NATIONAL INSTITUTE OF TECHNOLOGY WARANGAL

SCHEME OF INSTRUCTION AND SYLLABI

for M.Sc. Organic Chemistry Program

(Effective from 2021-22)

DEPARTMENT OF CHEMISTRY

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

Towards Serving as a Potential Hub of Knowledge in Chemical Sciences and Allied Areas So as to Uphold and Strengthen the Vision of the Institute as One among Many Pillars While Striving Continuously in Pursuit of Excellence in Chemical Education, Chemical Research, Chemical Industry and All Interfaces of Chemistry with Society

MISSION

- Imparting Total Quality Education in Basic and Applied Chemistry to Develop Innovative, Entrepreneurial and Environment Friendly Graduates of Chemical Sciences of International Standards.
- Offering Relevant Fundamental and Applied Attributes of Chemistry, the Central Science, to Engineering Students as an Integral Part of Technical Education.
- Promoting Chemical Industry and Societal Service Sectors towards Environment-Friendly and Green Chemical Protocols by Innovation and Research in Cutting Edge Areas of Chemical and Allied Sciences
- Augmenting the Country's Needs of Human Resources and Scientific Manpower in Basic and Advanced Chemistry through Learner-Centric and *Atma Nirbhar Bharath* Modern Education and Research.

Department of Chemistry:

Brief about the Department:

The Department of Chemistry was established in the year, 1959, as an integral part of the Regional Engineering College Warangal (RECW). Since its inception, the Department is rated as one of the most academically active Departments in the Institute. The Department has a two-year M.Sc. Chemistry with specializations in Organic and Analytical Chemistry and offers chemistry course to all branches of Engineering. A 5-Year Integrated M.Sc. Programme in Chemistry will commence from the Academic Year, 2021-22. The Department is actively engaged in research in cutting-edge areas of Chemistry and contemporary topics of Organic, Inorganic, Physical and Analytical and Computational Chemistry. It offers PhD program in all branches of Chemistry and cutting-edge areas of Chemistry. It had produced the highest number of PhDs to date from any single Department in not only NIT Warangal but also among any other NIT in the country. The faculty members of the Department are active in quality teaching, research, and out-reach programs. Many of them are carrying out sponsored R&D projects in frontier areas of Chemical Sciences and Technologies besides popularization of sciences among the school students and masses. The Department completed FIST project level 1 and now level 2 FIST program is currently under progress.

The Department houses various state-of-the-art facilities such as a 400 MHz NMR, X-Band ESR, FTIR, UV-Vis-NIR and Fluorescence Spectrometers, LC-HRMS Spectrometer, Gas Chromatographs, HPLC, Electrochemical Workstations, Advanced Molecular Modelling Chemistry Software, etc. besides access to ICP-OES, CD-ORD, Powder XRD, SEM, TGA-DTA-DSC, Fuel Cell Workstations, etc. As a part of continuing education and outreach activities, the Department has been organizing several National and International Conferences, Seminars, and Workshops.

List of Programs offered by the Department:

Program	Title of the Program
Integrated M.Sc.	Integrated M.Sc., Chemistry
M.Sc.	Organic Chemistry
M.Sc.	Analytical Chemistry
Minor	Chemistry
Ph.D.	Chemistry

Note: Refer to the following weblink for Rules and Regulations of PG programs:
https://nitw.ac.in/main/%20RulesandRegulations/PGProgrammes/

M.Sc. – Organic Chemistry

Program Educational Objectives

PEO-1	Demonstrate proficiency in the fundamentals and application of physical, organic, inorganic and analytical disciplines of chemistry.
PEO-2	Demonstrate critical thinking and analytical reasoning in the development of chemicals, molecular materials and chemical processes for sustainable domestic and industrial applications.
PEO-3	Develop solutions to chemistry related societal and industrial needs and difficulties with suitable research methodologies and life-long learning and research skills.
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**	**PEO1**	**PEO2**	**PEO3**	**PEO4**
Imparting Total Quality Education in Basic and Applied Chemistry to Develop Innovative, Entrepreneurial and Environment Friendly Graduates of Chemical Sciences of International Standards	**3**	**2**	**2**	**1**
Offering Relevant Fundamental and Applied Attributes of Chemistry, the Central Science, to Engineering Students as an Integral Part of Technical Education	**3**	**3**	**2**	**2**
Promoting Chemical Industry and Societal Service Sectors towards Environment-Friendly and Green Chemical Protocols by Innovation and Research in Cutting Edge Areas of Chemical and Allied Sciences	**2**	**3**	**3**	**3**
Augmenting the Country's Needs of Human Resources and Scientific Manpower in Basic and Advanced Chemistry through Learner-Centric and *Atma Nirbhar Bharath* Modern Education and Research	**1**	**2**	**3**	**3**

1-Slightly; 2-Moderately; 3-Substantially

M.Sc. – Organic Chemistry

Program Outcomes

PO-1	Gain and apply the knowledge of chemistry to meet specific needs with appropriate considerations towards public health, safety, culture, society and environment.
PO-2	Create, select, and apply appropriate analytical techniques, resources including prediction and computational modelling to complex chemistry activities with an understanding of the limitations.
PO-3	Devise organic materials for societal needs in pharmaceutical, agricultural, environmental, electrical and electronics 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.

SCHEME OF INSTRUCTION

M.Sc. Organic Chemistry – Course Structure

I - Year, I – Semester

S. No.	Course Code	Course Name	L	T	P	Credits	Cat. Code
1	CY4101	Analytical Chemistry	3	0	0	3	PCC
2	CY4102	Main Group and Transition Metal Chemistry	3	0	0	3	PCC
3	CY4103	Reaction Mechanism and Stereochemistry	3	0	0	3	PCC
4	CY4104	Thermodynamics and Electrochemistry	3	0	0	3	PCC
5	CY4105	Molecular Spectroscopy	3	0	0	3	PCC
6	CY4106	Analytical Chemistry Laboratory	0	0	3	1.5	PCC
7	CY4107	Organic Chemistry Laboratory-I	0	0	3	1.5	PCC
8	CY4108	Computational Chemistry Laboratory	0	0	3	1.5	PCC
		Total				**19.5**	

I - Year, II – Semester

S. No.	Course Code	Course Name	L	T	P	Credits	Cat. Code
1	CY4151	Applications of Organic Spectroscopy	3	0	0	3	PCC
2	CY4152	Symmetry, Group Theory and Solid State Chemistry	3	0	0	3	PCC
3	CY4153	Photochemistry and Pericyclic Reactions	3	0	0	3	PCC
4	CY4154	Chemical Kinetics and Quantum Chemistry	3	0	0	3	PCC
5	CY416X	Elective-1	3	0	0	3	PEC
6	CY4155	Inorganic Chemistry Laboratory	0	0	3	1.5	PCC
7	CY4156	Organic Chemistry Laboratory-II	0	0	3	1.5	PCC
8	CY4157	Physical Chemistry Laboratory	0	0	3	1.5	PCC
9	CY4198	Seminar-1	0	0	2	1	SEM
		Total				**20.5**	

Elective-1 (I Year, II Semester)		
S. No.	**Course Code**	**Course**
1	CY4161	Organic Reagents and Name Reactions
2	CY4162	Organometallic Chemistry
3	CY4163	Chemical Education and Research

SCHEME OF INSTRUCTION

M.Sc. Organic Chemistry – Course Structure

II - Year, I – Semester

S. No.	Course Code	Course Name	L	T	P	Credits	Cat. Code
1	CY5101	Organic Synthesis	3	0	0	3	PCC
2	CY5102	Stereo Selective Synthesis	3	0	0	3	PCC
3	CY5103	Heterocyclic Chemistry and Aromaticity	3	0	0	3	PCC
4	CY5104	Chemistry of Natural Products	3	0	0	3	PCC
5	CY511X	Elective-2	3	0	0	3	PEC
6	CY512X	Elective-3	3	0	0	3	PEC
7	CY5105	Organic Analysis Laboratory	0	0	3	1.5	PCC
8	CY5106	Organic Preparations Laboratory	0	0	3	1.5	PCC
9	CY5148	Seminar-2	0	0	2	1	SEM
		Total				**22**	

Elective-2 (II Year, I Semester)		
S. No.	**Course Code**	**Course**
1	CY5111	Green Chemistry
2	CY5112	Food Chemistry
3	CY5113	Medicinal Chemistry
Elective-3 (II Year, I Semester)		
S. No.	**Course Code**	**Course**
1	CY5121	Advanced Organic Spectroscopy
2	CY5122	Functional Organic Materials
3	CY5123	Industrial Pharmaceutical Chemistry

II - Year, II – Semester

S. No.	Course Code	Course Name	L	T	P	Credits	Cat. Code
1	CY516X	Elective-4	3	0	0	3	PEC
2	CY517X	Elective-5	3	0	0	3	PEC
3	CY5197	Comprehensive Viva-Voce				2	CVV
4	CY5199	Dissertation Work				10	DW
		Total				**18**	

Elective-4 (II Year, II Semester)		
S. No.	**Course Code**	**Course**
1	CY5161	Drug Development and Delivery Systems
2	CY5162	Advances in the Total Synthesis of Natural Products
3	CY5163	Carbohydrate Chemistry

Department Elective Courses

Elective-5 (II Year, II Semester)		
S. No.	**Course Code**	**Course**
1	CY5171	Advanced Topics in Optical and Resonance Techniques
2	CY5172	Chemistry of Biomolecules
3	CY5173	Advances in Quantum Chemistry
4	CY5174	Emerging Topics in Organic Synthesis
5	CY5175	Industrial Organic Chemistry
6	CY5176	Supramolecular Chemistry

Credits in Each Semester					
Cat. Code	**Sem-I**	**Sem-II**	**Sem-III**	**Sem-IV**	**Total**
BSC					
ESC					
PCC	19.5	16.5	15		51
PEC		3	6	6	15
OEC					
HSC					
MNC					
SEM		1	1		2
CVV				2	2
DW				10	10
Total	**19.5**	**20.5**	**22**	**18**	**80**

Note: BSC – Basic Science Courses
ESC – Engineering Science Courses
PCC – Professional Core Courses
PEC – Professional Elective Courses
OEC – Open Elective Courses
HSC – Humanities and Social Science Courses
MNC – Mandatory Non-credit Courses
SEM – Seminar
CVV – Comprehensive Viva-Voce
DW – Dissertation Work

DETAILED SYLLABUS

M.Sc. – Organic Chemistry

Course Code: CY4101	ANALYTICAL CHEMISTRY	Credits L-T-P: Cr 3-0-0: 3

Course Outcomes:

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

CO1	Understand the basic concepts of qualitative and quantitative analysis
CO2	Interpret the sources of errors in analytical results
CO3	Recognize the quality of experimental measurements
CO4	Apply the analytical techniques for qualitative and quantitative estimation of unknown samples
CO5	Evaluate the pattern of experimental data using statistics

Course Articulation Matrix:

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

Syllabus:

Chapter-1 Chemical Analysis, Errors and Statistical Treatment of Data: Relevance and Concepts of Qualitative and Quantitative Analysis, Stoichiometry as the Basis of Chemical Analysis, Concentration Representation and Interconversions, Standard Solutions and Literature Standards, Good Laboratory Practices (GLPs); Accuracy and Precision; Errors and Error Distributions; Data Presentation and Statistical Treatment of Data; Finite Data Analysis; Standard Deviation; Criteria for Rejection of Data – Q-test, z- test, t-test, F-test.

