New Delhi. 2008, 5th Ed.
- 2. D. Field; S. Sternhell; J. R. Kalman. *Organic Structures from Spectra*. John Wiley & Sons Ltd., Chichester. 2008, 4th Ed.
- 3. F. G. Mann; B. C. Saunders. *Practical Organic Chemistry*. Pearson Education India, New Delhi. 2009, 4th Ed.
- 4. W. Kemp. *Organic Spectroscopy*. Macmillan, London. 1994, 3rd Ed.
- 5. P. S. Kalsi. *Spectroscopy of Organic Compounds*. New Age International Pvt. Ltd., New Delhi. 2020, 8th Ed.
- 6. Y. R. Sharma. *Elementary Organic Spectroscopy Principles and Chemical Applications*. S. Chand & Company Ltd., New Delhi. 1992, 5th Ed.

#### CH5 AN106: ANALYTICAL CHEMISTRY LABORATORY (L-T-P-C: 0-0-8-4)

| Program: M. Sc. Chemistry (Analytical) | Semester: III                                |
|--|--|
| Course code: CH5 AN106                 | Course name: ANALYTICAL CHEMISTRY LABORATORY |

| I a at             | Practical  | Constitute Total |       | Evaluation Scheme |          |            |           |
|--------------------|------------|------------------|-------|-------------------|----------|------------|-----------|
| Lecture<br>(Hours) | (Hours)    | Credits          | Hours | Component         | Exam     | Max. Marks | Passing % |
| -                  | 8 per week | 4                | 120   | Lab               | CCE, ESE | 100        | 35        |

#### **Course Objectives:**

- Develop proficiency in classical and instrumental analytical techniques
- Determine acid dissociation constants (pKa), complex stability constants, and electrochemical parameters
- Gain hands-on experience in modern analytical methodologies

Course Learning Outcomes: At the end of this course, students will be able to

**CLO1:** Understand the potentiometric analysis of chemical compounds **CLO2:** Explain the use of pH meter in sample analysis of acid and base

**CLO3:** Apply the knowledge of conductometry in analysis of metal complexes **CLO4:** Demonstrate the application of polarography and electrogravimetry

| Sr. No. | Name of the Experiment  | Hours |
|---------|---|-------|
| 1       | Determination of carbonate and bicarbonate in a mixture by acid-base titration  | 8     |
| 2       | Determination of pKa values of: (i) Ethylenediamine, (ii) Glycine, (iii) Histidine  | 8     |
| 3       | Determination of binary stability constants: (i) Cu(II)-en, (ii) Ni(II)-His, (iii) Ni(II)-  | 8     |
|         | Gly systems   |       |
| 4       | Determination of stability constant for ternary o-Phen-Ni(II)-His complex   | 8     |
| 5       | Conductometric determination of complex composition: Cu(II)-oxine and Cu(II)-   | 8     |
|         | EDTA  |       |
| 6       | Conductometric analysis of pyrophosphate interaction with Mg <sup>2+</sup> , Ca <sup>2+</sup> , Mn <sup>2+</sup> , and Cu <sup>2+</sup> | 8     |
| 7       | Estimation of aspirin using KOH titration with pH or conductometric end-point   | 8     |
| 8       | Ion-selective electrode (ISE) method for fluoride estimation in water   | 8     |
| 9       | Ion-selective electrode (ISE) method for nitrate determination in water   | 8     |
| 10      | Ion-selective electrode (ISE) method for ammonia estimation in water  | 8     |
| 11      | Determination of E½ values of Cd <sup>2+</sup> and Pb <sup>2+</sup> by DC polarography  | 8     |
| 12      | Verification of the Ilkovic equation using Cd <sup>2+</sup> solution  | 8     |
| 13      | Determination of stability constants of Cd <sup>2+</sup> and Pb <sup>2+</sup> complexes via polarographic                               | 8     |
|         | measurements  |       |
| 14      | Electrogravimetric determination of copper and nickel individually  | 8     |
| 15      | Simultaneous electrogravimetric determination of Cu and Ni in a mixture   | 8     |

- 1. J. H. Kennedy. *Analytical Chemistry Practice*. Saunders College Publishing, Philadelphia. 1990, 2nd Ed.
- 2. J. Mendham. Vogel's Textbook of Quantitative Chemical Analysis. Pearson Education, New Delhi. 2002, 6th Ed.
- 3. A. I. Vogel. A Textbook of Quantitative Inorganic Analysis. ELBS Publication, London. 1969, 3rd Ed.
- 4. A. E. Martell; R. J. Motekaitis. *Determination and Use of Stability Constants*. VCH Publishers Inc., New York. 1988, 2nd Ed.
- 5. A. E. Martell; R. D. Hancock. *Metal Complexes in Aqueous Solutions*. Plenum Press, New York. 1996, 1st Ed.
- 6. G. D. Christian. *Analytical Chemistry*. John Wiley & Sons Inc., New York. 1994, 6th Ed.

