CURRICULUM & SYLLABI

M.Sc. CHEMISTRY

Effective from AY: 2024-25

NATIONAL INSTITUTE OF TECHNOLOGY WARANGAL

WARANGAL, TELANGANA - 506004

Table of Contents

Vision and Mission of the Institute
National Institute of Technology Warangal

VISION

Towards a Global Knowledge Hub, striving continuously in pursuit of excellence in Education, Research, Entrepreneurship and Technological services to the society

MISSION

- Imparting total quality education to develop innovative, entrepreneurial and ethical future professionals fit for globally competitive environment.
- Allowing stake holders to share our reservoir of experience in education and knowledge for mutual enrichment in the field of technical education.
- Fostering product-oriented research for establishing a self-sustaining and wealth creating centre to serve the societal needs.

Vision and Mission of the Department

DEPARTMENT OF CHEMISTRY

VISION

To provide excellent education, initiating research and inspiring environment in chemistry that ignites the young minds.

MISSION

- To encourage in the advancement of chemistry in all of its branches through education, research and service missions
- To appraise the significance of chemistry in day-to-day life and address the global challenges
- To empower with knowledge in all fields of chemistry and achieve excellence in teaching and research
- To nurture the young minds in chemistry towards the societal needs
- To produce qualified and responsible personnel to serve the society

Program: M.Sc. Chemistry

Program Educational Objectives

PEO-1	Impart proficiency in the fundamentals and applications of all disciplines of chemistry.
PEO-2	Inculcate critical thinking and analytical reasoning in the development of chemicals, materials and processes for sustainable domestic and industrial applications.
PEO-3	Provide solutions to chemistry related societal and industrial challenges with suitable research methodologies.
PEO-4	Formulate procedures and regulations with environmental and ecological dimensions for safe handling and endurable benefits of chemicals.

Program Articulation Matrix

PEO / Mission Statements	PEO-1	PEO-2	PEO-3	PEO-4
To encourage in the advancement of chemistry in all of its branches through education, research and service missions	3	2	2	2
To appraise the significance of chemistry in day-to-day life and address the global challenges	2	3	3	2
To empower with knowledge in all fields of chemistry and achieve excellence in teaching and research	3	3	2	3
To nurture the young minds in chemistry towards societal needs	1	2	1	2

1 - Slightly; 2 - Moderately; 3 - Substantially

Program: M.Sc. Chemistry

Program Outcomes

PO-1	Gain the knowledge of chemistry to meet specific needs with appropriate considerations towards public health, safety and environment
PO-2	Apply appropriate analytical techniques to complex chemistry activities with an understanding of the limitations
PO-3	Devise organic materials for societal needs in pharmaceutical, agricultural, environmental, materials fields
PO-4	Develop analytical strategies to elucidate nanomaterials, alloys and industrial materials comprehensively with high precision and to analyze complex real-world samples of biomedical, energy and environmental applications
PO-5	Develop new strategies for the synthesis and characterization of organic and bio-molecules using state-of-the-art technologies
PO-6	Utilize research-based knowledge in designing and executing new experiments through independent and life-long learning with up-to-date scientific skills.

Program Specific Outcomes

PSO-1	Understand the basic concepts of all disciplines of Chemistry
PSO-2	Apply the chemistry knowledge to provide solutions to the contemporary societal problems in fields of materials science, environmental science, and pharmaceutical chemistry
PSO-3	Able to Interpret the properties of various chemicals using the analytical techniques learned and relate the chemical characteristics to functioning and performance of various functional materials
PSO-4	Able to design synthetic schemes for the biologically active molecules

CURRICULUM
M.Sc. Chemistry

1st Semester

S.No.	Code	Course Title	L-T-P	Credits
1	CY16001	Main Group and Transition Metal Chemistry	4-0-0	4
2	CY16003	Chemical Kinetics and Electrochemistry	4-0-0	4
3	CY16005	Chemical and Statistical Thermodynamics	3-0-0	3
4	CY16007	Organic Reactions and Mechanism	3-0-0	3
5	CY160XX	Elective-1	3-0-0	3
6	CY16009	Inorganic Chemistry Laboratory-I	0-1-2	2
7	CY16011	Organic Chemistry Laboratory-I	0-1-2	2
			Total Credits	21

2nd Semester

S.No.	Code	Course Title	L-T-P	Credits
1	CY16002	Photochemistry and Pericyclic reactions	4-0-0	4
2	CY16004	Group Theory and Spectroscopy	4-0-0	4
3	CY16006	Quantum Chemistry	3-0-0	3
4	CY160XX	Elective-2	3-0-0	3
5	CY160XX	Elective-3	3-0-0	3
6	CY16008	Inorganic Chemistry Laboratory-II	0-1-2	2
7	CY16010	Physical Chemistry Laboratory-I	0-1-2	2
			Total Credits	21

3rd Semester

S.No.	Code	Course Title	L-T-P	Credits
1	CY17001	Organic Synthesis	4-0-0	4
2	CY17003	Organometallic Chemistry	3-0-0	3
3	CY170XX	Elective-4	3-0-0	3
4	CY170XX	Elective-5	3-0-0	3
5	CY17005	Organic Chemistry Laboratory-II	0-1-2	2
6	CY17007	Physical Chemistry Laboratory-II	0-1-2	2
7	CY17089	Seminar & Technical Writing	0-2-0	2
8	CY17091	Internship	0-0-4	2
			Total Credits	21

4th Semester

S.No.	Code	Course Title	L-T-P	Credits
1	CY170XX	Elective-6	3-0-0	3
2	CY170XX	Elective-7	3-0-0	3
3	CY17094	Comprehensive Viva-Voce	0-2-0	2
4	CY17098	Dissertation	0-2-10	8
			Total Credits	16

Professional Elective Courses:

Professional Elective-I

S.No.	Code	Course Title
1	CY16021	Bio-inorganic Chemistry
2	CY16023	Heterocyclic Chemistry
3	CY16025	Solid State Chemistry

Professional Elective-II

S.No.	Code	Course Title
1	CY16022	Chemistry of Natural Products
2	CY16024	Bio-organic Chemistry

Professional Elective-III

S.No.	Code	Course Title
1	CY16030	Nuclear and Radiochemistry
2	CY16032	Advanced Inorganic Materials

Professional Elective-IV

S.No.	Code	Course Title
1	CY17021	Spectroscopy for Structural Elucidation
2	CY17023	Chemical Education

Professional Elective-V

S.No.	Code	Course Title
1	CY17031	Applied Analytical Methods
2	CY17033	Electroanalytical Methods

Professional Elective-VI

S.No.	Code	Course Title
1	CY17022	Medicinal Chemistry
2	CY17024	Stereoselective Synthesis
3	CY17026	Advanced Organic Spectroscopy
4	CY17028	Emerging Topics in Organic Synthesis
5	CY17030	Advances in Total Synthesis of Natural Products
6	CY17032	Advances in Industrial Catalysis
7	CY17034	Microscopic and Diffraction Methods
8	CY17036	Supramolecular Chemistry

Professional Elective-VII

S.No.	Code	Course Title
1	CY17044	Green Chemistry
2	CY17046	Polymer Chemistry
3	CY17048	Chemistry of Nanomaterials
4	CY17050	Industrial Applications of Organic Chemistry
5	CY17052	Statistical Treatment of Data and Quality Control
6	CY17054	Surface Analytical Techniques
7	CY17056	Chemical and Electrochemical Energy Systems

SYLLABI

M.Sc. Chemistry

1st Semester

CY16001 **4-0-0 (4)**

Main Group and Transition Metal Chemistry

Pre-Requisites: **Basic inorganic chemistry**

Course Outcomes:

CO-1	Understand the structure, bonding and properties of metal carbonyls, metallocenes and main group compounds
CO-2	Apply the concepts of bonding for interpreting structural properties of coordination compounds
CO-3	Correlate the kinetics and mechanisms involved in inorganic reactions
CO-4	Analyze electronic spectra and magnetic properties of coordination compounds
CO-5	Interpret the role of various metal ions in biology and medicine

Course Articulation Matrix:

	PO-1	**PO-2**	**PO-3**	**PO-4**	**PO-5**	**PO-6**
CO-1	2	–	1	1	1	2
CO-2	2	1	1	2	–	3
CO-3	2	–	2	1	1	1
CO-4	2	2	1	–	–	1
CO-5	3	–	2	2	2	2

1 - Slightly; 2 - Moderately; 3 – Substantially

Syllabus:

Main group Chemistry: Structure and bonding in polyhedral boranes and carboranes, styx notation, Wade's rule electron count in polyhedral boranes; synthesis of polyhedral boranes, Isolobal analogy, boron heterocycles, borazine, P-N compounds, structural features and reactivity of S-N heterocycles, Isopoly & heteropoly acids.

Bonding in coordination compounds: Review of Crystal field theory (CFT) and its applications. Jahn-Teller effect. Molecular orbital theory of octahedral, tetrahedral and square planar complexes. Pi bonding in metal complexes.

Thermodynamic and Kinetic aspects of metal complexes: Stepwise and overall formation constants and their interaction, trends in stepwise constants. Factors affecting stability of metal complexes with reference to the nature of metal ion and ligand chelate effect. Methods for the determination of stability constants.

Reaction mechanism of transition metal complexes: Energy profile of a reaction, reactivity of metal complex, inert and labile complexes, kinetics of octahedral substitution, acid & base hydrolysis, conjugate base mechanism, anation reactions, substitution Reactions in octahedral complexes-A, D and I

Mechanisms, Substitution reactions in square planer complexes, Trans Effect-theories and applications, Electron Transfer Reactions-Outer Sphere and Inner Sphere.

Electronic and magnetic properties of transition metal complexes: Types of electronic transition, selection rules for d-d transitions. Spectroscopic ground states, Orgel and Tanabe-Sugano diagrams for transition metal complexes. Calculation of Racah parameters, Charge transfer spectra. Different types of magnetic behaviour. Factors affecting observed magnetic moments. Origin of magnetic moment, spin contribution, spin only formulas, orbital contribution, spin-spin coupling. Methods for magnetic susceptibility measurement, Ferro- and antiferromagnetism, mechanism of antiferromagnetic interaction, spin cross over and anomalous magnetic moments.

Coordination chemistry in biology: Metal ions in Biological Systems, Metal Binding Biomolecules, Metal Containing Units in Biology, Metal ion containing oxygen transport and electron transport proteins.

Learning Resources:

Text Books:

1. J.D. Lee, Concise Inorganic chemistry, Wiley India, 2015, 5th Edition.
2. C.E. Housecroft, A. G. Sharpe, Inorganic chemistry, Pearson, 2018, 5th Edition.

Reference Books:

1. J.H. Huheey, E.A. Keiter, R.L. Keiter, O.K. Medhi, Inorganic chemistry: principle of structure and reactivity, Pearson Education India, 2006, 4th Edition.
2. D.F. Shriver, P.W. Atkins, Inorganic chemistry, Oxford University Press, 2006, 4th Edition.

CY16003 **4-0-0 (4)**

Chemical Kinetics and Electrochemistry

Pre-Requisites: **Basic physical chemistry at undergraduate level**

Course Outcomes:

CO-1	Understand the theories of reaction rates
CO-2	Interpret the mechanism and kinetics of complex and enzymatic reaction
CO-3	Analyze the effect of various factors on reaction rates
CO-4	Interpret the electrochemical characteristics of electrolyte
CO-5	Apply the concepts of electro kinetic phenomenon for various physical insights

Course Articulation Matrix:

	PO-1	**PO-2**	**PO-3**	**PO-4**	**PO-5**	**PO-6**
CO-1	2	1	1	1	1	1
CO-2	1	2	1	1	2	1
CO-3	2	1	-	-	1	1
CO-4	2	1	1	-	-	1
CO-5	1	1	1	-	-	1

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Chemical Dynamics: Basic concepts of kinetics, Effect of temperature on reaction rates, Mechanism and kinetics of Complex reactions: Equilibrium approximation and Steady state approximation, theories of reaction rates, kinetics of fast reactions, reactions in solutions, photochemical reactions and polymerization

Catalysis: Acid-Base Catalysis, Enzyme Catalysis, Inhibition of Enzymatic Reactions, Langmuir-Hinshelwood mechanism for surface reactions, Autocatalysis and oscillatory chemical reactions

Electrolytic Conduction: DHO Theory of strong electrolytes, validity and deviations of DHO equation, Debye Hukel theory of activity coefficients-Debye Huckel Limiting law, validity, Debye-Huckel-Bjerrum equation, applications of conductance measurements

Electrodics and Interfacial Electrochemistry: Theories of Electrical DoubleLayer, Electrokinetic phenomena, Butler-Volmer Equation, Tafel Equation

Learning Resources:

Text Books:

1. K.J. Laidler, Chemical Kinetics, Pearson Education, 2003, 3rd Edition
2. Samuel Glasstone, An Introduction to Electrochemistry, East-West Publisher, 2006

Reference Books:

1. P. Atkins and J. de Paula, W. H. Freeman, Physical Chemistry, Oxford University press, 2006, 8th Edition
2. S. H. Maron, C. F. Prutton, Principles of Physical Chemistry, Macmillan, 1965, 4th Edition

CY16005 **3-0-0 (3)**

Chemical and Statistical Thermodynamics

Pre-Requisites: **Basic physical chemistry at graduation level**

Course Outcomes:

CO-1	Understand the relationship of thermodynamic variables
CO-2	Understand the Phase rule and Phase diagrams
CO-3	Apply the laws of thermodynamics to real systems to understand the stabilities
CO-4	Evaluate the thermodynamic parameters using partition function
CO-5	Analyze the microscopic parameters from macroscopic behavior of system

Course Articulation Matrix

	PO1	PO2	PO3	PO4	PO5	PO6
CO-1	2	2	1	3	1	3
CO-2	2	3	1	2	1	2
CO-3	2	2	2	2	3	3
CO-4	2	2	1	2	3	3
CO-5	2	3	1	2	3	3

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Classical Thermodynamics: Thermodynamic Variables, Laws of Thermodynamics, Thermodynamic Relationships and Applications, Partial Molar Quantities, Phase equilibria and Phase Rule, Fugacity, Activity and Activity Coefficient.

Statistical Thermodynamics: Statistical Treatment of Entropy; Maxwell Boltzmann Functions, Partition Functions and Their Relation to Thermodynamic Variables, Bose-Einstein and Fermi-Dirac Statistics.