Chapter-2 Separation methods: (a)Solvent extraction: Distribution Law, Extraction by Chelation, Extraction by Solvation, Extraction by Ion-Pair Formation, Batch and Continuous Extractions; Solid Phase Separation. (b) Chromatographic Separations: Basic Principle, Stationary and Mobile Phases, Planar (TLC) and Column Chromatography, HPLC, Size Exclusion Chromatography, Ion Exchange Chromatography, Affinity Chromatography, Separation of Enantiomers from Racemic Mixtures; Electrophoresis.

Chapter-3 Spectroanalytical Methods: Beer Lambert's law, Deviations of Beer's Law, absorption spectrophotometry – Instrumentation Schematics, Jablonski diagram, Fluorescence and Phosphorescence.

Chapter-4 Thermoanalytical Methods: Thermogravimetry; Differential Thermal Analysis (DTA); Differential Scanning Calorimetry (DSC); Temperature Control Methods-Thermostatic Circulators and Peltier Thermostats, Applications.

Chapter-5 Electroanalytical Methods: Conductometry; Potentiometry; Electrogravimetry; Coulometry; Fundamentals of Voltammetry.

Chapter-6 Bioassaying and Pharmacological Assaying: Sample Collection and Incubation;

Antibacterial and Antifungal Methods.

Chapter-7 Automated Methods of Analysis: Auto samplers, Microprocessor; Data Processing; Tandem Sensors; DA and AD Convertors; Spectral Libraries and Chemical Databases.

Learning Resources:

Text Books:

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

Reference Books:

1. Modern Analytical Chemistry, David Harvey, McGraw Hill, 1999 and 1st Edition.
2. Quantitative Analysis, Day and Underwood, PHI, 2009 and 6th Edition.

Course Code: CY4102	MAIN GROUP AND TRANSITION METAL CHEMISTRY	Credits L-T-P: Cr 3-0-0: 3

Course Outcomes:

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

CO1	Understand the structure, bonding and properties of metal carbonyls, metallocenes and main group compounds
CO2	Interpret the role of various metal ions in biology and medicine
CO3	Apply the concepts of bonding for interpreting structural properties of coordination compounds
CO4	Analyze electronic spectra and magnetic properties of coordination compounds
CO5	Correlate the kinetics and mechanisms involved in inorganic reactions

Course Articulation Matrix:

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

Syllabus:

Chapter-1 Coordination Chemistry: Review of CFT : Crystal field splitting in distorted octahedral, trigonal bipyramidal and square pyramidal complexes, Crystal field splitting energy and factors affecting it, CFSE values and its applications-Crystal structure of spinels, Correction in heat of hydration and lattice energy values, LS coupling scheme: Determination of ground state terms, Pigeon hole diagram method-Calculation of all possible term symbols: Hund's rules and its applications, Asymmetric and symmetric electron configurations and distortions, Jahn-Teller theorem-Calculation of JTSE and applications, Molecular orbital theory: MOED of octahedral, tetrahedral and square planar complexes of sigma and pi complexes.

Chapter-2 Stability, Magnetism and Electronic spectroscopy: Determination of Stoichiometry of a metal complex-Jobs methods, Mono variation, Continuous variation and Slope ratio methods, Stability constants-Stepwise and Overall stability constants and relation between them-Factors influencing the stability constants, Determination of stability constant of a metal complex by spectrophotometric method and pH metric method, Types, determination of magnetic susceptibility by Guoy's method, spin-only formula, spin-orbit coupling, Quenching of orbital contribution, Electron spectra of metal complexes- selection rules-relaxations-Mulliken term symbols-Electron transitions for octahedral and tetrahedral complexes, Orgel diagrams for d1-d9 electron configurations, Tanabe-Sugano diagrams for d2 configuration, Nephelauxetic series, Racah Parameter, Charge transfer spectra: M to L and L to M-Examples.

Chapter-3 Organometallic Compounds:18 electron rule-Calculations and applications, Metal carbonyls- classification of low nuclearity and high nuclearity carbonyl clusters, preparations and properties of Carbonyls. Bonding in carbonyl clusters, Metallocenes: Ferrocene-preparation methods and properties. Bonding and molecular orbital energy diagrams of

sandwich compounds.

Chapter-4 Inorganic Reaction Mechanism: Substitution Reactions in octahedral complexes-A, D and I Mechanisms, Acid hydrolysis, Factors affecting acid and base hydrolysis, Substitution reactions in square planar complexes; Trans Effect-theories and applications, Electron Transfer Reactions-Outer Sphere and Inner Sphere Mechanisms.

Chapter-5 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.

Chapter-5 Bio-inorganic Chemistry: Metal ions in Biological Systems; Metal Containing Units in Biology, Hemoglobin and Myoglobin; Electronic and Magnetic Aspects of Dioxygen Binding; Oxygen Adsorption Isotherms and Cooperativity in Hemoglobin and Its Physiological Significance. Electron transport proteins.

Learning Resources:

Text Books:

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

Reference Books:

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

Course Code: CY4103	REACTION MECHANISMS AND STEREOCHEMISTRY	Credits L-T-P: Cr 3-0-0: 3

Course Outcomes:

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

CO1	Understand kinetic and thermodynamic aspects of the chemical reactions
CO2	Classify chiral molecules using symmetry elements
CO3	Identify various types of organic reactions with mechanisms
CO4	Apply stereochemistry principles in interpreting molecular conformations
CO5	Predict the stereochemistry of the products

Course Articulation Matrix:

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

Syllabus:

Chapter-1 Structure and reactivity: Nomenclature, General rules as applied to bicyclic compounds, spiro and heterospiro compounds. Nature of reaction energy and kinetic considerations: Chemical kinetics, equilibria and energetics of reactions, Thermodynamics, kinetics, enthalpy, entropy, free energy, exergonic and endergonic reactions. Types of organic reactions, reactive intermediates: formation and stabilization, concept of tautomerism.

Chapter-2 Aliphatic and aromatic substitution reactions: SN^1, SN^2, SN^i, $SN^{i'}$, $SN^{1'}$, $SN^{2'}$, SE1, SE2, SEi mechanism, solvent effects, competition between SN^1 and SN^2 mechanism, General ideas about SE1, SE2, mechanisms. Methods of determination of reaction mechanisms, product analysis, determination of presence of intermediates, crossover experiments, isotopic experiments, Linear free energy relationships, Hammett equation, Taft treatment of polar effects in aliphatic compounds. Neighboring group participation of O, S, N, halogens, aryl groups, alkyl and cycloalkyl groups in nucleophilic substitution reactions. Sigma, Pi bond participation in acyclic and bicyclic systems (Non- classical carbocations).

Chapter-3 Elimination reactions: El, E1CB, E2 mechanisms, orientation in elimination reactions. Saytzeff and Hoffman eliminations, cyclic eliminations, stereochemistry of elimination in acyclic and cyclic systems, elimination versus substitution reactions, formation of carbon-carbon double bonds via elimination reactions; pyrolytic, syn and anti-elimination.
Addition Reactions: Addition to carbon multiple bonds - Addition reactions involving electrophiles, nucleophiles and free radicals, cyclic mechanisms, orientation and stereochemistry, hydrogenation of double and triple bonds, hydroboration, Birch Reduction. Michael reaction, addition of oxygen and Nitrogen; (b) Addition to carbon-hetero atom multiple bonds: Mannich reaction.

Chapter-4 Stereochemistry: Chirality and symmetry elements, classifications of chiral molecules based on symmetry (dissymmetric and asymmetric molecules) and energy criterion, chirality in trialkyl amines, phosphines etc. CIP rules for *R*, *S*-nomenclature, threo, erythro-nomenclature, classification of racemic mixtures, racemization methods, resolution methods, Geometrical isomerism (*cis*, *trans* and *E*, *Z*-nomenclature). Stereochemistry of the compounds containing –C=N and –N=N–, Dynamic enantiomerism.
Concept of Prochirality, Topicity (Homotopic and Heterotopic atoms, groups and ligands), Homotopic and Heterotopic faces.
Axis of chirality: Elongated tetrahedron, examples of axis of chirality, *R*, *S*-nomenclature of biphenyls (atropisomerism), Buttressing effect, allenes, spiro compounds etc.
Plane of chirality: Para cyclophanes, Ansa compounds, helicity (plus and minus helices), hexahelicene.

Chapter-5 Conformational analysis: cyclopentane, cyclohexane, mono and disubstituted cyclohexanes, 1, 2-dihaloethanes, chlorohydrin, 2, 2, 3, 3-tetrachlorobutane, stereochemistry and conformational analysis of decalins, octalins, hydrindanes, perhydro phenanthrenes, quinolizidines. Aziridine, piperidine, conformations of THP, exo-anomeric effect, Rabbit ear effect.

Learning Resources:

Text Books:

1. Reaction Mechanism in Organic Chemistry, S.M. Mukherjee and S. P. Singh, Macmillan India Limited, 2020.
2. Organic Chemistry, Francis A. Carey, Tata McGraw Hill publishing company Limited, New Delhi 2010, 8th Edition.
3. Organic Chemistry, Vol. I & II, I. L. Finar, Pearson Education India, 2002, 5th Edition.
4. Organic Reactions and Their Mechanisms, P. S. Kalsi, New Age International Private Limited, 2017, 4th Edition.

Reference Books:

1. A guidebook to mechanism in Organic Chemistry, Peter Sykes, ELBS, 2009, 6th Edition.
2. Advanced Organic Chemistry Reactions, Mechanism & Structure, Jerry March, Wiley, 2007, 6th Edition.
3. Stereochemistry of Organic Compounds: Principles and Applications, Fourth Edition, D. Nasipuri, New Age International Publishers, 2020.

Course Code: CY4104	THERMODYNAMICS AND ELECTROCHEMISTRY	Credits L-T-P: Cr 3-0-0: 3

Course Outcomes:

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

CO1	Understand the laws of thermodynamics and concepts of electrochemistry
CO2	Interpret the electrochemical characteristics of electrolytes
CO3	Apply thermodynamic principles to chemical reactions
CO4	Utilize the concepts of electrochemistry and electrokinetic phenomenon for various physical insights
CO5	Evaluate the thermodynamic parameters using partition function

Course Articulation Matrix:

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

Syllabus:

Chapter-1 Classical Thermodynamics: Introduction of Thermodynamic Laws and Various Thermodynamic Variables (Concept of Entropy, Changes in Entropy, and Free Energy, Reversible and Irreversible Processes, State Functions and Path Functions), Thermodynamic Relationships and Applications, Partial Molar Quantities, Phase equilibria and Phase Rule, Fugacity, Activity and Activity Coefficient, Third Law of Thermodynamics: Absolute Entropy of Solids, Liquids and Gases; Cryoscopic Evaluation of Absolute Entropy of Solids; Cryogenics of Asymptotic Approach to Absolute Zero Temperature.