#### CH5 EAN1: SEPARATION METHODS (L-T-P-C: 2-0-0-2)

| Program: M. Sc. Chemistry | Semester: III                   |
|---------------------------|---------------------------------|
| Course code: CH5 EAN1     | Course name: SEPARATION METHODS |

| Lockwas            | Practical Condition |         | Total |           | Evaluation Scheme |            |           |  |  |
|--------------------|---------------------|---------|-------|-----------|-------------------|------------|-----------|--|--|
| Lecture<br>(Hours) | (Houre)             | Credits | Hours | Component | Exam              | Max. Marks | Passing % |  |  |
| 2 per week         | -                   | 2       | 30    | Lecture   | CCE, ESE          | 50         | 18        |  |  |

#### **Course Objectives:**

- Understand the principles and mechanisms of solvent extraction and chromatographic techniques
- Explore the use of organic reagents in inorganic analysis
- Gain theoretical insight into advanced separation techniques

Course Learning Outcomes: At the end of this course students will be able to

**CLO1:** Explain the role of partition coefficient in solvent extraction

CLO2: Classify various solvent systems for extraction of natural and synthetic products

**CLO3:** Apply the knowledge in recovery and recycling of solvents

**CLO4:** Demonstrate the working principle of supercritical fluid extraction

| Units    | Content  | Hours |
|----------|--|-------|
| Unit I:  | <b>Solvent Extractions:</b> The distribution coefficient, distribution ratio, relation between KD& | 15    |
|          | D, and the percent extracted. Solvent extraction of metals – ion association complexes, metal      |       |
|          | chelates, the effect of pH and reagent concentration, the extraction process, separation           |       |
|          | efficiency of metal chelates, analytical separations – multiple counter current distribution,      |       |
|          | solid phase extraction, solvent extraction of flow injection analysis. Supercritical fluid         |       |
|          | extraction. Organic reagents in Inorganic analysis: Theoretical basis for the use of organic       |       |
|          | reagents in inorganic analysis. Extraction of metal ions by the use of organic reagents –          |       |
|          | acetylacetone, thionyl-trifluoro acetone, tri-n-octyl phosphine oxide. Applications to             |       |
|          | extractions of metal ions by chelating agent (Dithizone, 8-hydroxy quinoline, and cupferron)       |       |
|          | Determination of salts of organic acids and bases, determination of alkaloids in crude drugs       |       |
| Unit II: | <b>Supercritical Fluid chromatography (SFC) and Electrophoresis:</b> Instrumentation of SFC        |       |
|          | stationary and mobile phases used in SFC, Detectors, Advantages of SFC. Technique and              | 15    |
|          | applications of SFC. Size Exclusion Chromatography: Principle of Gel Chromatography,               |       |
|          | Filtration Chromatography, Instrumentation, retention behavior, resolution, selection of gel       |       |
|          | type – applications. Ion Exclusion – Principle and applications. Ultra-Performance Liquid          |       |
|          | Chromatography: Principle, Instrumentation   |       |
|          | <b>Electrophoresis:</b> Introduction, Definition Paper Electrophoresis: Principle, Experimental    |       |
|          | Requirements, Technique, Factors governing the migration of ions, Applications Capillary           |       |
|          | Electrophoresis: Electro osmotic flow, migration in CE, instrumentation, control of                |       |
|          | separation, applications Gel Electrophoresis: Principle, technique, applications Immuno            |       |
|          | electrophoresis: Principle, technique, applications.   |       |

- 1. M. N. Sastri. *Separation Methods*. Himalaya Publishing House, Mumbai. 1991, 1st Ed.
- 2. D. A. Skoog; F. J. Holler; T. A. Nieman. *Principles of Instrumental Analysis*. Harcourt College Publishers, Orlando. 1998, 5th Ed.
- 3. G. D. Christian. *Analytical Chemistry*. John Wiley & Sons Inc., New York. 1994, 6th Ed.
- 4. R. A. W. Johnstone; M. E. Rose. *Mass Spectrometry for Chemists and Biochemists*. Cambridge University Press, Cambridge. 1996, 2nd Ed.
- 5. E. A. V. Ebsworth; D. W. H. Rankin; S. Cradock. *Structural Methods in Inorganic Chemistry*. ELBS Publications, London. 1988, 2nd Ed.
- 6. R. P. W. Scott. *Introduction to Analytical Gas Chromatography*. Marcel Dekker Inc., New York. 1988, 2nd Ed.