Learning Resources:

Text Books:

1. Thermodynamics for Chemists, S. Glasstone, East-West Publishers, 2008.
2. Physical Chemistry: A Molecular Approach (Viva student edition), Donald A Mcquarrie, John D Simon, Viva Books-2015

Reference books:

1. Molecular Thermodynamics, Donald A. Macquarrie, John D. Simon, Viva Books-2018, Viva student edition
2. Physical Chemistry, P. Atkins and Julia de Paula, Oxford, 2011 and 9th Edition

CY16007 **3-0-0 (3)**

Organic Reactions and Mechanism

Pre-Requisites: **Basic Organic Chemistry, Functional group interconversion**

Course Outcomes:

CO-1	Understand kinetic and thermodynamic aspects of the chemical reactions
CO-2	Classify chiral molecules using symmetry elements
CO-3	Identify various types of organic reactions with mechanisms
CO-4	Apply stereochemistry principles in interpreting molecular conformations
CO-5	Predict the stereochemistry of the products

Course Articulation Matrix:

	PO-1	**PO-2**	**PO-3**	**PO-4**	**PO-5**	**PO-6**
CO-1	3	–	–	–	–	–
CO-2	–	–	–	–	–	–
CO-3	–	1	3	–	3	3
CO-4	–	2	3	3	3	3
CO-5	–	–	2	–	3	3

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Study of reaction intermediates: Generation and reactions of Carbocations, Carbanions, free radicals, carbenes, nitrenes, arynes, ylides

Types of organic reactions: Addition, substitution, elimination reactions in aliphatic and Aromatic systems

Stereochemical aspects of organic reactions: Isomerism, Basic concepts of stereochemistry, CIP rules, nomenclature, racemization and resolution methods, specific rotation, enantiomeric and diastereomeric excess, types of stereo chemical reactions (examples).

Experimental methods for studying reaction mechanisms: Theoretical and physical aspects of organic reactions

Oxidation reactions: Oxidation of hydrocarbons, alcohols, amines, nitro compounds, sulfides, reagents for the oxidation of specific functional groups

Reduction reactions: Reduction of unsaturated hydrocarbons, reductive dehalogenation, reaction of carbonyl compounds, nitro and nitriles, sulfones, sulfoxides

Learning Resources:

Text Books:

1. M.B. Smith and J. March, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, Wiley Interscience, 2016, 7th Edition.
2. E. L. Eliel, S. H. Wiley, Stereochemistry of Organic Compounds, Wiley Interscience, 2008, 1st Edition.

Reference Books

1. Stereochemistry of Organic Compounds: Principles and Applications, Fourth Edition, D. Nasipuri, New Age International Publishers, 2020.
2. Organic Chemistry, Francis A. Carey, Tata McGraw Hill publishing company Limited, New Delhi 2010, 8th Edition.

CY16009 **0-1-2 (2)**

Inorganic Chemistry Laboratory - I

Pre-Requisites: **Basic inorganic chemistry experiments at undergraduate level**

Course Outcomes:

CO-1	Gain hands on experience in the volumetric analysis, gravimetric and spectrophotometric analysis
CO-2	Acquire the knowledge in estimation of anions and cations
CO-3	Understand the principle involved in various types of volumetric titrations
CO-4	Estimate the metal ion contents by gravimetric analysis
CO-5	Analyze water samples for their alkalinity and quality parameters

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	1	3	–	1	–	–
CO-2	2	2	–	1	–	–
CO-3	1	1	–	1	–	–
CO-4	2	2	–	–	–	–
CO-5	2	1	–	1	2	–

1 - Slightly; 2 - Moderately; 3 – Substantially

Syllabus:

Determination of total alkalinity, and water quality analysis
Determination of cations and anions in environmental samples (e.g. Zn by complexometry, Cu by iodometry, sulphate by semi-gravimetry, Al by oxine method, Ni by DMG method)
Estimation of salt by ion-exchange method
Separation and estimation of Cu^{2+}- Ni^{2+} mixtures by volumetric and gravimetric methods
Separation of Mn and Fe using isoamyl alcohol and estimation of Mn
Estimation of sulfate by spectrophotometry
Determination of Iron by colorimetry
Determination of Cu^{2+} by electrogravimetry

Learning Resources:

Text Books:

1. G.H. Jeffery, J. Bassett, J. Mendham, R.C. Denney, Vogel's textbook of quantitative chemical analysis, Longman Inc., 1989, 5th Edition.
2. J. D. Woolins, Inorganic experiments, John Wiley & Sons, 2010, 3rd Edition.

Reference Books:

1. A.J. Elias, A Collection of interesting general chemistry experiments, Universities Press (India) Pvt. Ltd., 2002.
2. G. Pass, H. Sutfille, Practical inorganic chemistry: preparations, reactions and instrumental methods, Springer, 1979, 2nd Edition.
3. Z. Szafran, R. M. Pike, M.M. Singh, Microscale inorganic chemistry: A comprehensive laboratory experience, Wiley, 1991, 1st Edition.

CY16011 **0-1-2 (2)**

Organic Chemistry Laboratory - I

Pre-Requisites: **Basic organic chemistry experiments at undergraduate level**

Course Outcomes:

CO-1	Understand the principle involved in separation and purification techniques
CO-2	Obtain hands-on experience of chromatography techniques
CO-3	Analyze the functional groups in organic molecules
CO-4	Choose an appropriate technique for the purification of synthesized compound
CO-5	Understand the principle involved in separation of binary mixtures
CO-6	Obtain practical experience in the separation and identification of individual compounds in the binary mixtures

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	1	1	1	1	1	2
CO-2	1	2	2	2	1	2
CO-3	3	2	3	1	3	2
CO-4	2	-	2	-	2	1
CO-5	2	2	2	-	1	2

1 - Slightly; 2 - Moderately; 3 – Substantially

Syllabus:

Purification Techniques:

Crystallization, fractional crystallization, Sublimation,

Simple distillation, Fractional distillation, Vacuum distillation and Steam distillation.

Isolation and purification of products by chromatographic techniques:

TLC and column Chromatography.

Separation and Analysis of Single functional group and Binary Mixture:

Solubility tests for organic compounds, identification of single functional group in the organic compounds.

Separation of Binary mixture

Detection of elements N, Cl, Br, I, S and functional groups alcoholic/phenolic OH, carboxylic, aldehyde, ketone, ester, nitro, amino, amide, N-substituted amino, imido groups, unsaturation (C=C), aromatic hydrocarbons, and halogenated derivatives present in the organic molecules.

Synthesis of simple organic compounds:

Aspirin, Hippuric acid, *m*-Nitroaniline, Oxidative coupling reaction: BINOL.

Learning Resources:

Text Books:

1. R. K. Bansal, Laboratory Manual of Organic Chemistry, New Age International Private Limited, 2009, 5th Edition.
2. N. K. Vishnai, Advanced Practical Organic Chemistry, Vikas Publishing House Pvt Ltd, 2009, 3rd Edition.

Reference Books:

1. D.L. Pavia, G.M. Lampman, G.A. Kriz, R.G. Engel, Introduction to Organic Laboratory Techniques, Brooks/Cole 2010, 3rd Edition.

2nd Semester

CY16002 **4-0-0 (4)**

Photochemistry and Pericyclic Reactions

Pre-Requisites: **Basic reactions and stereochemistry**

Course Outcomes:

CO-1	Understand the photochemical and thermal reactions
CO-2	Classify the various types of pericyclic and photochemical reactions
CO-3	Apply the orbital correlation and frontier molecular orbital methods for pericyclic reactions
CO-4	Evaluate various types of organic photochemical and pericyclic reactions mechanisms with stereochemical outcome
CO-5	understand the aromaticity of various organic compounds

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	1	1	3	1	3	3
CO-2	3	1	3	1	3	3
CO3	3	1	2	1	3	3
CO4	2	1	3	1	3	3
CO5	3	1	3	1	3	3

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Organic Photochemistry: Photochemical energy, Frank Condon Principle, Jablonski diagram, Singlet and Triplet states, Dissipation of photochemical energy, Photosensitization, Quantum efficiency, Experimental methods of photochemistry.

Photochemical Reactions: Classification of photochemical reactions, Norrish type I and II cleavages, Patterno-Buchi reaction. Photoreduction, Photochemistry of enones, Rearrangement of, α,β-unsaturated ketones and cyclohexadienes, Photo-fragmentation reactions (Barton, Hofmann-Loffler-Freytag).

Pericyclic Reactions: Introduction, Molecular orbitals and their symmetry properties, MO's of ethylene, 1,3 Butadiene, 1,3,5- Hexatriene, Allyl system, Classification of pericyclic reactions, selection rules [Woodward-Hoffman correlation diagram, FMO and Perturbation of molecular (PMO)]

Electrocyclic Reactions: Conrotatory and disrotatory motions in (4n) and (4n+2), allyl systems and secondary effects; Antarafacial and suprafacial additions, Notation of cycloaddition of (4n) and (4n+2) systems, Secondary effects of substitutes on the rates of cycloaddition reaction, 1,3-dipolarcycloadditions;

Chelotropic reactions, Sigmatropic Reactions, Suprafacial and antarafacial shifts, retention and inversion of configurations, Claisen and Cope rearrangements, Ene-reactions, fluxional molecules.

Aromaticity: Localized and delocalised covalent bond, Concept of resonance and aromaticity, Huckel's rule for aromaticity in benzenoid and non-benzenoid compounds, Anti-aromaticity and homo-aromaticity, Aromaticity of various rings like annulenes, heteroannulenes, sydnones and Fullerenes (C60), Synthesis and properties of annulenes and Azulene, Craig's rule.

Learning Resources:

Text Books:

1. L. N. Ferguson, The modern structural theory in Organic Chemistry, Prentice Hall, 2008.
2. Charles Dupey, O. Chapman, Molecular reactions and photochemistry, Prentice Hall, 2006.
3. S.M. Mukherjee, Pericyclic reactions, Macmillan India Limited, 2009.

Reference Books:

1. Jerry March, Advanced Organic Chemistry Reactions, Mechanism & Structure, Wiley, 2006, 4th Edition.
2. Jack Hine, Physical Organic Chemistry, Mc. Graw Hill, 2007.

CY 16004 **4-0-0 (4)**

Group Theory and Spectroscopy

Pre-Requisites: Fundamentals of inorganic chemistry and physical chemistry at undergraduate level

Course Outcomes:

CO-1	Understand molecular symmetry, structure and motions with rotational, vibrational and electronic quantum levels and spectral properties
CO-2	Interpret molecular symmetry, symmetry operations and molecular point groups
CO-3	Analyze molecular structure and geometry with magnetic resonance spectral characteristics
CO-4	Justify molecular functionality and structure comprehensively
CO-5	Propose a relevant spectroscopic method for structural elucidation

Course Articulation Matrix:

	PO1	PO2	PO3	PO4	PO5	PO6
CO1	1	2	2	3	2	1
CO2	-	2	1	2	3	2
CO3	1	2	2	1	3	-
CO4	3	-	2	1	2	3
CO5	1	2	1	2	-	3

1 - Slightly; 2 - Moderately; 3 - Substantially

Syllabus:

Symmetry elements, Point Groups and Group Theory: Symmetry Elements, Symmetry Operations; Point groups, Assignment of point groups to molecules; Stereographic projections; Group generating elements, Group multiplication tables, Isomorphic groups, sub-groups, classes.

Matrix Representation and Applications of Group Theory: Matrix representation of symmetry elements and point groups; Character tables, Reducible and Irreducible Representations; Construction of character Tables, Mulliken Symbolism, The Standard Reduction Formula, The Direct Product. Symmetry of Normal Modes of Molecules, Infrared and Raman Activity, Criteria for Optical Activity; Symmetry Restrictions on Dipole Moment.

Microwave, Infrared and Raman Spectroscopy: Rotation of Molecules, Rigid and Non-rigid Rotors, Selection Rules of Transitions; Diatomic and Polyatomic Molecules, Applications; Selection Rules of Vibrational Transitions; Vibrational Rotational Spectra, Applications; Raman Effect; Quantum Mechanical Description; Rotational and Vibrational Raman Spectra; Mutual Exclusion and Complementarity

Magnetic Resonance Spectroscopy: Magnetic Nuclei and Nuclear Spin, ^{1}H NMR Spectroscopy: Chemical Shift; Spin-Spin Coupling; Pascal's triangle, Coupling constant, Relaxation Mechanism; spin-lattice and spin-spin relaxations, inversion recovery method, spin-echos methods; Nuclear Overhauser Effect, INDOR and NOE Methods; Nuclear quadrupole resonance spectroscopy; ^{13}C NMR Spectroscopy: Fourier Transform NMR; Off-Resonance and Spin-Decoupled ^{13}C NMR Spectroscopy; Applications; NMR

Spectroscopy of ^{19}F, ^{15}N and ^{31}P nuclides.^{19}F NMR heteronuclear coupling. Electron Spin and Its Magnetism; 'g'-Factor; ESR Spectral Phenomenon; Hyperfine structure, Line width and anisotropy; Zero-field splitting, Kramer's degeneracy, ENDOR and EEDOR methods, Applications.

Learning Resources:

Text Books:

1. K. Veera Reddy, Symmetry and spectroscopy of molecules, New Age International, 2020, 2nd Edition.
2. C. N. Banwell and E. M. McCash, Fundamentals of molecular spectroscopy, Tata McGraw Hill Education, 2017, 4th Edition.

Reference Books:

1. F. A. Cotton, Chemical Applications of Group Theory, Wiley Publishers, 2000, 3rd Edition.
2. D.C. Harris, M.D. Bertolucci, Symmetry and spectroscopy: an introduction to vibrational and electronic spectroscopy, Dover Publications 1989.

Other Suggested Readings:

1. A. Dutta, Symmetry and group theory https://onlinecourses.nptel.ac.in/noc22_cy40/preview .

CY16006 **3-0-0 (3)**

Quantum chemistry

Pre-Requisites: Basic physical chemistry and knowledge of atomic structure

Course Outcomes:

CO-1	Understand the behavior of electron
CO-2	Understand the first principles of calculation
CO-3	Apply first principles of calculation to real problems in chemistry
CO-4	Apply the concept of Molecular Orbital Theory to complex molecular systems
CO-5	Evaluate the electronic structure and properties of molecules

Course Articulation Matrix

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	2	1	1	1	1	2
CO-2	2	2	1	1	2	3
CO-3	3	2	1	2	3	3
CO-4	2	3	1	3	2	3
CO-5	2	3	1	3	3	3

1 - Slightly; 2 - Moderately; 3 - Substantially

Syllabus:

Emergence of quantum mechanics: Postulates of quantum mechanics, Time independent schrodinger equation and its application to Particle in a 3-D Box, Simple harmonic oscillator, Rigid rotor and H-Like atoms. quantum well and quantum tunneling.