Chapter-2 Statistical Thermodynamics: Statistical Treatment of Entropy; Maxwell-Boltzmann Functions, Partition Functions and Their Relation to Thermodynamic Variables, Bose-Einstein and Fermi-Dirac Statistics.

Chapter-3 Electrolytic Conduction: DHO Theory of strong electrolytes-Inter-Ionic Atmosphere, thickness of ionic atmosphere, time of relaxation of ionic atmosphere (no derivation) Debye Huckel Onsager treatment and derivation of conductance equation – validity of DHO equation and deviations – significance of degree of dissociation-Debye-Falkenhagen effect (Dispersion of conductance at high frequencies), Wein effect (conductance with high potential gradients) -Activity and Activity coefficients, Ionic strength-Numerical problems related Ionic strength, Debye Hukel theory of activity coefficients-Debye Huckel Limiting law (derivation) -validity-Concept of ion association (Debye-Huckel-Bjerrum equation) – ion pair formation association constant – conductance minima and triple ions.

Chapter-4 Electrodics and Interfacial Electrochemistry: Theories of Electrical Double-Layer-Electrodes, Electrokinetic phenomena-Electroosmosis, electrophoresis, streaming potential, zeta potential; Butler-Volmer Equation (Derivation); Polarisation of electrodes, decomposition potential and over voltage, Tafel Equation; Applications of over voltage;

Equilibrium Electrochemistry: Electrode Potentials, reference electrodes, electrochemical cells-Nernst equation for electrode potential and cell emf, thermodynamic formulation, applications of emf measurements, Concentration cells with and without transference, liquid junction potential and its determination

Chapter-5 Electroanalytical Methods and Electrochemical Energy Systems: Conductometric Titrations (Mixture of Acids and Mixture of Bases), Potentiometric Titrations: (acid-base, redox, and precipitation, pK_a of Polybasic Acids), Ion-Selective Electrodes: (glass electrode, fluoride electrode) and Chemically Modified Electrodes as sensors (urea sensor, glucose sensor) Rechargeable Batteries (Lead-acid batteries, Ni-Cd Cell, Li-ion Battery), types of Fuel Cells with examples, Photovoltaic Cells, Basic concepts of Electrochemical supercapacitors,Fundamentals of Cyclic voltammetry.

Learning Resources:

Text Books:

1. Thermodynamics for Chemists, S. Glasstone, East-West Publishers, 2008
2. Molecular Thermodynamics, Donald A. Macquarrie John D. Simon, Viva Books-2018, Viva student edition
3. An introduction to Electrochemistry, Samuel Glasstone, East-West Publishers 2006
4. A textbook of Physical Chemistry, K.L. Kapoor, volume 3, McGraw Hill Education, 2015 and 3rd edition.

Reference Books:

1. Physical Chemistry, P. Atkins and Julia de Paula, Oxford, 2011 and 9th Edition
2. Principles of Physical Chemistry, Puri, Sharma, Pathania, Vishal Publications, 2020 and 48th Edition
3. Advanced Physical Chemistry, Gurdeep Raj, Goel publishing, 2019 and 42 Edition
4. Physical Chemistry: A Molecular Approach (Viva student edition), Donald A Mcquarrie, John D Simon, Viva Books-2015

Course Code: CY4105	MOLECULAR SPECTROSCOPY	Credits L-T-P: Cr 3-0-0: 3

Course Outcomes:

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

CO1	Define interactions of electromagnetic radiation with matter
CO2	Understand molecular symmetry, structure and motions with rotational, vibrational and electronic quantum levels and spectral properties
CO3	Analyze molecular structure and geometry with magnetic resonance spectral characteristics
CO4	Evaluate molecular mass and fragmentation patterns with molecular structure and functionalities
CO5	Justify molecular functionality and structure comprehensively

Course Articulation Matrix:

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

Syllabus:

Chapter-1 Microwave Spectroscopy: Rotation of Molecules, Rigid and Non-rigid Rotors; Quantum Aspects of Molecular Rotational Energy and Selection Rules of Transitions; Diatomic and Polyatomic Molecules, Instrumentation; Applications of Microwave Spectroscopy.

Chapter-2 Infrared and Raman Spectroscopy: Quantum Aspects of Molecular Vibrational Energy and Selection Rules of Vibrational Transitions; Vibrational Rotational Spectra; Instrumentation; Applications; Raman Effect; Quantum Mechanical Description; Rotational and Vibrational Raman Spectra; Mutual Exclusion and Complementarity

Chapter-3 Electronic Spectroscopy: Types of Electronic Transitions; Instrumentation; Applications.

Chapter-4 Nuclear Magnetic Resonance Spectroscopy: Magnetic Nuclei and Nuclear Spin; NMR Spectral Phenomenon, Relaxation Mechanism; *^{1}H NMR Spectroscopy*: Chemical Shift; Instrumentation; Spin-Spin Coupling; Nuclear Overhauser Effect; 2-D NMR Spectroscopy (COSY) ; INDOR and NOE Methods.
^{13}C NMR Spectroscopy: Fourier Transform NMR; Off-Resonance and Spin-Decoupled ^{13}C NMR Spectroscopy; Applications; Magnetic Resonance Imaging (MRI); *NMR Spectroscopy of ^{19}F, ^{15}N and ^{31}P nuclides.*

Chapter-5 Electron Spin Resonance Spectroscopy: Electron Spin and Its Magnetism; 'g'-Factor; ESR Spectral Phenomenon; Instrumentation; Applications; Electron Spin-Nuclear Spin Coupling; *ENDOR*

Chapter-6 Mass Spectrometry: Mass spectrometry - Trajectories of Charged Bodies in Electrical and Magnetic Fields; Molecular Fragmentation; Resolution by Magnetic, Quadruple and Time of Flight Methods; Applications; Hyphenated Techniques.

Learning Resources:

Text Books:

1. Fundamentals of Molecular Spectroscopy, C N Banwell and E M McCash, Tata McGraw Hill Education, 4th Edn., 2017.
2. Modern Spectroscopy, Michael Hollas, Wiley, 4th Edn., 2013.
3. Atomic and Molecular Spectroscopy: Basic concepts and applications, Rita Kakkar, Cambridge, 2015
4. Infrared and Raman Spectra of Inorganic and Coordination Compounds, Nakamoto, Wiley Inter Science, 6th Edn., 2009.

Reference Books:

1. Molecular Structure and Spectroscopy, Aruldhas, PHI Learning, 2nd Edn, 2007.
2. Organic Spectroscopy, William Kemp, Macmillan, 2009, 3rd Edition.

Course Code: CY4106	ANALYTICAL CHEMISTRY LABORATORY	Credits L-T-P: Cr 0-0-3: 1.5

Course Outcomes:

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

CO1	Obtain hands-on experience in the volumetric analysis, gravimetric analysis and some instrumental methods
CO2	Apply the principles involved in conductometry, pH metry and potentiometry for determining various physical parameters
CO3	Utilize gravimetric analysis for quantifying metal ions
CO4	Analyze water samples for their hardness and alkalinity
CO5	Estimate metal content in domestic and industrial samples

Course Articulation Matrix:

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

Syllabus:

Determination of different types of alkalinity of a water by volumetric method.

Determination of Fe^{2+} in hematite by dichrometry.

Determination of available chlorine from bleaching powder.

Determination of different types of hardness of water by complexometric method.

Determination of sulphate by semi gravimetric method.

Determination of Ni^{2+} using DMG by Gravimetric method.

Determination of Al^{3+} using oxine by gravimetric method.

Determination of Cu^{2+} by gravimetric method and Ni^{2+} by volumetric method from a mixture.

Analysis of metal complexes by IR spectroscopy.

Potentiometric titration of a weak acid with strong base and determination of dissociation constant of the acid using quinhydrone electrode.

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

Determination of hydrolytic constant K_h of NH_4Cl solution pH-metrically.

To determine the acid and base dissociation constants of an amino acid and hence the isoelectric point of the acid by pH meter.

To determine the equivalent conductance of weak electrolyte at infinite dilution by Kohlrausch's law of independent migration of ions and verification of Ostwald's dilution law using conductometry.

Determination of strengths of HCl, KCl, NH_4Cl in a mixture conductometrically using standard NaOH and $AgNO_3$ solution.

To determine the surface tension of methyl alcohol, ethyl alcohol and n-hexane at room temperature and also to calculate atomic parachors of C, H, Oxygen.

Determination of Isosbestic Point of an Acid-Base Indicator spectrophotometry.

Learning Resources:

Text Books:

1. Vogel's Textbook of Quantitative Chemical Analysis, G H Jeffery, J Bassett, J Mendham and R C Denney, Longman Inc., 1989, 5th Edition
2. Physical Chemistry Laboratory Manual, Amritha Anand, Ramesh Kumari, Wiley, 2019

Reference Books:

1. Vogel's Textbook of Quantitative Chemical Analysis, G H Jeffery, J Bassett, J Mendham and R C Denney, Longman Inc., 1989, 5th Edition
2. Advanced Practical Physical Chemistry, J.B. Yadav, 38th Edition, 2019

Course Code: CY4107	ORGANIC CHEMISTRY LABORATORY-I	Credits L-T-P: Cr 0-0-3: 1.5

Course Outcomes:

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

CO1	Understand the principles involved in separation and purification techniques
CO2	Obtain hands-on experience of chromatography techniques
CO3	Demonstrate the skills of organic synthesis
CO4	Analyze the functional groups in organic molecules
CO5	Choose an appropriate technique for the purification of synthesized compound

Course Articulation Matrix:

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

Syllabus:

Chapter-1 Determination of physical constants (melting and boiling points) Purification Techniques: Crystallization, Decolourization, fractional crystallization, Sublimation, Simple distillation, Fractional distillation, Vacuum distillation and Steam distillation.

Chapter-2 Isolation and purification of products by chromatographic techniques: TLC & Column Chromatography.

Chapter-3 Solubility tests for organic compounds, identification of single functional group in the organic compounds.

Chapter-4 Synthesis of simple organic compounds, Aspirin, hippuric acid, *m*-nitroaniline, Oxidative coupling reaction: BINOL.

Learning Resources:

Text Books:

1. Laboratory Manual of Organic Chemistry, R. K. Bansal, New Age International Private Limited, 2009, 5th Edition.
2. Compressive Practical Organic chemistry, V. K. Ahluwalia, Universities Press, 2004.
3. Elementary Practical Part III (Quantitative Analysis) Organic Chemistry, Dorling Kindersley India Ptv Ltd., 2011, 1st Edition.