#### CH5 EAN4: APPLIED ANALYSIS AND GREEN ANALYTICAL CHEMISTRY (L-T-P-C: 2-0-0-2)

| Program: M. Sc. Chemistry | Semester: III                           |
|---------------------------|---|
| Course code: CH5 EAN4     | Course name: APPLIED ANALYSIS AND GREEN |
|                           | ANALYTICAL CHEMISTRY                    |

| Lockwas            | Practical | ctical  |       |           | Evaluation | n Scheme   |           |
|--------------------|-----------|---------|-------|-----------|------------|------------|-----------|
| Lecture<br>(Hours) | (Houre)   | Credits | Hours | Component | Exam       | Max. Marks | Passing % |
| 2 per week         | -         | 2       | 30    | Lecture   | CCE, ESE   | 50         | 18        |

#### **Course Objectives:**

- Understand the scope and real-world relevance of analytical chemistry.
- Gain practical insight into modern analytical protocols, including impurity profiling, stability testing, water quality analysis, and nutrient/adulterant detection.
- Explore the principles and techniques of Green Analytical Chemistry, focusing on solvent-free and sample preparation methods, green solvents, and environmentally friendly instrumentation.
- Evaluate case studies and analytical strategies.

Course Learning Outcomes: At the end of this course students will be able to

**CL01:** Face the real-world applications of analytical chemistry across industries.

**CLO2:** Bridge the gap between theoretical principles and analytical practices in research and quality control.

**CLO3:** Understand and apply the 12 principles of Green Analytical Chemistry.

**CLO4:** Choose and design greener alternatives for sample preparation, analysis, and waste management.

#### **Syllabus**

| Units  | Content  | Hours |
|--|--|-------|
| <b>Unit I:</b> Applied Analysis              | Introduction to Applied Analysis (Definition and scope, role of analytical chemists in industry and research), pharmaceutical applications (assay and impurity profiling, dissolution testing and drug release studies, stability testing and validation protocols), Environmental and Water Analysis (analysis of trace metals and pollutants, Water quality parameters - COD, BOD, TDS), Food and Agricultural Analysis (Nutrient profiling - Detection of adulterants, preservatives, pesticides), Role of FSSAI and ISO standards, Forensic and Clinical Applications: Analysis of toxins, drugs, and biological fluids, DNA and protein analysis. | 15    |
| Unit II:<br>Green<br>Analytical<br>Chemistry | Introduction to Green Analytical Chemistry: 12 principles and importance of Green Chemistry, Greening sample preparation: solvent-free methods: SPME, MAE, SFE, Solid-phase extraction (SPE) and microextraction, green solvents and miniaturization, Green instruments: Use of spectroscopic techniques (UV-Vis, FTIR, NIR, Raman), Electroanalytical methods (voltammetry, amperometry), Green chromatography and electrophoresis, Flow injection analysis (FIA). Case studies involving green analytical technique in food analysis, pharmaceuticals, environmental monitoring. Role of GAC in sustainable development goal.                        | 15    |

- 1. G. D. Christian. Analytical Chemistry. John Wiley & Sons Inc., New York. 1994, 6th Ed.
- 2. H. Marck; J. Rekniz. Kinetics Methods of Analysis. Marcel Dekker Inc., New York. Volume 25.
- 3. A. H. Beckett; J. B. Stenlake. *Practical Pharmaceutical Chemistry, Vol. 1 & Vol. 2.* CBS Publishers & Distributors, New Delhi. 1986, 3rd Ed.
- 4. M. De La Guardia; S. Armenta. *Green Analytical Chemistry: Theory and Practice*. Elsevier, Amsterdam. 2010, 1st Ed.
- 5. M. Koel; M. Kaljurand. *Green Analytical Chemistry*. RSC Publishing, Cambridge. 2010, 1st Ed.
- 6. A. Gałuszka; Z. Migaszewski; J. Namieśnik. *The 12 Principles of Green Analytical Chemistry. TrAC Trends in Analytical Chemistry*, Elsevier, Amsterdam. 2013, Vol. 50, pp. 78–84.