Approximation methods: Variational and Perturbation theory, first and second order perturbation corrections.

Chemical bonding: Molecular orbital theory; Hartree-Fock self consistent field (SCF) method, Roothaan Hartree-Fock equation, Huckel MO theory; Spin-orbit coupling.

Learning Resources:

Text Books:

1. D.A. McQuarrie, Quantum Chemistry (Student viva edition), Viva Books-2016

2. R. K. Prasad, Quantum Chemistry, New age international Limited, 1997. 5th Edition

Reference books:

1. L. Pauling, E.B. Wilson, Introduction to Quantum Mechanics: With Applications to Chemistry, Dover Books on Physics, 1985.
2. T.A. Albright, J.K. Burdett, M. H. Whangbo, Orbital Interactions in Chemistry, Wiley-Interscience; 2013.

CY16008 **0-1-2 (2)**

Inorganic Chemistry Laboratory-II

Pre-Requisites: **None**

Course Outcomes:

CO-1	Obtain hands-on experience in the spectrophotometry and electroanalytical methods
CO-2	Apply spectro- and electroanalytical methods for quantification of metal ions and other components in complex mixtures
CO-3	Predict characteristics of synthesized metal complexes
CO-4	Analyze metal ion content and other components
CO-5	Predict the order of metal ions in spectrochemical series

Course Articulation Matrix:

	PO-1	**PO-2**	**PO-3**	**PO-4**	**PO-5**	**PO-6**
CO-1	1	3	–	1	–	–
CO-2	2	3	–	1	–	–
CO-3	–	1	–	–	–	–
CO-4	2	1	–	1	–	–
CO-5	1	–	–	–	–	–

1 - Slightly; **2 - Moderately;** **3 – Substantially**

Syllabus:

Synthesis of Potassium bis(Oxalato)cuprate(II) dihydrate complex, Manganese(III) acetylacetonate, Mercury tetrathiocyanatocobaltate (II), Hexaamine cobalt (III) chloride

Characterization of the metal complexes by FT-IR/ESR/UV-Visible methods

Estimation of oxalate and copper in the potassium bis (oxalate) cuprate(II) dihydrate

Determination of Stoichiometry of a metal complex by mono variation and by continuous variation method

Simultaneous determination of two metal ions by spectrophotometric method

Determination of crystal field splitting of metal complexes and verification of spectrochemical series

Estimation of paracetamol in the given formulation using potentiometry

Estimation of Aspirin in the given formulation by pH-metry

Estimation of Ascorbic acid in the given formulation by potentiometry

Estimation of Ibuprofen in the given formulation by conductometry

Learning Resources:

Text Books:

1. G.H. Jeffery, J. Bassett, J. Mendham, R.C. Denney, Vogel's Textbook of Quantitative Chemical Analysis, Longman Inc., 1989, 5th Edition
2. J. D. Woolins, Inorganic Experiments, John Wiley & Sons, 2010, 3rd Edition.

Reference Books:

1. A.J. Elias, A Collection of Interesting General Chemistry Experiments, Universities Press (India) Pvt. Ltd., 2002.
2. G. Pass, H. Sutfille, Practical Inorganic Chemistry: Preparations, Reactions and Instrumental Methods, Springer, 1979, 2nd Edition.

CY16010 **0-1-2 (2)**

Physical Chemistry Laboratory - I

Pre-Requisites: **Fundamentals of physical chemistry, chemistry laboratory techniques and safety protocols**

Course Outcomes:

CO-1	Understand standard procedures of potentiometric, conductometric and pH-metric techniques and kinetics experiments
CO-2	Explain the principles of potentiometric, conductometric and pH-metric techniques and kinetics experiments
CO-3	Determine dissociation constants and reaction kinetics by performing titrations.
CO-4	Interpret the experimental data to identify trends and calculate relevant chemical parameters.
CO-5	Assess the accuracy and reliability of experimental results compared to theoretical values.

Course Articulation Matrix:

	PO-1	**PO-2**	**PO-3**	**PO-4**	**PO-5**	**PO-6**
CO-1	3	–	–	–	–	–
CO-2	2	1	–	–	–	1
CO-3	3	1	–	–	–	2
CO-4	3	2	–	–	1	2
CO-5	1	2	–	2	1	2

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Determination of concentration and dissociation constant of a weak acid/ weak base using potentiometer.

Determination of individual concentrations of mixture of acids with a strong base using potentiometer.

Determination of isoelectric point of an amino acid using potentiometer.

Determination of concentrations of reductant/oxidant using potentiometer.

Determination of concentrations of HCl and CH_3COOH in their mixture pH-metrically.

Determination of pk_a values of di and tribasic acids pH-metrically.

Determine the buffer capacity of various buffer solutions pH-metrically.

Determination of hydrolytic constant K_h of NH_4Cl solution using pH meter.

Effect of ionic strength on persulphate and iodide reaction.

Effect of temperature on rate of reaction and determination of activation energy.

Determination of catalytic constant of acid with respect to iodination of acetone.

Study the kinetics of interaction of Crystal Violet with NaOH colorimetrically.

Study the kinetics of base catalyzed hydrolysis of ester.

Determination of individual concentrations of weak acid, strong acid and salt mixture with a strong base using a conductometer.

Determination of solubility and solubility product constant (K_{sp}) of sparingly soluble salt conductometrically.

Learning Resources:

Text Books:

1. Amritha Anand, Ramesh Kumari, Physical Chemistry Laboratory Manual, Wiley, 2019
2. Physical Chemistry Laboratory Manual of NITW

Reference Books:

1. J.B. Yadav, Advanced Practical Physical Chemistry, 2019 and 38th Edition
2. D.P Shoemaker., C.W Garland and J.W.Nibler, Experiments in Physical chemistry, McGraw Hill, 2008, 8th Edition

3rd Semester

CY17001 **4-0-0 (4)**

Organic Synthesis

Pre-Requisites: **Basic knowledge of organic chemistry**

Course Outcomes:

CO-1	Understand the concepts involved in C-C and C=C bond formation reactions
CO-2	Demonstrate the applications of reagents in organic reactions
CO-3	Apply the knowledge of protecting and deprotection of functional groups
CO-4	Plan synthetic strategies using disconnections approaches
CO-5	Design the synthetic scheme for small and large organic molecules

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	1	-	3	-	2	2
CO-2	1	-	3	-	2	2
CO-3	1	-	3	-	2	2
CO-4	1	-	3	-	2	2
CO-5	1	-	3	-	2	2

1 - Slightly; 2 - Moderately; 3 – Substantially

Syllabus:

Carbon-Carbon Single bond formation reactions: Importance of enolates, alkylation of active methylene groups, Gama alkylation of 1,3-dicarbonyl compounds; dianions in the synthesis, enamine related reactions, kinetics of C- and O-alkylations, alkylation of alpha-thio and selenocarbanions, umpolung, allylic alkylation of alkenes, organolithium, magnesium and cuprates, applications of carbenes, carbenoids, formation of C-C bonds by addition of free radicals to alkenes, cyclisation reactions (3 to 7 membered rings),

Carbon-Carbon double bond formation reactions: Wittig and Wittig version of reactions, Fragmentation reactions, Wharton olefin synthesis, alkenes from tosylhydrazone, sulfone, titanium and chromium reagents, alkene metathesis, Oxidative decarboxylation of acids, stereospecific synthesis from 1,2-diols, Reactions at inactivated C-H bonds

Protecting groups: Protection and deprotection of hydroxy, carboxyl, carbonyl, carboxy amino groups and carbon-carbon multiple bonds; chemo-and regioselective protection and deprotection, protecting group free organic synthesis.

Disconnection approach to organic synthesis: Target selection, functional group interconversion, disconnection, synthons, synthetic equivalent, retron, topological studies, one group two group disconnections, 1,2-, 1,3-, 1,4-, 1,5-, 1,6- difunctions, reversal polarity, convergent and divergent synthesis, building block approach, biomimetic approach,

Stereochemistry in organic synthesis: Topology, Chemo-, regeo-stereoselectivity, substrate, reagent and catalyst controlled stereoselective reactions. Crams's rule, Felkin-Ahn's model, chiral oxidation and reduction reactions, Chiral oxidation and reduction reactions, stereoselective cyclization reactions (Baldwin rules).

Learning Resources:

Text Books:

1. W. Carruthers, I. Coldham, Some modern methods of organic synthesis, Cambridge University Press, Cambridge, 2015, 4th Edition.
2. M.B. Smith, Organic synthesis, Academic Press, 2016, 4th Edition.

Reference Books:

1. S. Warren, Organic synthesis: the disconnection approach, John Wiley & Sons, 2007.
2. G. Zweifel, M. Nantz, W. H. Freeman, Modern Organic Synthesis, John Wiley & Sons, 2006.

CY17003 **3-0-0 (3)**

Organometallic Chemistry

Pre-Requisites: **Basic knowledge of d- and f-block elements**

Course Outcomes:

CO-1	Understand the structure and bonding aspects of organometallic compounds
CO-2	Establish the structure-reactivity/activity relationship in organometallic chemistry
CO-3	Predict the chemical behavior and reactivity of metal organometallic compounds
CO-4	Understand the operating mechanisms in the catalytic processes
CO-5	Develop materials for various industrial processes

Course Articulation Matrix:

	PO-1	**PO-2**	**PO-3**	**PO-4**	**PO-5**	**PO-6**
CO-1	2	–	–	–	–	–
CO-2	2	–	–	–	2	–
CO-3	2	–	–	–	–	–
CO-4	1	–	–	–	–	–
CO-5	3	–	–	–	3	–

1 - Slightly; **2 - Moderately;** **3 – Substantially**

Syllabus:

Introduction: Overview of reactions in organometallic chemistry, metal sigma and pi complexes, Carbenes and Carbyne complexes and Metal clusters

Main Group Organometallics: Structure, Bonding and reactivity of main group organometallic compounds, Application of main group organometallic compounds.

Homogeneous Catalysis: Introduction to homogenous catalysis, Catalytic Cycles, Alkene Isomerization, Hydrogenation, Hydroformylation, Hydrocynation, Hydrosilyation and Hydroboration, Coupling Reactions, oxidation catalysis, cooperative catalysis.

Applications: Organic applications-carbon-carbon coupling, Metathesis, cyclopropanation, C-H insertion, Hydrogenation, Carbonylation, Oxidation, C-H activation, Click Chemistry. General Applications-Dimerization, Oligomerization and Polymerization of alkenes, Activation of CO and CO_2, Green Chemistry, Energy Chemistry, Nanoparticles, Organometallic Materials.

Learning Resources:

Text Books:

1. B.D. Gupta, A.J. Elias Basic organometallic chemistry- concepts, synthesis and applications, University Press Private Limited, India, 2011.
2. R. H. Crabtree, The organometallic chemistry of the transition metals, Wiley, 2014, 6th Edition.

Reference Books:

1. C. E. Housecroft, A. G. Sharpe, Inorganic chemistry, Pearson, 2018, 5th Edition.
2. D. F. Shriver, P. W. Atkins Inorganic chemistry, Oxford University Press, 2006, 4th Edition

CY17005 **0-1-2 (2)**

Organic Chemistry Laboratory – II

Pre-Requisites: **Organic Chemistry Laboratory-I**

Course Outcomes:

CO-1	Obtain hands-on experience in determining the purity of compound using volumetric and gravimetric methods.
CO-2	Estimate the acid, iodine and saponification values of oils.
CO-3	Apply the synthetic methodologies for the preparation of organic compounds
CO-4	Examine the greener methods of synthesis of organic compounds
CO-5	Develop the knowledge and skills in the synthetic organic chemistry useful for industrial applications

Course Articulation Matrix:

	PO-1	**PO-2**	**PO-3**	**PO-4**	**PO-5**	**PO-6**
CO-1	1	1	2	-	1	1
CO-2	1	2	2	-	2	2
CO-3	3	2	3	-	3	3
CO-4	3	1	3	-	3	2
CO-5	3	1	3	-	3	3

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Synthesis of organic compounds based on Oxidation: Benzyl chloride to benzoic acid, Reduction of nitrobenzene to aniline

Electrophilic aromatic substitution: Nitro benzene, sulphanilic acid, *p*-bromo acetanilide

Synthesis of optically active compounds: benzo pinacol

***O*-acylation & *N*-acylation**: *O*-Benzoylation: phenyl benzoate

Diazotization reaction: Azo-dye preparation

Preparation organic compounds by green chemistry methods: i) acetylation of Aniline, ii) base catalyzed aldol condensation, iii) Diels-Alder reaction, iv) Benzil-benzilic acid rearrangement.

Advanced reactions: L-Proline mediated asymmetric aldol reaction, Click reaction (in homogeneous and heterogeneous conditions), cross-coupling and acid-amine coupling reactions

Estimations: keto group of acetone, formaldehyde in formalin, sugars, acids in an oil, saponification value of an oil, acid and ester in a mixture, iodine value of an oil.

Learning Resources:

Text Books:

1. R. K. Bansal, Laboratory Manual of Organic Chemistry, New Age International Private Limited, 5th Edition, 2009.
2. Text Book of Practical Organic Chemistry, Vogel A. I., 5th Edition, ELBS, 2004.

Reference Books:

1. V. K. Ahulwalia, Sunita Dhingra, Comprehensive Practical Organic Chemistry Qualitative Analysis, Universities Press, 2008.
2. F. Clark, Jr. Most, Experimental Organic Chemistry, John Wiley & Sons, 2002.

CY17007 **0-1-2 (2)**

Physical Chemistry Laboratory - II

Pre-Requisites: Fundamentals of physical chemistry and chemistry laboratory techniques.