Reference Books:

1. Practical Organic Chemistry, F. G. Mann & B.C Saunders, Pearson Education India, 2009.
2. Text Book of Practical Organic Chemistry, Vogel A. I., ELBS, 2004, 5th Edition.

Course Code: CY4108	COMPUTATIONAL CHEMISTRY LABORATORY	Credits L-T-P: Cr 0-0-3: 1.5

Course Outcomes:

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

CO1	Understand the basics of computer and chemistry software
CO2	Demonstrate data presentation using software
CO3	Build the models related to chemistry
CO4	Apply the first principles to generate potential energy surface, hydrogen bonding, and reaction mechanism
CO5	Predict the structure & properties of molecules and reaction mechanisms using the tools of computational chemistry

Course Articulation Matrix:

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

Syllabus:

Chapter-1 Basics of Computer Hardware and Software Knowledge: Physical Components of Desktop Computer and Assembly; Operating Systems; Open-Access and Commercial OS.

Chapter-2 MS-Office for Chemical Applications: MS-Word for Chemical Documentation; MS-PowerPoint for Virtual Chemical Animations; MS-EXCEL for Data Processing, Graphical Representations and Curve-Fitting; Chemical Databases and Introduction to Cheminformatics.

Chapter-3 Golden Software: Surfer and Grapher: Contour and Surface 3-d Plots of z = f(x,y) Functions; Gridding of z = f(x, y) Kind Data Sets.

Chapter-4 Molecular Structure and Labware Drawing Software: ISIS Draw; ACD-Labs; ChemDraw.

Chapter-5 Molecular Modelling and Quantum Calculations
Introduction to Z-Matrix, Energy of Point Structure, Energy Minimization and Concept of PES, IR Spectra of Molecule and Minimum, Saddle Points on PES, Non-Covalent Interactions and Concept of BSSE, Reaction Mechanism (Kinetics and Thermodynamics).

Learning Resources:

Text Books:

1. Exploring Chemistry with Electronic Structure Methods, J.B. Foresman and AE. Frisch, Gaussian, Inc.: Wallingford, CT, 2015, 3rd Edition.
2. Avogadro: Molecular Editor and Visualization (Manual), Taylor Cornell and Geoffrey Hutchison, 2015.

Reference Books:

1. Handbook of Computational Chemistry, Jerzy Leszczynski, Springer, 2012.
2. Computational Chemistry: A Practical Guide for Applying Techniques to Real World Problems, David Young, Wiley, 2004.

Course Code: CY4151	APPLICATIONS OF ORGANIC SPECTROSCOPY	Credits L-T-P: Cr 3-0-0: 3

Course Outcomes:

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

CO1	Summarize the basic principles of spectroscopy
CO2	Identify the structure of organic compounds using spectroscopy
CO3	Analyze the structural aspects and stereochemistry of organic compounds using spectroscopy
CO4	Interpret molecular mass and fragmentation of organic compounds using mass spectrometry
CO5	Solve the structure of unknown organic compounds by using spectral data

Course Articulation Matrix:

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

Syllabus:

Chapter-1 Ultraviolet and Visible Spectroscopy: Origin and designations of bands. Characteristic absorptions of organic compounds. Factors influencing the position of UV bands. Woodward-Fieser rules for calculating absorption maxima of unsaturated compounds and related compounds. Applications of UV spectroscopy.

Chapter-2 Infrared Spectroscopy: Interpretation of illustrative examples. Coupled vibrations, Fermi Resonance, hydrogen bonding, I and M effects. Characteristic absorptions in common classes of compounds. Applications of IR spectroscopy.

Chapter-3 NMR spectroscopy-I (^{1}H-NMR): Chemical shifts, Equivalent and non-equivalent protons, enantiotopic and diastereotopic protons, Factors affecting the chemical shifts, electronegativity, effect of hydrogen bonding and anisotropy, shielding and deshielding effects, Signal integration, Spin-spin coupling: vicinal, germinal and long range coupling, coupling constants and factors affecting coupling constants. ^{1}H-NMR of organic molecules ethyl acetate, ethanol, anisole, paracetamol, *p*-Toluidine, ethyl benzoate, *N*-acetanilide and cinnamaldehyde. First order and non-first order spectra e.g., AX, AX2, AX3, A2X3, AMX and AB, AB2 ABC. Simplification of complex spectra: increased field strength, deuterium exchange, lanthanide shift reagents and double resonance techniques. Nuclear Over Hauser enhancement (NOE). Applications of ^{1}H-NMR spectroscopy.

Chapter-4 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.

Chapter-5 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: odd electrons and even electrons containing neutral and charged species (even electron rule), Nitrogen rule, isotopic peaks, metastable peaks. High resolution mass spectrometry. Determination of molecular formula. Salient features of fragmentation pattern of organic compounds including β-cleavage, Mc-Lafferty rearrangement, retro Diels – Alder fragmentation and ortho effect.

Learning Resources:

Text Books:

1. Organic Spectroscopy, William Kemp, Macmillan, 2009, 3rd Edition.
2. Spectroscopy of Organic Compounds, P. S. Kalsi, New Age International Publishers, 2020, 8th Edition.
3. Organic Spectroscopy: Principles & Applications, Jag Mohan, Narosa, 2020, 3rd Edition.

Reference Books:

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

Course Code: CY4152	SYMMETRY, GROUP THEORY AND SOLID STATE CHEMISTRY	Credits L-T-P: Cr 3-0-0: 3

Course Outcomes:

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

CO1	Understand structures of crystal systems and imperfections in crystals
CO2	Relate the knowledge of diffraction techniques for structure determination
CO3	Understand electrical, optical and dielectric properties of solids
CO4	Interpret molecular symmetry, symmetry operations and molecular point groups
CO5	Apply symmetry and group theory in electronic spectra of atoms and molecules

Course Articulation Matrix:

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

Syllabus:

Chapter-1 The crystal structure: Lattice Energy, Miller Indices, Imperfection in a crystal: Point defects and Line Defects, Types of crystals, X-ray diffraction: Single crystal and Powder Methods: The Debye Scherrer Method, Electron diffraction, Neutron diffraction.

Chapter-2 Properties of solids: Superconductivity: Low Temperature superconductivity, High Temperature Superconductivity, BCS theory, Electrical Properties, Magnetic properties and Optical & dielectric properties.

Chapter-3 Molecular Symmetry: Symmetry Operations and Elements of Symmetry: Rotational Axis of Symmetry, Plane of Symmetry, Improper Rotational Axis of Symmetry (Alternate Axis of Symmetry), Centre of Symmetry, Identity Element, Cartesian Coordinate System and Symmetry Elements, More about Symmetry Elements.

Chapter-4 Group Theory and Molecular Point Groups: Mathematical requirements for a point group, Group multiplication tables, Isomorphic groups, Group generating elements, Subgroups and Classes-exercises, Point groups, Identification of Molecular point groups, Notation of Point Groups, Systematic assignment of point groups to molecules, Descent in Symmetry of Molecules with substitution, Exercises on Point Groups, Matrix Representations of Symmetry Elements, Matrix Representations of Point Groups, Point Group and Character tables, Reducible and Irreducible Representations, Properties of Irreducible Representations.

Chapter-5 Application of Symmetry and Group Theory: Symmetry of Normal Modes of Vibrations of Molecules, Cartesian Coordinate and Internal Coordinate Methods, Infrared and Raman Activity, Internal Coordinates and Redundancy.General sequence of steps for normal mode analysis and exercises, Hybridization and Internal coordinate method, Symmetry and

Stereoisomerism, Symmetry Criteria for Optical Activity; Symmetry Restrictions on Dipole Moment.

Learning Resources:

Text Books:

1. Solid State Chemistry, An Introduction, Lesley Smart, Elaine Moore, CRC press, 2020, 5th Edition.
2. Symmetry and Group Theory in Chemistry, Mark Ladd, Marwood Publishers, London, 2000.

Reference Books:

1. Solid State Chemistry, D.K. Chakrabarty, New Age International (P) Limited, 2010, 2nd Edition.
2. Symmetry and Spectroscopy of Molecules, K. Veera Reddy, New Age International, 2020, 2nd edition.

Course Code: CY4153	PHOTOCHEMISTRY AND PERICYCLIC REACTIONS	Credits L-T-P: Cr 3-0-0: 3

Course Outcomes:

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

CO1	Understand the photochemical and thermal reactions
CO2	Classify the various types of pericyclic and photochemical reactions
CO3	Apply the orbital correlation and frontier molecular orbital methods for pericyclic reactions
CO4	Evaluate various types of organic photochemical reactions with mechanisms
CO5	Predict the stereochemical outcome of pericyclic and photochemical reactions

Course Articulation Matrix:

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

Syllabus:

Chapter-1 Organic Photochemistry: Photochemical energy, Frank Condon Principle, Jablonski diagram, Singlet and Triplet states, Dissipation of photochemical energy, Photosensitization, Quenching, Quantum efficiency and Quantum yield, Experimental methods of photochemistry, Photochemistry of carbonyl and non-carbonyl compounds.

Chapter-2 Photochemical Reactions: Norrish type I and Norrish type II cleavages, Patterno-Buchi reaction. Photoreduction, Photochemistry of enones, Rearrangement of, α, β-unsaturated ketones and cyclohexadienes, Photochemistry of p-Benzoquinones, Photochemistry of unsaturated systems - Olefins, cis trans Isomerisation and dimerization, Acetylenes dimerisation, Dienes - Photochemistry of 1,3 butadienes (2+2) additions leading to cage structures, Photochemistry of cyclohexadienes, Photochemistry of aromatic compounds.

Chapter-3 Pericyclic Reactions: Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3 Butadiene, 1,3,5- Hexatriene, Allyl system, Classification of pericyclic reactions, FMO approach, Woodward-Hoffman correlation diagram method and Perturbation of molecular (PMO) approach for the explanation of pericyclic reactions under thermal and photochemical conditions.

Chapter-4 Electrocyclic Reactions: Conrotatory and disrotatory motions in (4n) and (4n+2), allyl systems and secondary effects, Cycloadditions; Antarafacial and suprafacial additions, Notation of cycloaddition of (4n) and (4n+2) systems, Secondary effects of substitutes on the rates of cycloaddition reaction and cheletropic reactions, Sigmatropic Reactions; Suprafacial and antarafacial shifts, retention and inversion of configurations, Claisen and Cope rearrangements, fluxional molecules.

Learning Resources:

Text Books:

1. Advanced Organic Chemistry Reactions, Mechanism & Structure, Jerry March, Wiley, 2006, 4th Edition.
2. Molecular reactions and Photochemistry, Charles Dupey and O. Chapman, Prentice Hall, 2006.
3. Reaction Mechanism in Organic Chemistry, S.M. Mukherjee and S. P. Singh, Macmillan India Limited, 2009.
4. Pericyclic reactions, S.M. Mukherjee, Macmillan India Limited, 2009.