#### **SEMESTER IV**

#### CH5 AN201: RESEARCH OR INDUSTRIAL PROJECT (L-T-P-C: 0-0-20-10)

| Program: M. Sc. Chemistry | Semester: IV                                |
|---------------------------|---|
| Course code: CH5 AN201    | Course name: RESEARCH OR INDUSTRIAL PROJECT |

| T4                 | Practical   | C dit-  | Total |       | Evaluation | n Scheme |            |           |
|--------------------|-------------|---------|-------|-------|------------|----------|------------|-----------|
| Lecture<br>(Hours) | (Hours)     | Credits | Hours | Hours | Component  | Exam     | Max. Marks | Passing % |
| -                  | 20 per week | 10      | 150   | Lab   | CCE, ESE   | 100      | 35         |           |

**Course Description:** This is a compulsory course performed in the final semester where the students get a semester-long exposure to research.

- Students who work on research and industrial projects gain valuable training and experience that can help them in their future careers.
- Students can work on real-world research projects proposed by industry or public sector sponsors.
- This course helps to train individuals who contribute to human resources required in the chemical/pharmaceutical industry.
- The research work may lead to academic research articles as well.
- They also learn about patents, scientific publications, and literature search tools

Course Learning Outcomes: At the end of this course students will be able to

CLO1: Understand the real-world academic/industrial research problems

CLO2: Apply the knowledge gained during various theoretical and practical courses

**CLO3:** Design different projects with the knowledge of chemistry to solve existing problems in society

**CLO4:** Understand data interpretation and data analysis

**CL05:** Learn to reboot any experimental problems.

**Syllabus:** Lab-specific research topics.

#### CH5 AN202: PROJECT REPORT (L-T-P-C: 2-0-0-2)

| <b>Program:</b> M. Sc. Chemistry | Semester: IV                |
|----------------------------------|-----------------------------|
| Course code: CH5 AN202           | Course name: PROJECT REPORT |

| Lagtung            | Practical Credit |         | Total | Evaluation Scheme |          |            |           |
|--------------------|------------------|---------|-------|-------------------|----------|------------|-----------|
| Lecture<br>(Hours) | (Hours)          | Credits | Hours | Component         | Exam     | Max. Marks | Passing % |
| 2 per week         | -                | 2       | 30    | Lecture           | CCE, ESE | 100        | 35        |

**Course Description:** In this course, the students learn to summarise their learning experiences.

- They learn the proper ways to write a 'project thesis'.
- This contains a comprehensive overview of a project's objectives, progress, team performance, and milestone accomplishments.
- It also gives an account of the challenges faced during a project's execution, solutions devised to tackle them, and the lessons learned during the process.
- They also learn about different communication medium like Microsoft word, chemdraw etc.

Course Learning Outcomes: At the end of this course students will be able to

**CLO1:** Understand how to report a practical work into a thesis **CLO2:** Learn to publish their research results after the program

**CLO3:** Learn the art of written scientific communications

**Syllabus:** Depends on the research performed in respective labs.

#### CH5 AN203: PROJECT PRESENTATION (L-T-P-C: 3-0-0-3)

| Program: M. Sc. Chemistry | Semester: IV                      |
|---------------------------|-----------------------------------|
| Course code: CH5 AN203    | Course name: PROJECT PRESENTATION |

| Lockwas            | Practical Con- |         | Total | Evaluation Scheme |          |            |           |
|--------------------|----------------|---------|-------|-------------------|----------|------------|-----------|
| Lecture<br>(Hours) | (Hours)        | Credits | Hours | Component         | Exam     | Max. Marks | Passing % |
| 3 per week         | -              | 3       | 45    | Lecture           | CCE, ESE | 100        | 35        |

**Course Description:** In this course, the students mainly learn to communicate their work performed to the audience.

- They learn to use different communication mediums (for example Microsoft PowerPoint) and convince their audience about the research findings.
- This course helps students to increase confidence, presence, and enjoyment of public speaking.
- The students also learn to use vocal techniques; use tone, range, articulation, power, pace, and pausing to make an impact.
- The students learn the use of body language and gestures to create credibility.

Course Learning Outcomes: At the end of this course students will be able to

CL01: Develop proper communication skills.

**CLO2:** Defend their accomplished research in front of experts.

CLO3: Gain confidence in facing job interviews.

Syllabus: Depends on the research performed in respective labs.

~:The End:~