Course Outcomes:

CO-1	Understand the principles and analytical applications of diverse instrumental techniques
CO-2	Identify suitable methodologies and instrumental techniques for the study of physical and chemical properties
CO-3	Select appropriate analytical methods for determining analytes of interest
CO-4	Understand the usage of computer
CO-5	Understand the applications of computational chemistry

Course Articulation Matrix:

	PO-1	**PO-2**	**PO-3**	**PO-4**	**PO-5**	**PO-6**
CO-1	3	3	–	1	1	1
CO-2	2	2	1	2	2	1
CO-3	1	2	2	–	2	1
CO-4	–	1	–	–	–	2
CO-5	–	1	1	–	1	2

1 - Slightly; 2 - Moderately; 3 - Substantially

Syllabus:

Instrumental Analyses: Determination of redox potentials using cyclic voltammetry, Determination of binding constant by using spectrophotometry, Determination of Stern-Volmer quenching constant using fluorimetry, Determination of surface area and pore structure of graphite by BET analysis, Determination of crystal structure and particle size by XRD analysis, Measuring carbon monoxide in automobile exhaust by gas chromatography, DNA composition by high-performance liquid chromatography, Analysis of analgesic tablets by high-performance liquid chromatography, Optical rotatory dispersion of chiral compounds,

Computational experiments: Molecule drawing and visualization, Computation of single point energies, Geometry optimization, Molecular frequency calculation, Electron densities and electrostatic potentials, Reaction in Gas-phase

Learning Resources:

Text Books:

1. G H Jeffery, J Bassett, J Mendham, R C Denney, Vogel's textbook of quantitative chemical analysis, Longman Inc., 2009, 7th Edition.
2. D. C. Harris, Quantitative Chemical Analysis, 2015, 9th Edition.

Reference Books:

1. J.B. Yadav, Advanced Practical Physical Chemistry, 2019, 38th Edition.
2. R. D. Baun, Introduction to Instrumental Analysis, McGraw-Hill, NY, 1987.

CY17089 **0-2-0 (2)**

Seminar and Technical Writing

Pre-Requisites: None

Course Outcomes:

CO-1	Consolidate ideas based on expert talks attended
CO-2	Prepare a well-organized report employing elements of critical thinking and technical writing
CO-3	Demonstrate the ability to describe, interpret and analyze the subject matter and develop competence in presenting

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	2		2			3
CO-2	2		2			3
CO-3	2		2			3

1 - Slightly; 2 - Moderately; 3 - Substantially

Description:

In Seminar and Technical Writing, every student is expected to prepare a well-organized report based on one / all of the following:

- by attending at least 5 expert lectures/ invited talks/ Seminar/ Popular lectures etc. organized by the institute/any of the departments, ideally in a specific domain or with the same theme.
- prepare a business or marketing plan based on patent search

The student is expected to consolidate the ideas from these lectures/patent searches and may even include material from other sources to strengthen the content of the report. The student should prepare a well-organized report based on the above and present it to the panel constituted by the department, for evaluation.

Evaluation Criteria:

The student will be evaluated by the panel based on the below criteria.

Criteria	Description	Weightages
I	Clarity on the topic	
II	List of lectures attended	
III	Report	
IV	Presentation	
V	Response to questions	

Evaluation Criteria-CO Mapping

CO / Criteria	CO1	CO2	CO3
I	X		
II	X		
III		X	
IV			X
V			X

4th Semester

CY17094 **0-2-0 (2)**

Comprehensive viva-voce

Pre-Requisites: **None**

Course Outcomes:

CO-1	Comprehend the knowledge gained in the course work
CO-2	Demonstrate the ability in problem solving
CO-3	Communicate effectively using engineering terminology

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6	PO-7	PO-8	PO-9	PO-10	PO-11	PO-12	PSO-1	PSO-2	PSO-3	PSO-4
CO-1	3	3	3	3						2		3				
CO-2	3	3	3	3						2		3				
CO-3	2	2	2	2						3		3				

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Description:

In Comprehensive viva-voce each student will be evaluated for their overall comprehension of the course work and laboratory training that they have undergone. The students will be expected to answer questions orally, write down simple equations, draw plots, schematics, write simple code etc. as questioned by the panel. Assessment will be done by the panel based on the student response.

CY17098 **0-2-10 (8)**

Dissertation

Pre-Requisites: **None**

Course Outcomes:

CO-1	Identify a domain specific and contemporary topic
CO-2	Review literature to identify gaps and define objectives & scope of the work.
CO-3	Develop a prototype/model, experimental set-up or software systems to meet the objectives
CO-4	Analyze the results to draw valid conclusions

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	3	2			2	1
CO-2	2	2			1	2
CO-3	2	2	3	3	3	2
CO-4	2	2		3	3	

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Description:

Students are expected to choose real-world contemporary problem and apply the engineering principles learned, to solve the problem through building prototypes or simulations or writing codes or establishing processes/synthesis/correlations etc. The department constituted panel will decide the suitability and worthiness of the project

The method of evaluation should be as per the guidelines stipulated for the B.Tech. Project evaluation. The template for preparation of the project report may be downloaded from (https://www.nitw.ac.in/path/?dept=/nitwForms) under UG Forms. The students are required to submit a report showing that plagiarism is within 30%. The B.Tech. Project work will be evaluated for 100 marks, with the following weightages:

Component	Weightage
Periodic evaluation by Guide	40 marks
Mid-term review	20 marks
End Semester viva-voce examination	40 marks
Total	100 marks

The midterm review and the end semester viva-voce examination will be conducted by a committee constituted by the Head of the Department. If the performance of a student is not satisfactory, he/ she can be awarded ‘F’ grade. Such a student will be given a maximum time of three months to improve his/her performance. If the performance of such a student is not satisfactory even after the extended time period, he/ she will have to repeat the project work in the next academic year.

Evaluation Criteria:

The student will be evaluated by the panel based on the below criteria. Weightage for each criterion will be determined by the panel and will be informed to the students.

Criteria	Description	Weightages
I	Selection of Topic	
II	Literature Survey	
III	Objectives and Solution Methodology	
IV	Performance of the Task and clarity on the work	
V	Report Preparation	
VI	Presentation and Response to questions	

Evaluation Criteria-CO Mapping

CO / Criteria	CO1	CO2	CO3	CO4
I	X			
II		X		
III		X		
IV			X	
V				X
VI				X

Professional Electives

CY16021 **3-0-0 (3)**

Bioinorganic Chemistry

Pre-Requisites:

Course Outcomes:

CO-1	Understand role of metal ions in biological processes
CO-2	Interpret toxicological mechanisms of metals and the biological defenses against the toxic effects
CO-3	Identify metal sites in enzymes involved in the activation of molecules
CO-4	Understand medicinal applications of inorganic compounds
CO-5	Evaluate coordination chemistry principles in modulating properties of metal centers in enzymes

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	**3**	**–**	**–**	**–**	**–**	**–**
CO-2	**2**	**–**	**1**	**1**	**1**	**–**
CO-3	**2**	**–**	**–**	**–**	**–**	**–**
CO-4	**3**	**–**	**2**	**–**	**–**	**–**
CO-5	**2**	**–**	**1**	**1**	**1**	**–**

1 - Slightly; 2 - Moderately; 3 – Substantially

Syllabus:

Introduction: Fundamental concepts in biochemistry and biology: biosphere; living organisms; cells and cell compartments; biomolecules, distribution of elements in the earth's crust, seawater and organisms, inorganic elements in biological systems. Essential and trace metal ions in biology and their distribution, overview of metal ion function in metalloproteins and enzymes, metal ion transport and storage, function of special ligands - porphyrins, chlorin and corrin.

Principles of coordination chemistry and physical methods in Bioinorganic Chemistry: Overview of thermodynamics and kinetics aspects, electronic and geometrical aspects of metal ions, reactions of coordinated ligands, analysis of biomolecules by physical methods.

Functions of biomolecules: Sodium and potassium transport, dioxygen binding and activation by heme, non-heme and copper proteins, Iron transport and storage proteins in bacterial and mammalian systems, Electron transport–FAD, NAD, FMN, ubiquinone and blue copper proteins, Cytochromes, Iron- sulfur proteins – rubredoxin, ferredoxins, Photosynthesis.

Enzymes: Hydrolytic enzymes, enzymes deal with hydrogen peroxide and dioxygen, cobalt containing enzymes, Nitrogen-cycle enzymes.

Medicinal applications: metals in medicine, anti-cancer agents–cisplatin and other compounds, radiopharmaceuticals (Tc), diagnostic (Gd in MRI) and therapeutic agents Toxicity of Hg, Cd, Pb and As and chelation therapy.

Learning Resources:

Text Books:

1. S. J. Lippard, J. M. Berg, Principle of Bioinorganic chemistry, Univ. Science Books, 1994.
2. I. Bertini, H. B. Gray, E. I. Stiefel, J. S. Valentine, Biological Inorganic Chemistry: Structure & Reactivity, Univ. Science Books, 2007.

Reference Books:

1. G. N. Mukherjee, A. Das, Elements of Bioinorganic Chemistry, UN Dhur Pvt. Ltd, 1993, 4th Edition.
2. W. Kaim, B. Schwederski, A. Klein, Bioinorganic Chemistry -Inorganic Elements in the Chemistry of Life: An Introduction and Guide, Wiley, 2013, 2nd Edition.

CY16023 **3-0-0 (3)**

Heterocyclic Chemistry

Pre-Requisites: **Basic knowledge of organic functional groups**

Course Outcomes:

CO-1	Classify heterocyclic compounds and their nomenclature
CO-2	Understand the physical and chemical properties of simple and fused heterocyclic compounds
CO-3	Design the route to synthesize the heterocyclic compounds
CO-4	Apply the knowledge of heterocyclic chemistry to synthesize the natural products
CO-5	Apply the knowledge of heterocyclic chemistry to synthesize drug like molecules

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	2	-	2	-	1	1
CO-2	2	-	3	-	2	1
CO-3	3	-	3	-	3	1
CO-4	1	-	1	-	3	3
CO-5	1	-	1	-	3	3

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Non-Aromatic Heterocycles: Different types of strains, interactions and conformational aspects of non-aromatic heterocycles. Synthesis, reactivity and importance of following ring systems. Three and four membered heterocycles with O, N, S.

Aromatic Heterocyclic Compounds preparation properties and reactivities: Pyrrole, furan, thiophene and pyridine. Bicyclic ring systems derived from pyrrole, furan and Thiophene: Indoles, Isoindoles, carbazole, Benzofurans, Benzothiophene. Bicyclic ring systems derived from pyridine: Quinolines, Isoquinolines and Acridines. Five-membered heterocyclic compounds with two hetero atoms: Pyrazoles, Benzopyrazoles, Imidazoles, Bezimidazoles, Isoxazoles, Oxazoles, Benzoxazoles, Thiazoles. Six membered heterocyclics with two hetero atoms: Pyridazines, Pyrimidines, Quinazolines and Pyrazines. Synthesis of drug molecules based on the above heterocyclic rings.

Oxygen heterocyclic compounds: Coumarins, Chromones, Flavones and Isoflavones.

Mesoionic heterocycles: synthesis and aromaticity of sydnones, 1,3-dipolar addition reactions of mesoionic heterocycles.

Learning Resources:

Text Books:

1. J. A. Joule, K. Mills, Heterocyclic Chemistry, Wiley, 2010, 5th Edition.
2. V. K. Ahulwalia, Heterocyclic Chemistry, Narosa, 2012, 1st Edition.

Reference Books:

1. T. L., Gilchrist, Heterocyclic Chemistry, Pearson Education, 2008, 3rd Edition.
2. R. K. Bansal, Heterocyclic Chemistry, New Age International, 2017, 5th Edition.

CY16025 **3-0-0 (3)**

Solid State Chemistry

Pre-Requisites: **Basics of crystal structure**

Course Outcomes:

CO-1	Understand structures of crystal systems and imperfections in crystals
CO-2	Relate the knowledge of diffraction techniques for structure determination
CO-3	Selection of an appropriate technique for characterizing the new solid materials
CO-4	Impact of crystal structures on the solid materials
CO-5	Understand electrical, optical and dielectric properties of solids

Course Articulation Matrix:

	PO-1	**PO-2**	**PO-3**	**PO-4**	**PO-5**	**PO-6**
CO-1	1	-	1	-	-	-
CO-2	-	1	-	-	1	1
CO-3	1	-	1	-	-	-
CO-4	-	1	-	-	-	-
CO-5	1	2	-	1	1	2
CO-6	1	-	1	-	-	-

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Crystal structure: Lattice Energy, Miller Indices, Crystal defects, Types of crystals, Solid-Solutions, Phase diagram and their interpretations, Some Important Structure: Perovskite, Spinel, Pyrochlore.

Synthesis and Characterization of Crystals: Shake 'n Bake, Chimie Douce, Hydrothermal and Microwave Methods; X-ray diffraction: Single crystal and Powder Methods: The Debye Scherrer Method, Electron diffraction, Neutron diffraction.

Properties of solids: Superconductivity, Low- and High-temperature Superconductivity, BCS theory, Electrical Properties, Magnetic properties, and Optical & dielectric properties.

Learning Resources:

Text Books:

1. Lesley Smart, Elaine Moore, Solid State Chemistry, An Introduction, CRC press, 5th Edition 2020.
2. Anthony R. West, Solid State Chemistry and its Applications, Wiley publication, 2nd Edition 2022.

Reference Books:

1. V. Keer, Principles of the Solid State, New Age International 2nd Edition, 2017.
2. Weller, T. Overton, J. Rourke, and F. Armstrong, Inorganic Chemistry, Oxford University Press, 6th Edition, 2014. (South Asia Edition 2015)

CY16022 **3-0-0 (3)**

Chemistry of Natural Products

Pre-Requisites: **Basic knowledge of Organic Synthesis**

Course Outcomes:

CO-1	Understand the concept of structure elucidation of natural compounds
CO-2	Build the synthetic schemes of natural products and bioactive molecules
CO-3	Analyze the stereochemistry of drug molecules
CO-4	Apply the knowledge of biosynthesis in total synthesis of organic molecules.
CO-5	Design new synthetic methodologies

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	2		3		3	2
CO-2	2		3		3	2
CO-3	3	1	3	1	3	2
CO-4	3		3		3	2
CO-5	3	1	3	1	3	2
CO-6	3		3		3	3

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Introduction: Classification of Natural Products, isolation of natural products, general methods of structural elucidation and stereochemistry.