Reference Books:

1. The modern structural theory in Organic Chemistry, L. N. Ferguson, Prentice Hall, 2008.
2. Physical Organic Chemistry by Jack Hine, Mc. Graw Hill, 2007.
3. Mechanisms and Theory in Organic Chemistry by T.H. Lowry and K.S. Rich Gadson, 2006.

Course Code: CY4154	CHEMICAL KINETICS AND QUANTUM CHEMISTRY	Credits L-T-P: Cr 3-0-0: 3

Course Outcomes:

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

CO1	Understand the theories of reaction rates and first principles of calculation
CO2	Interpret the mechanism and kinetics of complex and enzymatic reactions
CO3	Apply first principles of calculation to real problems in chemistry
CO4	Analyze the effects of temperature, catalyst, solvent, salt and substituents on reaction rates
CO5	Assess approximation methods for chemical bonding

Course Articulation Matrix:

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

Syllabus:

Chapter-1 Chemical Dynamics: Basic concepts of kinetics, Effect of temperature on reaction rates-Arrhenius equation; Mechanism of Complex reactions: Equilibrium approximation and Steady state approximation, Kinetics of Complex reactions: Derivation of first order rate expression for parallel, opposing and consecutive reactions, chain reactions and their reaction mechanisms; Kinetics and flow methods of fast reactions; Theories of Reaction Rates**:** Collision theory of bimolecular gaseous reactions (overview), absolute reaction rate theory of bimolecular reactions (ACT), thermodynamic formulation of ACT-Eyring equation (numerical problems), Lindemann theory of unimolecular gaseous reactions and its limitations, Hinshelwood modification; Kinetics of Reactions in Solution: Effect of Solvent, Salt and Substituent on Reaction Rates; Linear Free Energy Relationships

Chapter-2 Catalysis: Homogeneous Catalysis: Acid-Base Catalysis; Enzyme Catalysis: Rate –Substrate Concentration Profile of Enzymatic Reactions. Michaelis - Menten Model; Inhibition of Enzymatic Reactions, Heterogeneous catalysis-Langmuir-Hinshelwood mechanism-unimolecular and bimolecular surface reactions, Autocatalysis and oscillatory chemical reactions

Chapter-3 Emergence of Quantum Mechanics and: Incompatibility of Classical Explanation of Blackbody Radiation, Schrodinger Equation Photoelectric Effect, Franck-Hertz Experiment; Colours of Gold Colloids, de Broglie Equation; 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. Approximation methods: Introduction to Variational and Perturbation theory, first and second order corrections.

Chapter-4: Chemical Bonding and Intermolecular Interactions: Molecular Orbital Theory; Schrodinger Equation to H_{2^+} and H_2 Molecule. Hartree-Fock Self Consistent Field (SCF) Method,

Huckel MO Theory; Spin-Orbit Coupling; Supramolecular Interactions; Quantum Mechanical Interpretation of Nanoparticle Properties: Size-Dependent Properties; Quantum Well and Quantum Tunnelling; Quantum Dots; Tunnelling Microscopy.

Learning Resources:

Text Books:

1. Chemical Kinetics, K.J. Laidler, Pearson Education, 2003 and 3rd Edition.
2. Quantum Chemistry, I. N. Levine, Phi, 2006.
3. A textbook of Physical Chemistry by K L Kapoor, volume 5, McGraw Hill Education, 2015, 3rd Edition
4. Principles of Physical Chemistry, Samuel H. Maron, Carl F. Prutton, CBS Publishers 2017 4th Edition

Reference Books:

1. Quantum Chemistry (Student viva edition), Donald A. McQuarrie, Viva Books-2016
2. Quantum Mechanics of Molecular Rate Processes, R. D. Levine, Dower Publications, 2011
3. Principles of Physical Chemistry, Puri, Sharma, Pathania, Vishal Publications, 2020, 48th Edition
4. Advanced Physical Chemistry, Gurdeep Raj, Goel publishing, 2019, 42nd Edition

Course Code: CY4155	INORGANIC CHEMISTRY LABORATORY	Credits L-T-P: Cr 0-0-3: 1.5

Course Outcomes:

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

CO1	Obtain hands-on experience in the spectrophotometry, potentiometry, flame photometry, electrogravimetry and ion exchange methods
CO2	Apply spectro- and electroanalytical methods for quantification of metal ions in complex mixtures
CO3	Synthesize and characterize metal complexes
CO4	Determine metal ion content and other components present in metal complexes
CO5	Predict the order of metal ions in spectrochemical series

Course Articulation Matrix:

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

Syllabus:

Simultaneous determination of two metal ions by spectrophotometric method

Determination of Ni^{2+} by colorimetry

Determination of Fe^{2+} by Potentiometric method

Determination of Cu^{2+} in brass by electrogravimetric method

Determination of the concentration of a salt by ion exchange method

Synthesis and characterization of the following complexes

Potassium bis(Oxalato)cuprate(II) dehydrate

Manganese(III) acetylacetonate

Mercury tetrathiocyanatocobaltate (II) (Characterization by thermal/magnetic/FT-IR/ESR/UV-Visible methods)

Determination of Stoichiometry of a metal complex by Job's methods (mono and continuous variation)

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

Determination of sodium by flame photometry

Determination of optical rotation of metal complexes

Conductometric analysis of coordination compounds

Learning Resources:

Text Books:

1. Vogel's Textbook of Quantitative Chemical Analysis, G H Jeffery, J Bassett, J Mendham and R C Denney, Longman Inc., 1989, Fifth edition
2. Inorganic Experiments, J. D. Woolins, John Wiley & Sons, 2010, Third edition.

Reference Books:

1. Elias, A. J., A Collection of Interesting General Chemistry Experiments, Universities Press (India) Pvt. Ltd., 2002
2. Practical Inorganic Chemistry: Preparations, reactions and instrumental methods, Springer, 1979, Second edition.
3. Microscale Inorganic Chemistry: A Comprehensive Laboratory Experience, Z. Szafran; R. M. Pike; M. M. Singh, Wiley, 1991, First edition.

Course Code: CY4156	ORGANIC CHEMISTRY LABORATORY-II	Credits L-T-P: Cr 0-0-3: 1.5

Course Outcomes:

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

CO1	Understand the principles involved in separation of binary mixtures
CO2	Obtain practical experience in the separation and identification of individual compounds in the binary mixtures
CO3	Apply the synthetic methodologies for the preparation of organic compounds
CO4	Examine the greener methods of synthesis of organic compounds
CO5	Develop the knowledge and skills in the synthetic organic chemistry useful for industrial applications

Course Articulation Matrix:

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

Syllabus:

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 organic compounds based on Oxidation: Benzyl chloride to Benzoic acid, Reduction: 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, preparation organic compounds by green chemistry methods i) acetylation of Aniline, ii) base catalysed aldol condensation, iii) Diels-Alder reaction, iv) Benzil-benzilic acid rearrangement.

Learning Resources:

Text Books:

1. Practical Organic Chemistry, F. G. Mann & B.C Saunders, Pearson Education India, 2009.
2. Advanced Practical Organic Chemistry, N. K. Vishnai, Vikas Publishing House Pvt Ltd, 2009, 3rd Edition.

Reference Books:

1. Introduction to Organic Laboratory Techniques, Randall G. Engel, George. Kriz Gary M. Lampman, Donald L. Pavia, Cengage Learning 2011, 3rd Edition.
2. Text Book of Practical Organic Chemistry, Vogel A. I., ELBS, 2004, 5th Edition.

Course Code: CY4157	PHYSICAL CHEMISTRY LABORATORY	Credits L-T-P: Cr 0-0-3: 1.5

Course Outcomes:

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

CO1	Acquire pragmatic experience on the experimental techniques to measure various physico-chemical parameters
CO2	Demonstrate conductometry and polarimetry to study the kinetics of reactions
CO3	Estimate various thermodynamic properties of different systems
CO4	Evaluate some physical parameters using spectroscopic techniques
CO5	Analyze and interpret the experimental data

Course Articulation Matrix:

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

Syllabus:

Conductometric determination of rate constant of alkaline hydrolysis of methyl acetate
Determination of Isosbestic Point of an Acid-Base Indicator spectrophotometrically
To determine the Buffer action and Buffer Capacity of various buffers
Kinetics of Iodine-Clock Reaction
Evaluation of E^o values of $Zn|Zn^{+2}$, $Cu|Cu^{+2}$ electrodes
Polarimetry- determination of molar rotation and, Polarimetric studies of acid catalyzed hydrolysis of sucrose
Study of Effect of temperature on rate of a chemical reaction, determination of activation energy
Evaluation of Thermodynamic Functions by Potentiometry
Determination of Force constants of some selected chemical bonds using FTIR spectroscopy
Verification of Freundlich's Adsorption isotherm for the adsorption of acetic acid on charcoal
Determination of partition coefficient of acetic acid between i. water and cyclohexane ii. Water and n-butanol at room temperature
Potentiometric titration of mixture of halides (KCl, KI) with $AgNO_3$
Determination of pKa values of dibasic acid (e.g. oxalic acid) and tribasic acid (H_3PO_4) pH metrically
To determine the Enthalpy of neutralization and Enthalpy of ionization of Weak Acid and Weak Base
To study the kinetics of the reaction between acidified acetone and iodine colorimetrically or spectrophotometrically (initial rate method)
Determination of relative viscosity of a given liquid with respect to water at room temperature by Ostwald's viscometer
Determination of Band Gap in CdS semiconductor and CdS-Cu_2S phosphor by UV-Vis-NIR Spectroscopy

Learning Resources:

Text Books:

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

Reference Books:

1. Advanced Practical Physical Chemistry, J.B. Yadav, 2019 and 38th Edition
2. Experiments in Physical chemistry, Shoemaker D.P., Garland C.W. and Nibler J.W. McGraw Hill, 2008, 8th Edition
3. Systematic Experimental Physical Chemistry by S.W. Rajbhoj and T.K. Chondheka, Anjali Publication, 2013, 3rd Edition

Course Code: CY4161	ORGANIC REAGENTS AND NAME REACTIONS	Credits L-T-P: Cr 3-0-0: 3

Course Outcomes:

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

CO1	Understand the reactivity of reagents
CO2	Classify the types reagents and name reactions
CO3	Apply the concepts of named reactions in synthetic organic chemistry
CO4	Adopt new protocols industrial chemicals and synthetic drugs
CO5	Propose the reaction mechanism for the organic transformations

Course Articulation Matrix:

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

Syllabus:

Chapter-1 Oxidizing reagents:
Determination of the oxidation numbers in molecules that contain covalent bonds and examples of common redox reactions. Oxidation of alcohols to aldehydes, ketones and carboxylic acids: Chromium reagents [CrO_3, $H_2Cr_2O_7$, CrO_3-H_2SO_4), CrO_3-pyridine complexes (PCC, PDC), $KMnO_4$]. Oxidation of alcohols via activation of DMSO: (Swern Oxidation, Mofatt oxidation, Corey-Kim), OsO_4/NMO, Dess-Martin periodinane, tetrapropylammonium perruthenate (TPAP), TEMPO, over oxidation of alcohols into carboxylic acids. Oxidations of hydrocarbons: Oxidation of sp^3-carbon (allylic, benzylic) into alcohol/carboxylic acid ($KMnO_4$, MnO_2, SeO_2). Oxidation of sp^2 Carbon: Hydroboration-oxidation, Oxymercuration [$Hg(OAc)_2$], Dihydroxylation ($KMnO_4$, OsO_4), $Pb(OAc)_4$, Epoxidation (peracids), aziridination, oxidation with RuO_3 and $Tl(NO_3)_3$. Oxidation of C-H bond: Halogenation (Appel reaction, NCS, NBS, molecular bromine) Oxidation of ketones into lactones, Oxidation of amines, oxidation of nitro compounds. Dissociation of 1, 2-diols ($Pb(OAc)_2$/$NaIO_4$ and RuO_2/$NaIO_4$), Dissociation of C-C double bond (ozonolysis), Over oxidation of aromatic compounds (V_2O_5).

Chapter-2 Reducing agents: Hydrogenation of unsaturated compounds: Catalytic hydrogenation under homogeneous (Wilkinson's catalyst) and heterogeneous (Landler catalyst) conditions], supported catalysts for hydrogenation, Dissolving metals (Na/Liq NH_3), hydrazine, selectivity in reduction (reduction of alkynes) Dehalogenation (Tin reagents), reductive cleavage of ethers (KI and other metal catalysts)

Chapter-3 Reduction of carbonyl compounds: Reduction of aldehydes, ketones, carboxylic acids, amides, esters, lactones, lactams (Boron and Aluminium reagents: Borane, $NaBH_4$, $LiAlH_4$, DIBAL-H, Catechol borane, Disiamylborane, Thexyl borane, Diisopinocampyl borane, Super hydrides and other modified boron and aluminum reagents), Hydrazines. Reduction of nitro compounds and nitriles: Reduction of nitro compounds (hydrogenation using metals).

Chapter-4 Name Reactions: Achmatowicz reaction, McMurry reaction, Sakurai reaction, Nazarov reaction, Julia olefination, Peterson olefination. Prins reaction, Baylis-Hillman reaction, Corey-Fuchs reaction, Nozaki-Hiyama-Kishi reaction, Kulin-kovich reaction, Ritter reaction, Cross-coupling name reactions, Metathesis, Bamford-Stevens rearrangement, Schmidt Glycosylation Brook rearrangement, Smiles.

Learning Resources:

Text Books:

1. Some Modern Methods of Organic Synthesis W. Carruthers, Cambridge University Press, Cambridge, 2007, 4th Edition.
2. Name Reactions: A Collection of Detailed Mechanisms and Synthetic Applications, Jie Jack Li, Springer, 2014, 5th Edition.

Reference Books:

1. Advanced Organic Chemistry Reactions, Mechanism & Structure, Jerry March, Wiley, 2007, 4th Edition
2. Organic Synthesis, Michael B. Smith. Academic Press, 2016, 4th edition.

Course Code: CY4162	ORGANOMETALLIC CHEMISTRY	Credits L-T-P: Cr 3-0-0: 3

Course Outcomes:

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

CO1	Understand the structure and bonding aspects of organometallic compounds
CO2	Apply different electron counting rules to predict the shape/geometry of metal carbonyl clusters
CO3	Predict the chemical behaviour and reactivity of main group and transition metal organometallic compounds
CO4	Establish the structure-reactivity/activity relationship in organometallic chemistry and the operating mechanisms in the catalytic processes
CO5	Apply the above concepts to different catalytic reactions

Course Articulation Matrix:

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

Syllabus:

Chapter-1 Introduction: Definition, History and Importance of Organometallic Chemistry, Revision of 18-electron rule, Spectator ligands: Phosphine and N-Heterocyclic carbenes.

Chapter-2 Reactions in Organometallic Chemistry: Oxidative addition and reductive elimination, insertion and elimination reactions, Ligand substitution reactions, Fluxionality.

Chapter-3 Metal sigma and pi complexes: alkyls, Alkene and alkyne: Synthesis, bonding and reactivity β-hydride elimination, Agostic alkyls, Cyclic and acyclic polyenes: Cyclopentadiene-Synthesis, structure and properties of sandwich compounds, Ferrocene-preparation, properties, structure, bonding and MOED of ferrocene. Arene sandwich compounds, Allyl and 1,3 butadiene: Synthesis, bonding and reactivity, Davies Green Mingos rules.

Chapter-4 Metal-Ligand multiple bonds and clusters: Carbenes and Carbyne complexes: Synthesis and reactivity of carbine and carbine complexes, Metal clusters: Dinuclear, multinuclear clusters.

Chapter-5 Main group organometallics and Homogeneous catalysis: Structure and bonding Organolithium, Organomagnesium, organoaluminum, Homogeneous catalysis: Hydrogenation, Hydroformylation, Hydrocyanation, hydrosilylation and hydroboration, alkene isomerization, C-C coupling reactions.

Learning Resources:

Text Books:

1. Basic Organometallic Chemistry- Concepts, Synthesis and Applications, BD Gupta and AJ Elias, Universities Press Private Limited, India, 2011.
2. The Organometallic Chemistry of the Transition Metals, Robert H. Crabtree, Wiley, 2014, Sixth edition.

Reference Books:

1. Inorganic Chemistry, Catherine E. Housecroft and Alan G. Sharpe, Pearson, 2018, Fifth edition.
2. Inorganic Chemistry, D. F. Shriver and P. W. Atkins, Oxford University Press, 2006, Fourth edition.

Course Code: CY4163	CHEMICAL EDUCATION AND RESEARCH	Credits L-T-P: Cr 3-0-0: 3

Course Outcomes:

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

CO1	Understand the importance of chemical education and ethical standards
CO2	Identify promising modern research trends with their strength, growth and application
CO3	Discover the strengths of chemical education in modern world and mankind in future
CO4	Examine safety and ecological approaches in dealing hazardous compounds and effluents
CO5	Recommend models and tools helping effective dissemination of trends in chemical education and research

Course Articulation Matrix:

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

Syllabus:

Chapter-1: 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.

Chapter-2 Chemical Hazards and Disasters: Chemistry of Explosives, Poisons and Pollutants; GLPs; Models and Tools of Chemical Education: Models and Virtual Experiments

Chapter-3 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. Research and Practice in Chemistry Education: Advances from the 25th IUPAC International Conference on Chemistry Education, M Schultz, S Schmid, G A Lawrie, Springer; 1st ed. 2019.
4. Argumentation in Chemistry Education: Research, Policy and Practice: Volume 2 (Advances in Chemistry Education Series), S Erduran, RSC, 2019.

Reference Books:

1. Chemical Education: Towards Research-based Practice: 17 (Contemporary Trends and Issues in Science Education), J K Gilbert, O Jong, R Justi, D F Treagust, J H Driel, Springer; 2003.
2. Research in Chemistry Education, L Mammino, J Apotheker, Springer; 1st ed. 2021.

Course Code: CY5101	ORGANIC SYNTHESIS	Credits L-T-P: Cr 3-0-0: 3

Course Outcomes:

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

CO1	Understand the concepts of C-C and C=C bond formation reactions.
CO2	Demonstrate the applications of reagents in organic reactions.
CO3	Apply the knowledge of protecting and deprotection of functional groups.
CO4	Plan synthetic strategies using disconnections approaches.
CO5	Design the synthetic scheme for small organic molecules.

Course Articulation Matrix:

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

Syllabus:

Chapter-1 C-C Single Bond Formation Reactions: Alkylation importance of enolate anions, alkylation of relatively acidic methylene groups, Gama alkylation of 1,3-dicarbonyl compounds; dianions in the synthesis, alkylation of ketones, the enamine related reactions under basic conditions, enamines, Alkylation and Acylation in acidic medium alkylation of alpha-thio and alpha-selenocarbanions, umpolung, allylic alkylation of alkenes, reactions of lithium organocuprates: copper-catalysed reactions of Grignard reagents, synthetic applications of carbenes and carbenoids, formation of C-C bonds by addition of free radicals to alkenes, some photocyclization reactions.

Chapter-2 Carbon-Carbon Double Bond Formation Reactions: Wittig reaction, Phosphonium Ylide preparation, reaction mechanism, olefin synthesis, Modified Wittig reactions, stereoselective synthesis of substituted ethylenes, Fragmentation reactions, Wharton olefin synthesis, alkenes from tosylhydrazone, sulfone, alkenes from titanium and chromium reagents, alkene metathesis reaction, Oxidative decarboxylation of acids, stereospecific synthesis from 1,2-diols, Oxidation & electro organic oxidations. Reactions at unactivated C-H bonds, the cyclisation reactions of nitrenes, and photolysis of N-nitroso amides, reaction of monohydric alcohols with lead tetra acetate (LTA), miscellaneous reactions.

Chapter-3 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.

Chapter-4 Design of Organic Synthesis: Synthetic strategies: Introduction and target selection and terminology, aims and objectives, introduction, target selection, structural

verification, biological activity, topological studies, new reactions and reagents, retro synthetic analysis, terms used in retro synthetic analysis, target molecule, functionalization, functional group interchange, disconnection synthons, synthetic equivalent transform, retron different strategies in retro synthetic analysis, C-C disconnection, introduction one group C-C disconnection, two group disconnections, 1,2-, 1,3-, 1,4-, 1,5-, 1,6- difunctional compounds, applications of some important strategies in organic synthesis, chemo selectivity, regioselectivity, stereoselectivity, cyclisation reactions(3 to 7 membered rings), reversal polarity, amine synthesis, consecutive and convergent synthesis and some selected synthesis. Biomimetic approach to retrosynthesis, Johnson polyene cyclization, retro mass spectral degradation, Yamaguchi esterification, Corey-Nicolaou macro lactonization.

Learning Resources:

Text Books:

1. Organic Synthesis, Michael B. Smith. Academic Press, 2016, 4th Edition.
2. Organic Synthesis, The disconnection Approach, S. Warren, Wiley India Edition, John Wiley & Sons, 2007.
3. Some Modern Methods of Organic Synthesis, W. Carruthers, I. Coldham, Cambridge University Press, Cambridge, 2015, 4th Edition.

Reference Books:

1. Modern Organic Synthesis, George Zweifel, Michael Nantz, W. H. Freeman and company New York, 2006.
2. Organic Synthesis Strategy and Control, Paul Wyatt and Stuart Warren, Wiley and Sons, 2013.
3. Organic Chemistry, J. Clayden, N. Greeves, S. Warren, Oxford, 2012, 2nd Edition.