Terpenoids: Classification, Structure and synthesis of Mono, sesqui, di, tri terpenoids, biogenesis of terpenoids (Geraniol, Alpha- Terpineol, Alpha-pinene, Camphor, Cadenene, Abeitic acid)

Steroids: Classification, structure, stereochemistry and synthesis of steroids (Cholesterol).

Alkaloids: Structure and chemistry of papaverine, Quinine, Morphine, Lysergic acid and Resepine, nicotine, atropine.

Vitamins: Structure and synthesis of vitamins B1

Learning Resources:

Text Books:

1. I. L. Finar, Organic Chemistry, Vol. I & II, Pearson Education India, 2002, 5th Edition.
2. O.P. Agarwal, Organic Chemistry Natural Products -Vol. I, Krishna Prakashan Media (P) Ltd, 2015.

Reference Books:

1. R. Cooper, G. Nicola, Natural Products: Chemistry Sources, Separations, and Structures, CRC Press. 2015.
2. J.J. Li, E.J. Corey, Total Synthesis of Natural Products: At the Frontiers of Organic Chemistry, Springer, 2015

CY16024 **3-0-0 (3)**

Bio-organic Chemistry

Pre-Requisites: **Structure and properties of organic compounds**

Course Outcomes:

CO-1	Understand the importance of biomolecules
CO-2	Illustrate the structure and functions of bioorganic molecules
CO-3	Interpret the physiological role of RNA, DNA and enzymes
CO-4	Utilize the concepts of protein purification and synthesis in bio-pharma industry
CO-5	Apply the concepts of enzyme catalysis for industrial applications

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	3	1	3	1	3	3
CO-2	3		3		3	3
CO-3	3	1	3	2	3	3
CO-4	3		3		3	3
CO-5	3	1	3	2	3	3

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Amino acids: Amino acids: structure, acid-base chemistry, and chemical synthesis; Asymmetric Synthesis of Amino Acids.

Proteins and Peptides: Introduction, Quaternary Structure of Proteins, Protein Purification Methods, amino acid analysis and peptide sequencing; peptide bond formation and coupling reagents-carbodiimides and phosphonium reagents; orthogonal protecting groups; solid-phase peptide synthesis: (Fmoc/Boc strategies); native peptide ligation; cyclic peptides; Enzyme chemistry: Introduction, proteases and phosphatases; proteins as drug targets, Enzyme technology, Enzyme catalysis.

Coenzymes: Structure and biological function of coenzyme A, thiamine pyrophosphate (TPP), pyridoxal phosphate (PLP), oxidized and reduced forms of NAD^+, NADH, $NADP^+$, NADPH, ATP.

Nucleosides, nucleotides and nucleic acids: Introduction to nucleic acids: biological importance, discovery, structure; chemical synthesis of nucleosides and protecting groups for nucleobase, sugar and phosphates; solution and solid phase synthesis of oligonucleotides: PCR; enzymatic synthesis of nucleic acids; principle behind sequencing; nucleic acid as drug targets.

Lipids: Fatty acids, essential fatty acids, structure and function of triacylglycerols, glycerophospholipids, sphingolipids, cholesterol, bile acids, prostaglandins. Lipid metabolism -β-oxidation of fatty acids.

Learning Resources:

Text Books:

1. A.L. Lehninger, Principles of Biochemistry, Worth Publishers, 2017, 7th Edition.
2. H.B. Dugas, Bioorganic Chemistry, Springer, 1996, 3rd Edition.
3. L. Stryer, W.H.F. Freeman, Biochemistry, 2006, 6th Edition.

Reference Books:

1. O.P. Agarwal, Organic Chemistry Natural Products -Vol. I, Krishna Prakashan Media (P) Ltd, 2015.
2. D. Voet, J.G. Voet, C.W. Pratt, Biochemistry Wiley, 2018.

CY16032 **3-0-0 (3)**

Advanced Inorganic Materials

Pre-Requisites: **None**

Course Outcomes:

CO-1	Understand the concepts involved in synthesizing advanced inorganic materials.
CO-2	Apply the concept to design new inorganic materials.
CO-3	Understand the structure-property correlation in these materials.
CO-4	Understand and identify societal issues and design new inorganic materials to solve them.
CO-5	Apply the concept to develop new devices for renewable energy applications

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	2	–	–	2	–	1
CO-2	3	1	–	1	–	2
CO-3	2	1	–	2	–	1
CO-4	3	–	–	1	–	1
CO-5	3	1	–	2	–	2

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Introduction to advanced inorganic materials. Definition and classes of materials. Molecular design of materials. From the molecule to the material. Basic experimental techniques for the characterization of materials: General aspects.

Methods of Synthesis: Chemical Method, High-Pressure Method, Arc Technique, and Skull Method.

Different methods for single crystal growth: Crystal Growth from Melt: Bridgman and Stockbargar, Czochralski and Vernuil methods; Crystal growth from liquid solution: Flux growth and temperature gradient methods; Crystal growth from vapor phase: Epitaxial growth methods.

Thin film preparation: Physical and Chemical methods.

Solid Solutions: Formation of Substitutional, Interstitial and Complex Solid Solutions; Mechanistic Approach; Study of Solid solutions by X-ray Powder Diffraction and Density Measurement.

Properties: Application of MXene. Gallium-nitride, Gallium-arsenide and their semiconducting properties in LED, Indium-tin-oxide (ITO) and its transparent conducting property, Allotropes of carbon (graphite, diamond, fullerene, graphene, carbon nanotube) and their properties. Thermoelectric materials, Superconducting property of Inorganic materials, Topological insulator materials and their properties, Inorganic materials for solar cell application, and Battery materials. Microporous, mesoporous, and macroporous materials. Zeolites and other porous materials. Applications.

Learning Resources:

Text Books:

1. F. A. Cotton, G. Wilkinson, C. A. Murillo, M. Bochmann, Advanced inorganic chemistry, John Wiley and Sons, New York, 1996, 6th Edition.
2. E. Smart and E. A. Moore, Solid state chemistry –An introduction, CRC Press, 2012, 4th Edition.

Reference Books:

1. W. Henderson, Main group chemistry, Royal Society of Chemistry, Cambridge, 2000.
2. J. E. Huheey, E. A. Keiter, R. L. Keiter, Inorganic chemistry-principles of structure and reactivity, Harper-Collins, NY, 1993, 4th Edition.

CY16030 **3-0-0 (3)**

Nuclear and Radiochemistry

Pre-Requisites: **None**

Course Outcomes:

CO-1	Understand the general concept of radioactivity
CO-2	Identify various methods and instrument used in measuring radioactivity
CO-3	Know the applications of radioactivity in various human endeavour
CO-4	Describe about various effects of radiation exposure
CO-5	Know about management of hazardous nuclear waste

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	3	–	–	1	–	1
CO-2	2	2	–	1	–	2
CO-3	2	–	–	2	–	2
CO-4	2	–	–	1	–	1
CO-5	3	–	–	2	–	1

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Introduction: Radioactivity in nature, Radioelements, Isotopes, Radionuclides, Physical Properties of atomic nuclei and elementary particles, Radioactive decay and decay modes.

Nuclear Radiation and Measurement: General properties, Alpha, beta and gamma radiation, Neutrons, Short-lived elementary particles in atoms and molecules, Activity and counting rate, Detectors, Spectrometry, Determination of absolute disintegration rates, Neutron detection, Statistics and errors of counting.

Nuclear Reactions and Chemical effects of nuclear reactions: Mono and binuclear reactions, Energetics, projectiles, yields and mechanisms of nuclear reactions, low and High energy reactions, Heavy ion reactions, Nuclear fission, Nuclear fusion. Recoil effects, Excitation effects, Szilard Chalmers reactions, Recoil and self-labelling, Dependence of Half-lives and Radiation emission on chemical bonding.

Nuclear Energy: Energy production by nuclear fission, Nuclear Fuel and Fuel Cycles, Fuel elements, Nuclear reactors, Moderators and coolants, Reprocessing, Radioactive waste, Nuclear reactors, Controlled thermo nuclear reactors, Nuclear explosives.

Applications of Radio Chemistry: Dating by Nuclear Methods, Radiotracers in chemistry, Radionuclides in the life sciences, Industrial applications of Radionuclides and Nuclear radiation

Radiation Protection: Dosimetry, External and Internal radiation sources, Effects of radiation in humans, animals and plants, radiation exposure, safety recommendations and regulations.

Learning Resources:

Text Books:

1. K. H. Lieser, Nuclear and Radiochemistry: Fundamentals and applications, Wiley VCH, 2001, 2nd Edition.
2. G. Choppin, J.-O. Liljenzin, J. Rydberg, Radiochemistry and nuclear chemistry, Butterworth-Heinemann, Woburn, MA, 2002, 3rd Edition.

Reference Books:

1. G. F. Knoll, Radiation Detection and measurement, Wiley, New York, 2000, 3rd Edition.
2. W. D. Ehmann, D. E. Vance, Radiochemistry and nuclear methods of analysis, Wiley Interscience, New York, 1991.

CY17021 **3-0-0 (3)**

Spectroscopy for Structural Elucidation

Pre-Requisites: **Molecular Spectroscopy**

Course Outcomes:

CO-1	Summarize the basic principles of spectroscopy
CO-2	Identify the structure of organic compounds using spectroscopy
CO-3	Analyze the structural aspects and stereochemistry of organic compounds using spectroscopy
CO-4	Interpret molecular mass and fragmentation of organic compounds using mass spectrometry
CO-5	Solve the structure of unknown organic compounds by using spectral data

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	1	3	-	-	-	-
CO-2	1	3	-	-	1	-
CO-3	1	3	-	-	1	-
CO-4	1	3	-	-	1	-
CO-5	1	3	-	-	1	-

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Ultraviolet and Visible Spectroscopy: Factors influencing the position of UV bands. Woodward-Fieser rules for calculating absorption maxima of unsaturated compounds and related compounds. Applications of UV spectroscopy.

Infrared Spectroscopy: Interpretation of illustrative examples. Characteristic absorptions in common classes of compounds. Applications of IR spectroscopy.

NMR spectroscopy-I (^{1}H-NMR): Chemical shifts, Equivalent and non-equivalent protons, enantiotopic and diastereotopic protons, Spin-spin coupling: ^{1}H-NMR of organic molecules ethyl acetate, ethanol, anisole, paracetamol, *p*-Toluidine, ethylbenzoate, *N*-acetanilide and cinnamaldehyde. First order and non-first order spectra, lanthanide shift reagents and double resonance techniques. Nuclear Over Hauser enhancement (NOE). Applications of ^{1}H-NMR spectroscopy.

Introduction, Types of ^{13}C-NMR spectra: coupled, proton-decoupled and off-resonance decoupled (ORD) spectra. ^{13}C chemical shifts, factors affecting the chemical shifts.

Mass spectrometry: Principle of EI, CI, Electrospray (ESI) ionization, Fast Atom Bombardment (FAB). Principles of different ionization techniques (EI, CI, FAB etc.). Types of fragments: Nitrogen rule, isotopic peaks, metastable peaks. High resolution mass spectrometry. Determination of molecular formula.

Learning Resources:

Text Books:

1. W. Kemp, Macmillan, Organic Spectroscopy, 2009, 3rd Edition.
2. P. S. Kalsi, Spectroscopy of Organic Compounds, New Age International Publishers, 2020, 8th Edition.

Reference Books:

1. D. L. Pavia, G. M. Lampman, G. S. Kriz, Introduction to Spectroscopy, Brooks/Cole,Thompson Learning, 2001, 3rd Edition.
2. R. M. Silverstein, F. X. Webster, D. J. Kiemle, D.L. Bryce, Spectrometric Identification of Organic Compounds, Wiley, 2014, 8th Edition.

CY17023 **3-0-0 (3)**

Chemical Education

Pre-Requisites:

Course Outcomes:

CO-1	Understand the importance of chemical education and ethical standards
CO-2	Identify promising modern research trends with their strength, growth and application
CO-3	Discover the strengths of chemical education in modern world and mankind in future
CO-4	Examine safety and ecological approaches in dealing hazardous compounds and effluents
CO-5	Recommend models and tools helping effective dissemination of trends in chemical education and research

Course Articulation Matrix:

	PO-1	**PO-2**	**PO-3**	**PO-4**	**PO-5**	**PO-6**
CO-1	1	-	-	-	-	1
CO-2	2	-	1	-	-	2
CO-3	2	1	-	1	-	1
CO-4	3	1	2	2	2	3
CO-5	3	2	-	-	1	3

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Chemistry as the Central Science: Uniqueness of Chemical Stoichiometry; Chemistry of Inanimate and Living Materials, Chemistry and Civilization; Chemistry in Product Industry; UN Slogan, ‘Chemistry- Our Life and Our Future’; Amazements in Chemistry: Amusement in Chemistry Classroom; Chemistry and Magic.

Chemical Hazards and Disasters: Chemistry of Explosives, Poisons and Polluttants; GLPs; Models and Tools of Chemical Education: Models and Virtual Experiments

Thrust Areas of Chemical Research: Topic by Relevance to Health, Nutrition, Energy, Environment, Sanitation, Technology, Rural Employment, Harnessing Natural Resources; IPR and Patents in Chemical Research and Innovations: Intellectual Property Rights in Chemical Innovations and Products; Patent Paradigms

Learning Resources:

Text Books:

1. Chemical Education, S. Ladage and S.D. Samant, Narosa Publishing House, 2012
2. Affective Dimensions in Chemistry Education, M. Kahveci and M. Orgill, Springer (e-Book), 2015.

3-0-0 (3)

CY17031

Applied Analytical Methods

Pre-Requisites: None

Course Outcomes:

CO-1	Understand the basic concepts of analytical chemistry
CO-2	Identify the sources of errors in analytical results
CO-3	Identify the importance of separation methods for purifying the mixture of compounds
CO-4	Choose the appropriate analytical technique for qualitative and quantitative estimation of unknown samples
CO-5	Evaluate the pattern of experimental data using the analytical techniques studied.

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	2	2	1	1	1	1
CO-2	2	1	1	1	1	1
CO-3	1	1	1	3	2	1
CO-4	1	1	1	3	3	2
CO-5	1	1	1	3	2	3

1 - Slightly; 2 - Moderately; 3 - Substantially

Syllabus:

Errors and Statistical Treatment of Data: Accuracy and Precision; Errors and Error Distributions; Standard Deviation; Confidence limits and intervals, Criteria for Rejection of Data – z- test, t-test, F-test, Q-test.