Course Code: CY5102	STEREOSELECTIVE SYNTHESIS	Credits L-T-P: Cr 3-0-0: 3

Course Outcomes:

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

CO1	Understand the principles and applications of stereoselective synthesis.
CO2	Demonstrate types of stereo chemical models.
CO3	Apply the concepts of stereoselective transformations in organic synthesis.
CO4	Utilize the advanced chiral reagents for asymmetric synthesis.
CO5	Design the synthetic strategies for cyclic molecules using Boldwin rules.

Course Articulation Matrix:

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

Syllabus:

Chapter-1 Asymmetric Synthesis: Principle of stereoselectivity, strategies of asymmetric synthesis, substrate diastereoselectivity, product stereoselectivity, product composition, determination of product composition, diastereomeric excess (*de*), and enantiomeric excess (*ee*), double stereo differentiating reactions. Strategies for stereo control in enantio and diastereoselective synthesis, small ring templates, molecular walls, ring formation reactions, pericyclic reactions coordination to metal centers, use of π-donors complexes, π-π interactions with aromatic substituents, directed π-facial diastereoselectivity chiral auxiliaries, achiral auxiliaries, intraanular and extraanular stereocontrol. Nucleophilic additions to cyclic and acyclic carbonyl compounds, Cram's rule, Felkin's model, addition to chelated carbonyl compounds, Prelog's rule and its applications, addition to chelated carbonyl compounds of H and R to cyclic ketones (formation of axial and equatorial alcohols), Electrophilic initiated cyclization, Aldol reactions: (1) Achiral enolates with achiral aldehydes (2) Achiral enolates with achiral aldehydes. (3) Chiral enolates with achiral aldehyde. (4) Chiral enolates with chiral aldehydes, organocatalysis.

Chapter-2 Stereo selective Reactions: Stereo selective reactions of C=C double bond, Diastreoselective transformations involving catalytic hydrogenation; Hydrogenation over heterogeneous catalysts; Directed hydrogenation with soluble catalysts; synthetic applications of organoboranes and organosilanes, hydroboration, reactions of organoboranes, corbonylation of organoboranes, reactions with alpha halo carbonyl compounds, reactions of alkenylboranes and trialkenylboranes, free radical reactions of organoboranes, alkenyl silanes and allylsilanes, control of rearrangement reactions involving silicon, trimethylsilyl cyanide, trimetylsilyliodide and trimethylsilyltrifliate; Stereochemistry of free radical cyclization reactions,

Prevost hydroxylation, Simon-Smith reaction.

Chapter-3 Enantioselective Reactions. Enantioselective synthesis with chiral racemic catalysts, hydroboration reactions involving chiral boranes, chiral organometallic complexes, chiral enolate aggregates, reductions with chiral complexes hydrides. Catalysis by chiral transition metal complexes, enantioselective epoxidation of alkenes. Enantioselective hydrogenations.

Chapter-4 Principles of Cyclization Reactions and C-H activation: Thorpe-Ingolde effect, Bredt rule, macro lactonization, Corey-Nicholaou procedure, Baldwin rules for cyclization reactions, required trajectories for Baldwin ring closure, Exo and endo displacement involving enolate ions, Iodo lactonization, C-H activation of organo zinc compounds.

Learning Resources:

Text Books:

1. Stereochemistry of Organic Compounds, Ernest L. Eliel and Samuel H. Wilen, Wiley-India, 2008.
2. Stereochemistry of Organic Compounds: Principles and Applications, Fourth Edition, D. Nasipuri, New Age International Publishers, 2020.
3. Stereochemistry: Conformation and Mechanism, P.S. Kalsi, New Age Publishers, 2019, 10th Edition.

Reference Books:

1. Catalytic Asymmetric Synthesis, edited by Iwao Ojima , John Wiley &Sons, Hoboken , New Jersey, USA. 2012.
2. Advanced Asymmetric Synthesis, edited by G. R. Stephenson. Chapman & Hall, Springer Science, 1996.

Course Code: CY5103	HETEROCYCLIC CHEMISTRY AND AROMATICITY	Credits L-T-P: Cr 3-0-0: 3

Course Outcomes:

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

CO1	Classify heterocyclic compounds and their nomenclature
CO2	Understand the physical and chemical properties of simple and fused heterocyclic compounds
CO3	Apply the knowledge of heterocyclic chemistry to synthesize the natural products and drug molecules
CO4	Distinguish aromatic and homoaromatic compounds using spectral data
CO5	Predict the aromaticity of organic compounds and their stabilities

Course Articulation Matrix:

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

Syllabus:

Chapter-1 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.

Chapter-2 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, Benzoisoxazoles, Oxazoles, Benzoxazoles, Isothiazoles, Benzoisothazoles, Thiazoles and Bezoisothazoles; Six membered heterocyclic compound with two hetero atoms: Pyridazines, Cinnolines, Phthalazines, Pyrimidines, Quinazolines, Pyrazines and Quinaxalines. Synthesis of drug molecules based on the above heterocyclic rings.

Chapter-3 Oxygen heterocyclic compounds: Coumarins, Chromones, Flavones and Isoflavones.

Chapter-4 Mesoionic heterocycles: synthesis and aromaticity of sydnones, 1, 3 dipolar addition reactions of mesoionic heterocycles.

Chapter-5 Aromaticity and Antiaromaticity: 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 (C_{60}), Synthesis and properties of annulenes and Azulene.

Learning Resources:

Text Books:

1. Heterocyclic Chemistry: Volume II: Five-Membered Heterocycles, Radha R. Gupta, Mahendra Kumar, Vandana Gupta, Springer, 1999.
2. Heterocyclic Chemistry, V. K. Ahulwalia, Narosa Publishers, 2012, 1st Edition.
3. Heterocyclic Chemistry, Raj K. Bansal, New Age International, 5th Edition.

Reference Books:

1. Heterocyclic Chemistry, Joule, J. A. and Mills, K, Wiley, 2010, 5th Edition.
2. Chemistry, Gilchrist, T. L., Pearson Education, 2008, 3rd Edition.

Course Code: CY5104	CHEMISTRY OF NATURAL PRODUCTS	Credits L-T-P: Cr 3-0-0: 3

Course Outcomes:

At the end of the course, the student t will be able to:

CO1	Understand the concept of structure elucidation of natural compounds
CO2	Build the synthetic schemes of natural products and bioactive molecules
CO3	Analyze the stereochemistry of drug molecules
CO4	Apply the knowledge of biosynthesis in total synthesis of organic molecules.
CO5	Design new synthetic methodologies

Course Articulation Matrix:

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

Syllabus:

Chapter-1 Introduction: Classification of Natural Products, isolation of natural products, general methods of structural elucidation and stereochemistry.

Chapter-2 Terpenoids: Classification, Structure and synthesis of Mono, sesqui, di, tri terpenoids, biogenesis of terpenoids (Geraniol, Alpha- Terpineol, Alpha-pinene, Camphor, Cadenene, Abeitic acid.

Chapter-3 *Steroids*: Classification, structure, stereochemistry and synthesis of steroids (Cholesterol).

Chapter-4 *Alkaloids*: Structure and chemistry of papaverine, Quinine, Morphine, Lysergic acid and Resepine, nicotine, atropine.

Chapter-5 *Vitamins*: Structure and synthesis of vitamins B6, B12.

Learning Resources:

Text Books:

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

Reference Books:

1. The Alkaloids, Bently, Oxford University Press, 2000.

2. Natural Products: Chemistry Sources, Separations, and Structures. Raymond Cooper and George Nicola. CRC Press. 2015.
3. Total Synthesis of Natural Products: At the Frontiers of Organic Chemistry, Jie Jack Li, E.J. Corey, Springer, 2015.

Course Code: CY5111	GREEN CHEMISTRY	Credits L-T-P: Cr 3-0-0: 3

Course Outcomes:

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

CO1	Understand the basic principles of Green Chemistry
CO2	Know about the renewable and non-renewable sources
CO3	Demonstrate the applications of green solvents and reagents
CO4	Apply concepts of atom economy and green catalysis in the organic synthesis
CO5	Adopt green protocols for sustainable environment

Course Articulation Matrix:

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

Syllabus:

Chapter-1 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, Avoidance of unnecessary derivatization, careful use of blocking/protection groups, Use of catalytic reagents (wherever possible) in preference to stoichiometric reagents, Designing biodegradable products.

Chapter-2 Examples of green synthesis/reactions: Green starting materials, Green reagents, real world cases (Traditional processes and green ones): Ibuprofen, Paracetamol, Seldinafil, Nylons, 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; non-covalent derivatization. Biomass conversion, emission control.

Chapter-3 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, Fluorous phase reactions, Fluorous separating techniques, isolation of soybean oil and caffeine.
Nonconventional energy sources: Microwave assisted reaction, Ultrasound assisted reactions, photochemical reactions using sunlight.

Chapter-4 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. New trends in green chemistry, V. K. Ahluwalia, M. Kidwai, Springer, 2012, 1st Edition.
2. Green Chemistry: Environment Friendly Alternatives, Rashmi Sanghi, M.M Srivastava, Alpha Science International, 2009, 4th Edition.

Reference Books:

1. Green Chemistry: Theory and Practice. P.T. Anastas and J.C. Warner. Oxford University Press, 2000, 1st Edition.
2. Introduction to green chemistry, Albert S. Matlack, CRC Press, 2001, 2nd Edition.

Course Code: CY5112	FOOD CHEMISTRY	Credits L-T-P: Cr 3-0-0: 3

Course Outcomes:

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

CO1	Understand the problems related to the chemical composition in food.
CO2	Apply theoretical concepts of food chemistry in day-to-day life.
CO3	Identify the advantages and disadvantages of additives in food.
CO4	Choose foods that are helpful in reducing community health.
CO5	Develop healthy food processes.

Course Articulation Matrix:

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

Syllabus:

Chapter-1 Role of Water & Biomolecules in Food: Water, Lipids, Amino acids, Proteins, Carbohydrates, enzymes, nutrients and natural toxicants in foods

Chapter-2 Food additives: Artificial sweeteners – saccharin, cyclamate, and aspartame – food flavors. Emulsifying agents, Modern food: Snack foods. Production of bread, bun and biscuits. Raw materials, methods and machinery required. Candy manufacturing, Caramelization, Fast foods, Instant foods, dehydrated foods.

Chapter-3 Beverages: Processing and technologies of alcoholic and non-alcoholic beverages, basic concepts of quality assurance and quality control applicable to the beverage industry, Soft drinks, soda, fruit juices.

Chapter-4 Storage & other aspects of Food: Introduction to refrigeration, slow freezing, quick freezing, introduction to thawing, changes during thawing and its effect on food, Food Irradiation- Introduction, kinds of ionizing radiations used in food irradiation, emulsions, properties of emulsions, formation of emulsion, emulsifying agent, food foams.