Separation Methods: Solvent extraction, Distribution Law; Extraction by Chelation, Extraction by Solvation, Extraction by Ion-Pair Formation, Batch and Continuous Extractions; Solid Phase Separation; Chromatographic Separations, Basic Principle, Stationary and Mobile Phases, void time, retention rime, and retention factor, separation factor, Electrophoresis.

Spectroanalytical Methods: Atomic Spectroscopy: Atomic Absorption, Atomic Emission, and Atomic Fluorescence; Molecular Spectroscopy: Beer's law, Deviations of Beer's Law, standard-addition method, steady-state fluorescence, life-time, fluorescence quenching, Phosphorescence, turbidimetry and nephelometry, refractometry; Mossbauer Spectroscopy: Recoilless Gamma Ray Absorption; Mossbauer Effect; Chemical Shift (Isomer Shit); Quadrupole Shift; Zeeman Effect; Applications; Polarimetry: Optical Rotatory Dispersion and circular dichroism in Qualitative and Quantitative Analysis of Chiral Compounds.

Thermoanalytical Methods: Thermogravimetric Analysis (TGA); Differential Thermal Analysis (DTA); Differential Scanning Calorimetry (DSC); Applications.

Radioanalytical Methods: Radioactive nuclides, Neutron activation analysis (NAA), isotope dilution analysis.

Learning Resources:

Text Books:

1. D. A. Skoog, D. M. West, F. J. Holler, S. R. Crouch, Fundamentals of Analytical Chemistry, Saunders College Publishing, 2004, 8th Edition.
2. G. D. Christian, Analytical Chemistry, Wiley India, 2009, 6th Edition.

Reference Books:

1. D. Harvey, Modern Analytical Chemistry, McGraw Hill, 1999, 1st Edition.
2. R.A. Day Jr, A.L. Underwood, Quantitative Analysis, PHI, 2009, 6th Edition.

CY17033 **3-0-0 (3)**

Electroanalytical Methods

Pre-Requisites: Fundamentals in analytical and physical chemistry, and basic mathematics. Familiarity with electrochemistry concepts is recommended.

Course Outcomes:

CO-1	Understand the basic principles of stationary and dynamic electroanalytical methods
CO-2	Identify strengths of pulse methods for superior quantitative analysis
CO-3	Analyze the results of micro- and rotating disc electrodes for interpreting mechanisms of electrochemical reactions
CO-4	Evaluate the efficiency and capacity of electrochemical energy storage materials
CO-5	Choose a combination of electroanalytical methods for comprehensive analysis of electrochemical materials and devices

Course Articulation Matrix:

	PO-1	**PO-2**	**PO-3**	**PO-4**	**PO-5**	**PO-6**
CO-1	3	2	1	2	1	2
CO-2	1	2	2	2	-	2
CO-3	3	2	1	1	3	1
CO-4	1	-	2	-	2	3
CO-5	2	1	3	-	2	2

1 - Slightly; 2 - Moderately; 3 - Substantially

Syllabus:

Steady-state and potential step techniques: Open circuit potential, Stern layer thickness, Linear sweep voltammetry, Cyclic voltammetry, Reversibility and accompanied chemical and catalytic reactions, Principles and applications. Microelectrodes, Capacitance, Turnover number, Surface electrochemistry.

Pulse voltammetry and hydrodynamic analysis: Normal and differential pulse voltammetry, Square wave voltammetry: Anodic stripping and cathodic stripping voltammetry and applications. Hydrodynamic measurements, rotating disk and rotating ring disk electrodes, and flow-cell analysis, capillary systems and lab-on-chip analysis.

Chronomethods: Principles, instrumentation and applications in Electrocatalysis (Oxygen and hydrogen evolution reactions), electrochemical sensors, development of capacitors and electrochemical supercapacitors, cyclic charging discharging processes, C rate and electrochemical capacitance. Electrochemical supercapacitors: Ragone plot, comparison with batteries, energy and power densities of storage devices, Pseudocapacitance, Ruthenium and porous materials, applications.

Electrochemical impedance and polarization methods: Electrochemical impedance spectroscopic measurements, principles and applications, equivalent circuits, Nyquist and Bode plots, potentiodynamic polarization studies, Randles model, Tafel methods. Electrochemical quartz crystal microbalance, principle, Thin layer coatings, Adlayer formations, electrodeposition of metals, applications.

Hyphenated methods: Electrochemical scanning tunneling microscopy, principles, instrumentation, Potential-UV-VIS measurements, Potential-Infrared measurements, applications.

Learning Resources:

Text Books:

1. A.J Bard, L. R Faulkner, Electrochemical methods: Fundamentals and applications, John Wiley, 2022
2. F. Scholz, Electroanalytical methods: Guide to experiments and applications, Springer, 2014

Reference Books:

1. B. E. Conway, Electrochemical supercapacitors - Scientific fundamentals and technological applications, Springer, 2014.
2. P. M. S Monk, Fundamentals of Electroanalytical Chemistry, John Wiley, 2008
3. P. Ceroni, A. Credi, M. Venturi, Electrochemistry of Functional Supramolecular Systems, John Wiley, 2010.

CY17022 **3-0-0 (3)**

Medicinal Chemistry

Pre-Requisites: **None**

Course Outcomes:

CO-1	Understand basic concepts of drug discovery
CO-2	Apply the concepts in lead discovery
CO-3	Identify the importance of Lipinski rule and bioisosterism
CO-4	Evaluate the concepts of SAR and QSAR
CO-5	Design and develop a molecule with drug like property

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	3	-	3	1	1	3
CO-2	3	-	3	1	3	2
CO-3	3	-	3	-	3	-
CO-4	3	-	3	-	-	-
CO-5	3	-	3	1	3	3

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Basics of Drug Discovery: Origin, comparison with ayurveda and homeopathic medicines, drug efficacy, potency, assay development, IC_{50}, LD_{50}, ED_{50}, Therapeutic index, margin of safety, agonist, antagonist, IND, NDA, quantal dose and graded dose. pharmacophore identification, lead modification, Lipinski rule, drug-like properties, druggability, bioisosterism, ADME, Factors affecting on ADME, Toxicity (CYPs, Glucuronidation)

Drug targets: Macromolecules as targets (receptors, enzymes, nucleic acids, cell organelles).

Drug discovery stages and strategies: SAR and QSARS, tereo chemical and metabolic aspects of drugs, serendipitous drug discovery, drug discovery without lead, natural products, fragment and metabolites based drug discovery (examples), clinical observations, random screening and non-random screening.

Chemistry of Drugs: Pharmacological activity, uses and limitations of Antipyretics, Analgesics, Sedatives, Hypnotics, Barbiturates, Sulpha drugs, Anaesthetics, Antiseptics, Antibacterial, Diuretics, Anthelmintic, Anticoagulants, Anticonvulsants, Antihistamines, Psychotherapeutics, Anti TB Drugs, Diagnostic agents and Antimalarial drugs (selective examples)

Drug Delivery Systems: Introduction to the necessity of Drug Delivery Systems, Types of drug delivery systems, Micelles, Vesicles, Polymers, Dendrimers, Nano spheres, Nano tubes etc., Osmatic Oral Drug Delivery Systems, Transdermal Drug Delivery Systems, Implantable Drug Delivery Systems.

Combinatorial synthesis: Combinatorial and building block approaches for the drugs and role of biomarkers (examples).

Learning Resources:

Text Books:

1. A. Kar, Medicinal Chemistry, New Age Publications, 2007.
2. G. L. Patrick, An Introduction to Medicinal Chemistry, Oxford Press, 2009, 4th Edition.

Reference Books:

1. Burger, Medicinal Chemistry Vol-I & II, Wiely Int.Sci., 1999.
2. R. B. Silverman, M. W. Holladay, The organic chemistry of Drug Design and Drug Action Academic Press, 2014, 3rd Edition.

CY17024 **3-0-0 (3)**

Stereoselective Synthesis

Pre-Requisites: **None**

Course Outcomes:

CO-1	To understand the 3-dimentional behavior of the organic/organometallic compounds during the reaction
CO-2	To predict the possible product from the 3-dimentional orientation of the intermediate that participate in the reaction
CO-3	Apply the knowledge of stereoselective synthesis for the preparation of active pharmaceutical ingredients and drug like compounds
CO-4	Apply the knowledge of stereoselective synthesis for the preparation of materials in materials and agriculture industry
CO-5	To understand and apply the knowledge of separation techniques for small and large scale reactions

Course Articulation Matrix:

	PO-1	**PO-2**	**PO-3**	**PO-4**	**PO-5**	**PO-6**
CO-1	2	1	3	1	3	3
CO-2	2	2	2	1	2	3
CO-3	2	2	3	2	3	3
CO-4	3	2	3	1	3	3
CO-5	1	1	1	1	3	3

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Strategies of asymmetric synthesis: Strategies of asymmetric synthesis, double stereo differentiating reactions, diastereoselective synthesis, Nucleophilic addition to cyclic carbonyl compounds, Aldol reactions based on achiral enolates, chiral enolates, small ring templates, chiral auxiliaries, achiral auxiliaries, intraanular and extraanular setreocontrol.

Stereo selective Reactions: Stereo selective reactions of C=C double bond, Asymmetric hydrogenation, Oganoboranes, organosilanes

Enantioselective Reactions. Enantioselective synthesis with chiral organometallic complexes, oxidation and reductions with chiral complexes, complex hydrides, Organocatalysis, asymmetric cross-coupling reactions, asymmetric metathesis reactions, directed asymmetric synthesis of natural and drug like molecules.

Learning Resources:

Text Books:

1. L. Ernest , Eliel ,H. Samuel H. Wilen Stereochemistry of Organic Compounds, , Wiely-India, 2008.
2. Stereochemistry: Conformation and Mechanism, P.S. Kalsi, New Age Publishers, 2019, 10th Edition.

Reference Books:

1. I. Ojima, Catalytic Asymmetric Synthesis, John Wiley & Sons, Hoboken, New Jersey, USA. 2012.

2. G. R. Stephenson. Chapman, Hall, Advanced asymmetric synthesis, Springer Science, 1996.

CY17026 **3-0-0 (3)**

Advanced Organic Spectroscopy

Pre-Requisites: Molecular spectroscopy, Spectroscopy for structural elucidation

Course Outcomes:

CO-1	Understand the concepts of spectroscopy
CO-2	Summarize the principles of PMR and CMR spectroscopies
CO-3	Analyze the concepts of ^{19}F spectroscopy in determining the structures of molecules
CO-4	Apply the principles of 2D NMR spectroscopy in resolving the structures of organic molecules
CO-5	Discuss the principle of ^{31}P and mass spectrometry and their applications

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	1	3	-	-	-	-
CO-2	1	3	-	-	1	-
CO-3	1	3	-	-	1	-
CO-4	1	3	-	-	1	-
CO-5	1	3	-	-	1	-

1 - Slightly; 2 - Moderately; 3 - Substantially

Syllabus:

Spectroscopy II (^{1}H-NMR): Applications of ^{1}H-NMR spectroscopy: Reaction mechanisms E,Z isomers, study of conformational changes through NMR of cyclohexane and decalins, study of dynamic processes using NMR spectroscopy. Chiral lanthanide shift reagents and Mosher's acid.

^{13}C NMR spectroscopy: Calculation of chemical shifts of alkanes, alkenes and alkynes. Homonuclear (^{13}C, ^{13}C J) and heteronuclear (^{13}C, ^{1}H J and ^{13}C, 2H J) coupling. ^{13}C-NMR spectral editing techniques: principle and applications of APT, INEPT and DEPT methods.

2D-NMR spectroscopy: Principles of 2D NMR, Classification of 2D-experiments. Homonuclear and Heteronuclear 2D-J-resolved spectroscopy, ROESY, NOESY and 2D- INADEQUATE experiments and their applications.

^{19}F NMR spectroscopy: Introduction, ^{19}F chemical shifts, spin-spin coupling, coupling constants. Homonuclear couplings, Applications of ^{19}F NMR involving coupling with ^{19}F, ^{1}H and ^{31}P: 1, 2 dichloro-1, 1 difluoro ethane, BrF_5, SF_4, PF_5, ClF_3, IF_5, CF_3CH_2OH.

^{31}P NMR spectroscopy: ^{31}P chemical shifts, coupling constants. Applications of ^{31}P NMR involving coupling with ^{31}P, ^{19}F, ^{1}H and ^{13}C: Simple molecules ^{31}P, P_4S_3, H_3PO_4, H_3PO_3, H_3PO_2 and HPF_2.

Advanced Mass spectrometry: Mass Analyzers: Quadruple, Ion traps, Time of flight (TOF) mass analyzers Mass Spectrometry / Mass Spectrometry: Tandem Mass Spectrometry, Instrumentation, Applications. Hyphenated Techniques: GC-MS Principle, instrumentation, LC-MS, ICP – MS -

Principle Instrumentation, and Applications, Desorption ionization methods, Spectroscopic Solutions of Structural Problems.

Learning Resources:

Text Books:

3. D. Pavia, G. M. Lampman, G. S. Kriz, J. R. Vyvyan, Introduction to Spectroscopy, Cengage Learning, 2015, 5th Edition.
4. P. S. Kalsi, Spectroscopy of Organic Compounds, New Age International Publishers, 2020, 8th, Edition.

Reference Books:

1. W. Kemp, Organic Spectroscopy, Palgrave Publishers, 2007, 3rd Edition.
2. R. M. Silverstein, F. X. Webster, D. J. Kiemle, D. L. Bryce, Spectrometric Identification of Organic Compounds, Wiley, 2014, 8th Edition.

CY17028 **3-0-0 (3)**

Emerging Topics in Organic Synthesis

Pre-Requisites: **None**

Course Outcomes:

CO-1	Understand the concepts of multicomponent reactions and their mechanisms
CO-2	Understand the tandem reactions in organic synthesis
CO-3	Apply the principles of click chemistry in drug discovery, biology and materials chemistry
CO-4	Utilize the soft metal catalyst in organic synthesis
CO-5	Discuss the flow chemistry, micro reactors, separation techniques and process chemistry in organic synthesis

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	3	–	3	–	3	3
CO-2	2	–	3	–	3	3
CO-3	2	–	3	–	3	3
CO-4	–	–	3	–	3	3
CO-5	3	–	3	–	3	3
CO-6	3	–	3	–	3	3

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Recent developments in the multicomponent reactions (MCRs): General Approaches of MCRs, Synthesis of different heterocyclic compounds using 3, 4 and 5 component reactions, MCRs using homogeneous and heterogeneous catalysts.

Importance of click chemistry, applications of click chemistry in drug discovery, biology and materials chemistry. alternative solvent systems in organic synthesis, recent developments in ionic liquids, deep eutectic solvents.

Tandem (cascade/domino) reactions in organic synthesis, metal carbenes in organic synthesis, *n*-heterocyclic carbenes in organic synthesis, hypervalent iodine reagents in organic synthesis.

Soft metals in organic synthesis: silver in organic synthesis, indium in organic synthesis, gold in organic synthesis. nanomaterials in catalysis and organic synthesis, photocatalysis.

Recent advances in flow chemistry and micro reactors, separation techniques, process chemistry, trouble shooting in organic synthesis.

Learning Resources:

Text Books:

1. R. P. Herrera, E. Marqués-López, Multicomponent Reactions: Concepts and Applications for Design and Synthesis, John Wiley & Sons. 2015, 1st Edition.
2. L. F. Tietze, G. Brasche, K. Gericke, Domino Reactions in Organic Synthesis, John Wiley & Sons, 2006.

Reference Books:

1. T. Wirth, Microreactors in Organic Synthesis and Catalysis, John Wiley & Sons, 2008.
2. K H Dtz, Metal Carbenes in Organic Synthesis, Springer Science & Business Media, 2004.

CY17030 **3-0-0 (3)**

Advances in Total Synthesis of Natural Products

Pre-Requisites: **Organic synthesis**

Course Outcomes:

CO-1	Understand the concepts and tactics used in total synthesis of natural products
CO-2	Illustrate the multistep organic synthesis using different reagents
CO-3	Develop the retrosynthetic analysis for complex natural products
CO-4	Analyze the different concepts and strategies in total synthesis
CO-5	Choose the synthon approach in total synthesis of natural products

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	1	-	3	-	2	2
CO-2	1	-	3	-	2	2
CO-3	1	-	3	-	2	3
CO-4	1	-	3	-	2	3
CO-5	1	-	3	-	2	3

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Concepts and tactics in organic synthesis, linear synthesis, Convergent, Divergent and Building block approaches.

Practical difficulties in large scale synthesis, Symmetry driven total synthesis of Resolvin E2.

Dearomatization strategies in natural product synthesis, protecting group free synthesis, Solid-phase chemistry in the total synthesis of non-peptidic natural products.

Structure, absolute configuration and total synthesis of natural products: Taxol.

Learning Resources:

Text Books:

1. E. M. Carreira, L. Kvaerno, Classics in Stereoselective Synthesis, Wiley-VCH, 2008.
2. E. J. Corey, X.-M. Cheng, The Logic of Chemical Synthesis, John Wiley & Sons Inc. 1995.

Reference Books:

1. K. C. Nicolaou, E. J. Sorensen, Classics in total synthesis-I: Targets Strategies, Methods, Wiley-VCH, 2000.

2. K. C. Nicolaou, Scott A. Snyder, Classics in total synthesis-II: More Targets Strategies, Methods, Wiley-VCH, 2003.

CY17032 **3-0-0 (3)**

Advances in Industrial Catalysis

Pre-Requisites:

Course Outcomes:

CO-1	Understand the synthesis and properties of Molecular sieves
CO-2	Classify catalysts based on the properties
CO-3	Analyze mechanisms of new catalytic reactions
CO-4	Evaluate the mechanisms of enzymatic catalysis
CO-5	Modify the catalyst to meet the required industrial applications

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	2	-	-	-	-	-
CO-2	1	1	-	-	-	-
CO-3	1	1	-	-	-	-
CO-4	-	1	-	-	-	-
CO-5	1	-	-	-	-	3

1 - Slightly; 2 - Moderately; 3 - Substantially

Syllabus:

Chapter-1: Introduction: The Phenomenon Catalysis; Mode of Action; Turnover Number, Turnover Frequency, Selectivity, Classification of Catalysts, Comparison of Homogeneous and Heterogeneous Catalysis and Langmuir Hinshelwood mechanism of Heterogeneous catalysis.

Chapter-2: Catalysts Preparation Methods: Ceramic Method; Microwave Method; Sol-gel Method; Co-Precipitation Method; Hydrothermal Method, Chemical Vapour deposition Method; Examples, Advantages, Limitations and Applications.

Chapter-3: Characterization of Catalysts: Elemental Analysis (Surface and Bulk), Low and Wide angle XRD, SEM – EDAX, TEM, TG/DTA, TPD-NH3, TG-MS, BET-Surface area, FT-IR, Raman, ESR, UV-Vis., XPS, MASNMR, and Cyclic voltammetry.

Chapter-4: Catalysis by Solid acids/bases/redox and multifunctional catalysts: Liquid phase, and Gas phase Catalysis, Examples, Solid acids/base: Alkylation, Cracking, Isomerization, Aromatization, and Methanol to olefin reaction. Solid redox catalysts: Phenol & Benzene hydroxylation, Ammoxidation, Alkane oxidation, Alcohol oxidation, Alkene epoxidation, Oxidative dehydrogenation, and Dye degradation. Multifunctional: Photocatalysis, Electrocatalysis, Applications in Petrochemical and Fine Chemical synthesis and one pot multicomponent synthesis.

Chapter-5: Other Industrially important catalysts and processes: Wilkinson catalyst, Zeigler Natta catalyst, Zeolites, Mesoporous materials, Hollow Silica, Metal Organo Framework, Nanocomposites, Fisher trope

synthesis, Heck reaction, Suzuki coupling reaction, Haber process, Bio-diesel production

Chapter–6: Biocatalysis: Mechanisms and Applications: Introductions, Mechanisms, Applications of Enzymes in Organic Synthesis, Oxidoreductase, Transferase, Hydrolase, and Lyase.

Learning Resources:

Text Books:

1. B. Viswanathan, S. Sivasanker, A.V. Ramaswamy, Catalysis: Principles and Applications, , Narosa Publishing House, New Delhi 2007.
2. Jens Hagen, Industrial Catalysis: A Practical Approach, Wiley-VCH, Verlag GmbH & Co. KGaA, 2006.

Reference Books:

1. R. Szostak, Van Nostrand Reinhold catalysis series, Molecular sieves of synthesis and Identification, New York, 1989.
2. R. Szostak, Hand book of molecular sieves, International zeolite association, 2010.
3. Mark E. Davis, Mesoporous Zeolites, Preparation, Characterization and Applications, Wiley-VCH, Verlag GmbH & Co. KGaA, 2015.
4. Lesley Smart and Elaine Moore, Solid State Chemistry an Introduction, Stanley Thomes (Publishers) Ltd., 2004, 2nd Edition.

CY17034 **3-0-0 (3)**

Microscopic and Diffraction Methods

Pre-Requisites: **Basic physical chemistry at bachelor level**

Course Outcomes:

CO-1	Analyze electron microscopic images for morphological and in-depth material characteristics
CO-2	Interpret X-ray and particle diffraction patterns in assigning the crystallographic aspects of materials
CO-3	Understand the concepts of X-ray spectroscopy and electron microscopy for qualitative and quantitative analysis of solid samples
CO-4	Evaluate atomic arrangements and interatomic forces in solid materials
CO-5	Choose an appropriate microscopic and diffraction technique along with sample preparation methodology for analysis of materials

Course Articulation Matrix:

	PO-1	**PO-2**	**PO-3**	**PO-4**	**PO-5**	**PO-6**
CO-1	2	1	2	2	1	3
CO-2	1	2	1	3	2	1
CO-3	3	1	3	1	–	2
CO-4	1	3	–	1	3	1
CO-5	2	–	2	2	3	2

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Scanning Electron microscopy: Scanning electron microscopy, instrumentation, electron sources – Thermionic and Field emission guns, electromagnetic lenses, resolution and contrast, environmental SEM, FE-SEM, Sample preparation, Backscatter and secondary electron detectors, Energy dispersive X-ray spectrometry (EDX), Environmental SEM, Applications.

Transmission Electron Microscopy: Transmission electron microscopy (TEM): Principle, instrumentation, Sample preparation, imaging, electron diffraction, reflection electron microscopy, applications.

Probe microscopy: Scanning tunneling microscopy (STM), principles, basic parameters, atomic resolution, surface imaging, lithography. Atomic force microscopy: Principles, Static and dynamic probes, Contact and Non-contact operation modes, Advantages and applications. Chemical force microscopy, AFM Lithography, applications.

Diffraction methods: Introduction, X-ray diffraction, small-angle X-ray diffraction, Electron diffraction, Principle, Instrumentation, Applications. Reflection high-energy electron diffraction (RHEED), Principle, Instrumentation, and Applications.

Learning Resources:

Text Books:

1. S. Holler, Crouch, Principles of Instrumental Analysis, Cengage Learning, 2020.
2. R F Egerton Physical principles of electron microscopy: an introduction to TEM, SEM and AEM, Springer, 2016.
3. J Goldstein, D Newbury, D Joy, C Lyman, P Echlin, E Lifshin, L Sawyer, J R Michael, Scanning electron microscopy and X-ray microanalysis, Springer, 2003 and 3rd Edition.

Reference Books:

1. J. C Vikerman, I. Gilmore, Surface Analysis: The Principal Techniques, Wiley 2009, 2nd Edition.
2. A. Rouessac, F. Rouessac Chemical Analysis – Modern Instrumentation Methods and Techniques, John Wiley, 2010, 6th edition.

CY17036 **3-0-0 (3)**

Supramolecular Chemistry

Pre-Requisites: **None**

Course Outcomes:

CO-1	Understand the importance of non-covalent interactions in chemistry
CO-2	Identify the importance of cation and anion complexation in organic chemistry
CO-3	Identify the significance of supramolecular interactions in guest recognition
CO-4	Explain how supramolecular chemistry is used in organic chemistry, materials science, chemical biology and nanotechnology
CO-5	Discuss how supramolecular chemistry can be used to facilitate sustainable development

Course Articulation Matrix:

	PO-1	**PO-2**	**PO-3**	**PO-4**	**PO-5**	**PO-6**
CO-1	2	1	1	1	1	3
CO-2	3	2	2	1	1	3
CO-3	2	1	1	1	2	2
CO-4	1	1	2	1	2	3
CO-5	2	2	2	1	1	3

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Non-covalent interactions: Ion pairing, Ion-Dipole Interactions, Dipole-Dipole interactions, Dipole-Induced Dipole and Ion-Induced Dipole interactions, *vander Waals* or Dispersion Interactions, Hydrogen bonding, Cation-p interactions, Anion-p interactions, p-p interactions, Closed shell interactions, Aromatic-Aromatic Interactions

Cation Complexation and applications: The High Dilution Rule, Templated Cyclizations, Crown Ether, Cryptands, Spherand and Hemipherand, Calixarenes, ion channels; complexation by ammonium ions.

Anion Complexation: Halide Ion Receptors, Complexation Properties of Macrocyclic Polyamines, Ditopic Receptors, Anion Receptors, Guanidinium Ions, Complexation of Ion Pairs

Applications of cation and anion complexation: Phase Transfer Catalysis and Anion Activation, Cation and Anion Sensors, Molecular Switches, Ion Selective Membrane Electrodes, Applications in Chromotographic Separations, Allosteric Effects; Rotaxanes and Catenane,

Complexation of Neutral molecules: Hydrophobic Pockets at the Active Sites of Enzymes and Antibodies, Cyclophane Receptors, Electronic Effects in Cyclophane Complexes with Aromatic Substrates and polyaromatic Hydrocarbons, Combination of Apolar Binding and Ion Pairing; Cryptophanes for Neutral Guest and Onium Ion Inclusion

Hydrogen Bonding: Synthons, Secondary Electrostatic Interactions in Hydrogen Bonding Arrays, Hydrogen Bonding Receptors, Hydrogen Bonding in Cleft-Type Synthetic Receptors, Macrocyclic

Hydrogen Bonding Receptors, Chiral Recognition in Supramolecular Complexes, Carbohydrate Recognition

Learning Resources:

Text Books:

1. J. W. Steed, J. L. Atwood, Supramolecular Chemistry, John Wiley & Sons Ltd., 2nd Edition, 2013.
2. J. M. Lehn, Supramolecular Chemistry: Concepts and Perspectives, VCH, Weinheim, 1st Edition, 1995.

Reference Books:

1. G. R. Desiraju, T. Steiner, The Weak Hydrogen Bond, Oxford Science Publications, 1999.
2. H. J. Schneider, A. Yatsimirsky, Principles and Methods in Supramolecular Chemistry, Wiley, Chichester, 2nd Edition. 2000.

CY17044 **3-0-0 (3)**

Green Chemistry

Pre-Requisites: **None**

Course Outcomes:

CO-1	Understand the principles of Green Chemistry
CO-2	Explain pollution causes and its prevention measures
CO-3	know about the renewable and non-renewable sources
CO-4	Apply concepts of green chemistry in organic synthesis
CO-5	Adopt green protocols for sustainable environment

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	2	2	1	1	1	2
CO-2	2	1	2	1	2	1
CO-3	2	1	2	2	1	3
CO-4	2	3	2	1	2	3
CO-5	–	–	–	–	–	–

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Introduction to Green chemistry: Basic principles of Green Chemistry and their illustrations with examples. Prevention of waste/by-products, Prevention/Minimization of hazardous/toxic products, Atom Economy, Green metrics, Designing safer chemicals - different basic approaches, Selection of appropriate auxiliary substances (solvents, separation agents etc), Energy requirements for reactions-use of microwave, ultrasonic energy, Selection of starting materials—use of renewable starting materials.

Examples of green synthesis/reactions: Green starting materials, Green reagents, real world cases (Traditional processes and green ones): Ibuprofen, Paracetamol, Seldinafil, Nylons, Pregabalin, and Prostaglandin. Hazard assessment and mitigation in chemical industry, Future trends in Green Chemistry: OHSA rules, Oxidation-reduction reagents and catalysts; biomimetic, multifunctional reagents; Combinatorial green chemistry (MCRs); Proliferation of solvent less reactions; Noncovalentderivatization. Biomass conversion, emission control.

Green solvents: Aqueous medium: Enhancement of selectivity, efficiency, and industrial applicability, Ionic liquids, Supercritical fluids, Solvent free neat reactions in liquid phase, Solvent free solid phase reactions, Flourous phase reactions, Flourous separating techniques, isolation of soybean oil and caffeine. Nonconventional energy sources: Microwave assisted reaction, Ultrasound assisted reactions, photochemical reactions using sunlight.

Green catalysis: Heterogeneous catalysis: Use of zeolites, silica, alumina, clay, polymers, cyclodextrin, and supported catalysts, Biocatalysis: enzymes, microbes, Phase-transfer catalysis (micellar/ surfactant etc), Green industrial processes- case studies, Green analytical methods.

Learning Resources:

Text Books:

1. V. K. Ahluwalia, M. Kidwai, New trends in green chemistry, Springer, 2012, 1st Edition.

2. R. Sanghi, M.M Srivastava, Green Chemistry: Environment Friendly Alternatives, Alpha Science International, 2009, 4th Edition.

Reference Books:

1. P.T. Anastas, J.C. Warner. Green Chemistry: Theory and Practice, Oxford University Press, 2000, 1st Edition.

CY17046 **3-0-0 (3)**

Polymer Chemistry

Pre-Requisites: **Organic Reactions and Mechanism, Thermodynamics and Kinetics**

Course Outcomes:

CO-1	To understand the relationships between polymer molecular weight, molecular weight distribution, and the properties of various polymers
CO-2	To demonstrate an ability to distinguish different polymerization reactions, mechanisms and kinetics of polymerization process
CO-3	To analyze polymerization data and predict the conversion, which will lead to critical thinking about how to improve the setup for better polymerization
CO-4	To expand their skills in performing and analyzing the thermal and mechanical properties of polymers, and demonstrate an ability to predict how the molecular weight and other parameters will affect these properties
CO-5	To propose plan on plastic manufacturing from resins and polymers

Course Articulation Matrix:

	PO-1	**PO-2**	**PO-3**	**PO-4**	**PO-5**	**PO-6**
CO-1	–	–	–	1	1	2
CO-2	1	1	–	–	2	3
CO-3	2	2	1	–	2	3
CO-4	1	2	3	1	2	3
CO-5	1	–	3	–	1	3

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Introduction to polymers: Classification, physical and chemical properties.

Polymerization methods: Step, chain, and living radical polymerization, thermoplastic and thermosetting, polymerization techniques and kinetics

Characterization methods, structure-activity relationships

Reactions of macromolecules

Specialty polymers

Plastic processing and fabrication

Learning Resources:

Text Books:

1. P. Bahadur, N. V. Sastry, Principles of Polymer Science, Narosa Publishing House, 2002.

2. M. P. Stevens, Polymer Chemistry, An introduction, Oxford University Press, 1999, 3rd Edition,

Reference books:

1. Mark, James E., Physical Properties of Polymer Handbook, 2nd edition, Springer, 2007
2. George Odian, Principles of Polymerization, 4th Edition, 2004

CY17048 **3-0-0 (3)**

Chemistry of Nanomaterials

Pre-Requisites: Basics of materials chemistry

Course Outcomes:

CO-1	Understand the history of nanoscience
CO-2	Classify nanomaterials based on structural properties
CO-3	Model suitable nanomaterials with desired shape, size and structure towards diverse applications
CO-4	Select an appropriate technique for characterizing new nanomaterial
CO-5	Predict the impact of nanomaterials on the environment

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	1	-	-	-	-	-
CO-2	-	1	-	-	-	-
CO-3	1	-	1	1	-	2
CO-4	-	3	-	3	-	-
CO-5	2	-	-	2	-	-

1 - Slightly; 2 - Moderately; 3 - Substantially

Syllabus:

Introduction: Nanostructure - an overview, Quantum confinement, dimensionality and size dependent phenomena, surface to volume ratio, surface dependent properties at nanoscale, Dimensionality based classification.

Synthesis and Characterization of Nanomaterials: Bottom-up approach: Sol-gel, microemulsions, co-precipitation, hydrothermal-solvothermal methods. Top-down approach: High energy ball milling, photolithography, waste to wealth creations; Characterization of nanomaterials using diffraction and microscopic methods, adsorption, light-scattering and electroanalytical techniques,

Applications: Solar energy harvesting and storage, catalysis, nanoelectronics, topological insulator, environmental remediations i.e CO_2 reduction, organic waste degradation.

Learning Resources:

Text Books:

1. T. Pradeep, Textbook of Nanoscience and Nanotechnology, Tata McGraw Hill Education Pvt. Ltd, 2012, 1st Edition

2. G. Dieter Vollath, Nanomaterials: An Introduction to Synthesis, Properties and Applications, Wiley-VCH Verlag GmbH & Co. KGaA, Germany, 2013, 2nd Edition

Reference Books:

1. C. N. R. Rao, A. Muller, K. Cheetham, Nanomaterials Chemistry, Wiley-VCH, 2007.
2. G. Cao, Nanostructures & Nanomaterials; Synthesis, Properties & Applications, Imperial College Press, 2007.

CY17050 **3-0-0 (3)**

Industrial Applications of Organic Chemistry

Pre-Requisites: **Organic synthesis and reaction mechanism**

Course Outcomes:

CO-1	Understand the concepts of organic chemistry to synthesize value added chemicals from various sources
CO-2	Apply the knowledge in industrial chemical transformations
CO-3	Analyse synthetic approaches economically viable industrial transformation
CO-4	Design the synthetic process using sustainable approach
CO-5	Develop industrially significant chemicals

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	2	–	1	–	2	2
CO-2	2	–	2	–	2	2
CO-3	2	1	2	–	3	3
CO-4	2	–	3	1	3	3
CO-5	3	1	3	2	3	3

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Value-added chemicals from non-renewable resources and further organic transformations.

Natural gas: conversion to value-added chemicals and materials.

Chemicals derived from renewable resources: Source, value-added chemicals, and products.

Bulk preparation methods.

Industrial chemicals derived by the Fermentation process.

Surface Active Agents, detergents, and pharmaceuticals.

Learning Resources:

Text Books:

1. M. A. Benvenuto, Industrial Organic Chemistry, Berlin, Boston: De Gruyter, 2017.
2. B. G. Reuben, J. S. Plotkin, H. A. Wittcoff, Industrial Organic Chemicals, Wiley, 3rd Edition, 2012

Reference Books

1. H. H. Szmant, Organic Building Blocks of the Chemical Industry, Wiley & Sons, 1989.

2. E. R. Riegel, J. A. Kent. Riegel's Handbook of Industrial Chemistry, 2007

CY17052 **3-0-0 (3)**

Statistical Treatment of Data and Quality Control

Pre-Requisites: None

Course Outcomes:

CO-1	Understand the significance of statistical concepts in chemical analysis
CO-2	Identify the type of errors occurring in the measurements and minimize them
CO-3	Apply appropriate calibration method in achieving results with highest precision
CO-4	Evaluate statistical tools for improving the quality of analytical measurements
CO-5	Develop a standard method for optimizing experimental procedures in analytical chemistry laboratories

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO1	2	2	-	1	1	1
CO2	2	1	-	1	3	2
CO3	3	1	-	2	-	2
CO4	2	3	-	2	2	1
CO5	2	-	1	1	1	2

1 - Slightly; 2 - Moderately; 3 - Substantially

Syllabus:

Significance tests: Comparison tests, t-test, paired t-test, t-test for means, F-test (one sided, two sided), Outliers, Q-test, G-test, ANOVA calculations

Quality of Analytical Measurements: Propagation of error, Quality control methods-property control charts, Precision control charts, Collaborative tests and uncertainty of measurements, Numerical calculations

Analytical methods Metrological Quality: Various types of analytical methods, Regression analysis, Limit of detection, Limit of quantification, Random error, Calibration of equipment and instruments, Curvilinear and outlier analysis.

Standard Method Development and Validation: Optimization of experimental procedures in analytical chemistry, Standard addition, External standard, internal standard and dilution methods, Experimental design-fractional factorial designs, Validation testing parameters and their calculation with numerical examples

Learning Resources:

Text Books:

1. J. N. Miller, J. C. Miller, Statistics and Chemometrics for Analytical Chemistry, Pearson, 2005, 5th Edition.

2. P. C. Meier, R. E. Zund, Statistical Methods in Analytical Chemistry, John Wiley & Sons, 2000, 2nd Edition.

Reference Books:

1. P. Konieczka, J. Namiesnik, Quality Assurance and Quality Control in the Analytical Chemical Laboratory, CRC Press, 2009, 2nd Edition.
2. D. B. Hibbert, Quality Assurance in the Analytical Chemistry Laboratory, Oxford University Press, New York, 2007, 1st Edition.

CY17054 **3-0-0 (3)**

Surface Analytical Techniques

Pre-Requisites: Understanding of general and physical chemistry. Familiarity with instrumental analyses is recommended

Course Outcomes:

CO-1	Understand the basic principles and instrumentation of surface analytical techniques
CO-2	Illustrate the methodology and applications of surface analytical techniques
CO-3	Identify suitable analytical technique for studying surface characteristics of diverse materials
CO-4	Analyze the data obtained from the analytical techniques to know the surface properties
CO-5	Design appropriate instrumental techniques for analysis of samples

Course Articulation Matrix:

	PO-1	PO-2	PO-3	PO-4	PO-5	PO-6
CO-1	2	2	1	1	1	1
CO-2	2	2	1	1	1	1
CO-3	1	1	3	2	1	1
CO-4	1	1	1	1	2	3
CO-5	1	1	1	2	2	3

1 - Slightly; 2 - Moderately; 3 - Substantially

Syllabus:

Surface structural analysis: Introduction to surface structural analysis and surface heterogeneity. Atomic force microscopy. Electron Spectroscopy for Chemical Analysis (ESCA) and Auger Electron

Spectroscopy (AES): Principles, Instrumentation, Quantification methods and standards,

Analytical Applications. Depth Profile Analysis.

Secondary Ion Mass Spectrometry (SIMS): Principle, Instrumentation, Specific Applications.

Surface-Enhanced Raman Spectroscopy (SERS): Principles, Electromagnetic theory of SERS, Sensitivity factor, Quantitative analysis, SERRS of Ag and Au metal colloids.

Electron Energy Loss Spectroscopy (EELS) and Electron Microprobe Analysis (EMPA): Principle, Instrumentation, Specific Applications.

Low Energy Ion Scattering Spectroscopy (LEISS): Principle, Instrumentation, Specific Applications.

Learning Resources:

Text Books:

1. J. F Watts, J. Wolstenholme, An introduction to surface analysis by XPS and AES, Wiley, 2003, 2nd Edition.
2. S. Schlucker, W. Kiefer, Surface enhanced Raman spectroscopy, Wiley VCH, 2011.

Reference Books::

1. D J O'Connor, Brett A Sexton, Roger S C Smart, Surface analysis methods in materials science, Springer Series in surface sciences, 2010, 2nd Edition.
2. J. C Vikerman, I. Gilmore, Surface Analysis: The Principal Techniques, Wiley, 2009, 2nd Edition.

CY17056 **3-0-0 (3)**

Chemical and Electrochemical Energy Systems

Pre-Requisites: Fundamentals in chemistry. Knowledge in electrochemistry is recommended.

Course Outcomes:

CO-1	Understand basic concepts of thermochemistry and chemical kinetics of energy Sources
CO-2	Illustrate principles of electrochemical energy storage systems and their applications
CO-3	Interpret principles of solar energy harnessing for promising applications
CO-4	Design new materials based on band gap engineering for energy harvesting
CO-5	Develop pilot devices for energy storage applications

Course Articulation Matrix:

	PO-1	**PO-2**	**PO-3**	**PO-4**	**PO-5**	**PO-6**
CO-1	3	1	–	1	–	1
CO-2	1	1	–	3	–	2
CO-3	1	1	–	3	1	2
CO-4	1	–	–	3	2	2
CO-5	–	1	–	3	1	2

1 - Slightly; **2 - Moderately;** **3 - Substantially**

Syllabus:

Thermochemistry and Chemical Kinetics of Energy Sources: Heats of Combustion of Fuels; Differential Scanning Calorimetry; Ignition Point, Flash Point; Coal Carbonization and Gasification; Chemical Energy Sources; Chemistry of Conventional and Non-Conventional Energy Materials: Petroleum Products, Petroleum Refinery; Biomass and Gober Gas; Hydrogen as a Fuel.

Electrochemical Energy Systems: Battery & Supercapacitors: Introduction about batteries, Solid state and molten solvent batteries, Metal ion batteries, Metal-air Battery, Supercapacitors and its applications. Fuel cells: Current-Voltage and Current Interrupt measurements; Porosity, Solid Oxide Fuel Cells.

Band gap engineering of materials for Solar Energy Harnessing: Concept of metal, semiconductor, insulator and their band structure. P-N junction and its behaviour in forward and reverse biasing, Metal semiconductor junctions i.e., schottky junction and ohmic contact and its behaviour in forward and reverse biasing, concept of band bending & band gap engineering. Photovoltaic and Photogalvanic energy storage, Regenerative Photoelectrochemical Cells; Photocorrosion; Electrodes with chemically modified surfaces. Photochemical and Photoelectrochemical Water Splitting: Chemically Modified Electrodes for Water Splitting; E-pH (Pourbaix) diagram of water.

Environmental Concerns and Green Methods of Energy Sources: Quality of Chemical Energy Sources; Monitoring of Energy Extraction from Materials; Nanochemical Methods in Energy Extraction; Modeling of Combustion and Other Energy Tapping from Materials

Learning Resources:

Text Books:

1. F. Vanek, L. Albright, L. Argenent, Energy Systems Engineering – Evaluation and Implementation, Mc Graw-Hill, 2016, 3rd Edition
2. R. Narayan and B. Viswanathan, Chemical and Electrochemical Energy Systems, University Press, 1998

Reference Books:

1. Lucia Gauchia, Javier Sanz, Dynamic Modeling of Electrochemical Energy Systems, LAP Lambert Academic Publishing, 2010
2. Peter Hoffmann, Byron Dorgan, Tomorrow's Energy: Hydrogen, Fuel Cells, and the Prospects for A Cleaner Planet, MIT Press, 2012
3. Piotrowiak, Laurie Peter, Heinz Frei and Tim Zhao, Solar Energy Conversion – Dynamics of Interfacidal Electron and Excitation Transfer, RSC, 2013