Chapter-5 Food Adulteration: Contamination of wheat, rice, dhal, milk, butter, etc., Food poisons: natural poisons (alkaloids, nephrotoxins), pesticides (DDT, BHC, Follidol), Chemical poisons (KCN), Objectives of packaging, flexible packaging, properties of the following packaging materials.

Learning Resources:

Text Books:

1. Food Science, Srilakshmi B., New Age International Pvt. Ltd. Publishers, 2003, 3rd Edition.
2. Principles. Textbook of medical biochemistry, Ramakrishnan S., Prasannam K. G and Rajan R. Orient Longman Ltd., 2001, 3rd Edition.

Reference Books:

1. Food Processing and Preservation. Siva Sankar B., Prentice–Hall of India Pvt. Ltd., New Delhi. 2002.

Course Code: CY5113	MEDICINAL CHEMISTRY	Credits L-T-P: Cr 3-0-0: 3

Course Outcomes:

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

CO1	Understand basic concepts of drug discovery.
CO2	Apply the concepts in lead discovery.
CO3	Identify the importance of Lipinski rule and bioisosterism.
CO4	Evaluate the concepts of SAR and QSAR.
CO5	Design and develop a molecule with drug like property.

Course Articulation Matrix:

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

Syllabus:

Chapter-1 Basics of Drug Discovery: *Introduction to Modern drug discovery:* Origin, current approaches, comparison with Ayurveda and homeopathic medicines*; Definitions:* 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)*; Concept of pharmacophore:* Definition, identification and impact of modification of pharmacophore*; Lead structure:* Identification, optimization and modification, Preclinical, clinical phases, identification of lead structure*; Lipinski rule:* Lipinski rule of five, drug like properties, druggability (Examples)*; Bioisosterism:* Bioisosterism, classical and non-classical isosteres, examples.

Chapter-2 Drug targets: Macro molecules as targets (receptors, enzymes, nucleic acids, cell organelles).

Chapter-3 Drug discovery stages and strategies: *Pharmacodynamics and Pharmacokinetics:* Pharmacological action and mechanism at molecular level (ADME), Factors affecting Absorption, Distribution, Metabolism, Elimination and Toxicity (CYPs, Glucuronidation), Stereo chemical and metabolic aspects of drugs*; Serendipitous drug discovery:* Identification of lead (examples), drug discovery without lead; *Current approaches to drug discovery:* a) natural products based b) fragment based c) metabolites based d) clinical observations e) random screening and non-random screening*; Structure-activity relationships:* Importance of rational approaches of lead discovery, and introduction to structure activity relationship.

Chapter-4 Combinatorial synthesis: Combinatorial and building block approaches for the drugs and role of biomarkers (examples).

Chapter-5 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.

Learning Resources:

Text Books:

1. Medicinal Chemistry, Ashutosh Kar, New Age Publications, 2007.
2. An Introduction to Medicinal Chemistry, Graham L. Patrick, Oxford Press, 2009, 4th Edition.
3. Fundamentals of Medicinal Chemistry by Gareth Thomas, John Wiley & Sons Ltd., 2003.

Reference Books:

1. Medicinal Chemistry Vol-I & II – Burger, Wiley Int.Sci., 1999.
2. The organic chemistry of Drug Design and Drug Action by Richard B Silverman and Mark W Holladay, Academic Press, 2014, 3rd Edition.
3. Medicinal Chemistry and Drug Design, Edited by Deniz Ekinci, Published by InTech, Croatia, 2012.

Course Code: CY5121	ADVANCED ORGANIC SPECTROSCOPY	Credits L-T-P: Cr 3-0-0: 3

Course Outcomes:

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

CO1	Understand the concepts of spectroscopy.
CO2	Summarize the principles of PMR and CMR spectroscopies.
CO3	Analyze the concepts of ^{19}F spectroscopy in determining the structures of molecules.
CO4	Apply the principles of 2D NMR spectroscopy in resolving the structures of organic molecules.
CO4	Discuss the principle of ^{31}P and mass spectrometry and their applications.
CO5	Solve the structures of organic compounds using spectral data.

Course Articulation Matrix:

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

Syllabus:

Chapter-1 Spectroscopy II (^{1}H-NMR): Applications of ^{1}H-NMR spectroscopy: Reaction mechanisms (cyclic bromonium ion, electrophilic and nucleophilic substitutions, carbocations and carbanions), E, Z isomers, study of conformational changes through NMR of cyclohexane and decalins, study of dynamic processes using NMR spectroscopy. Keto-enol tautomerism, hydrogen bonding, valence tautomerism, proton exchange on electronegative atoms, C-N restricted rotation. Discrimination of enantiomers by use of chiral NMR solvents (CSAs), chiral lanthanide shift reagents and Mosher's acid.

Chapter-2 ^{13}C NMR spectroscopy: Chemical shifts of organic compounds. 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. Applications of ^{13}C-NMR spectroscopy: Structure determination, stereochemistry, reaction mechanisms and dynamic processes in organic molecules. ^{13}C-NMR spectral editing techniques: principle and applications of APT, INEPT and DEPT methods.

Chapter-3 2D-NMR spectroscopy: Principles of 2D NMR, Classification of 2D-experiments. Correlation spectroscopy (COSY) HOMOCOSY (1H-1H COSY) , TOCSY (Total Correlation Spectroscopy), Hetero COSY (^{1}H, ^{13}C COSY, HMQC), long range ^{1}H, ^{13}C COSY (HMBC), Homonuclear and Heteronuclear 2D-J-resolved spectroscopy, ROESY, NOESY and 2D-INADEQUATE experiments and their applications.

Chapter-4 ^{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.

Chapter-5 ^{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.

Chapter-6 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, Interfaces- Direct coupling interface and open split interface. Application based on gas chromatography/mass spectrometry-Analysis of metabolite of drug Imipramine. LC-MS-principle, Instrumentation – Interfaces- Moving belt interface, particle beam interface, thermospray interface, Electrospray interface, atmospheric pressure chemical ionization interface. ICP – MS - Principle Instrumentation, and Applications. Secondary Ion Mass Spectrometry (SIMS), Matrix Assisted Laser Desorption Ionization (MALDI) methods. Introduction to principle and applications of Liquid Chromatography-Mass Spectrometry. Spectroscopic Solutions of Structural Problems.

Learning Resources:

Text Books:

1. Introduction to Spectroscopy, Donald Pavia, G. M. Lampman, George S. Kriz, Thomson/Brooks/Cole, 2001, 3rd Edition.
2. Spectroscopy of Organic Compounds, P. S. Kalsi, New Age International Publishers, 2020, 8th, Edition.
3. Organic Spectroscopy: Principles & Applications, Jag Mohan, Narosa, 2020. 3rd Edition.

Reference Books:

1. Organic Spectroscopy, William Kemp, Palgrave Publishers, 2007, 3rd Edition.
2. Spectrometric Identification of Organic Compounds, Robert M. Silverstein, Francis X. Webster, David J. Kiemle, David L. Bryce, Wiley, 2014, 8th Edition.

Course Code: CY5122	FUNCTIONAL ORGANIC MATERIALS	Credits L-T-P: Cr 3-0-0: 3

Course Outcomes:

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

CO1	Understand the structural features and functionalization of carbon nanotubes.
CO2	Illustrate the non-linear optical properties of functional organic materials.
CO3	Apply combinatorial approach in cross-coupling reactions and coordination chemistry.
CO4	Design synthetic routes for the preparation of chiral-conjugated molecules.
CO5	Discuss significance of electron transfer in π-functional molecules for building light harvesting systems.

Course Articulation Matrix:

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

Syllabus:

Chapter-1 Introduction and Functionalization of Carbon Nanotubes: Introduction to Carbon Nanotubes, Functionalization of Carbon Nanotubes, Defect Functionalization, p-Conjugated Oligomers, Electron Transfer of π-Functional Systems and Applications. Introduction, Synthesis of Cyclophenacene p-Conjugated Systems from [60]Fullerene, π-Conjugated Oligomers.

Chapter-2 Nonlinear Optical Properties of Organic Materials: Introduction to Nonlinear Optics, Linear and Nonlinear Polarization, Second-order Nonlinear, Measurement Techniques.

Chapter-3 Diversity- oriented Synthesis of organic materials: Combinatorial Syntheses of Chromophores, Combinatorial Cross-coupling Reactions, Combinatorial Coordination Chemistry.

Chapter-4 Synthesis of Chiral Conjugated Materials: Introduction, Synthetic Approaches to Highly Annelated Chiral, π-Conjugated Systems, Chiral Polycyclic Aromatic Hydrocarbons, Strong Chiroptical Properties in Absorption, Emission and Refraction, Absorption and Emission.

Chapter-5 Electron Transfer of π-Functional Systems and Applications: Introduction, Efficient Electron-transfer Properties of Zinc Porphyrins, Fullerenes, Photoinduced Electron Transfer in Electron Donor- Acceptor, Linked Molecules Mimicking the Photosynthetic, Organic Solar Cells Using Simple Donor-Acceptor Dyads, Organic Solar Cells Composed of

Multi-porphyrin/C_{60}, Supramolecular Assemblies, electronic and bio applications of assembled organic materials.

Learning Resources:

Text Books:

1. Functional Organic materials: Syntheses, Strategies and Applications, Thomas J. J. Miller and Uwe H. F. Bunz (WILEY-VCH), 2007.
2. Molecular Organic Materials: From molecules to crystalline solids, Jordi Froxedas; Cambridge Press, 2006.
3. Molecular Materials; Duncan W. Bruce, Dermot O'Hare, Richard Walton, Wiley, 2010.

Reference Books:

1. Introduction to Organic Electronic and Optoelectronic Materials and Devices, Sam-Shajing Sun, Larry R. Dalton, CRC Press, 2008, 1st Edition.

Course Code: CY5123	INDUSTRIAL PHARMACEUTICAL CHEMISTRY	Credits L-T-P: Cr 3-0-0: 3

Course Outcomes:

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

CO1	Understand the concepts of unit processes.
CO2	Apply the principles of pharmaceutical manufacturing to drugs.
CO3	Analyze the principles of quality control and quality assurance.
CO4	Evaluate quality control and standard operational methods.
CO5	Discuss effluents and their purification methods.

Course Articulation Matrix:

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

Syllabus:

Chapter-1 Unit Processes: Concept of unit processes in systematization of chemical reactions, explanation of one example each for unit processes: Thermodynamic and kinetic aspects of Alkylation, amination, (by ammonolysis, reduction), esterification, halogenation, hydroformylation, hydrogenation, nitration, oxidation and reduction. Mechanistic aspects of carbonylation and carboxylation.

Chapter-2 Industrial Synthesis: Introduction to pharmaceutical manufacturing - raw materials, detailed manufacturing procedure, therapeutic function, common name, chemical name, structural formulae of the following drugs. Acyclovir, alprazolam, Ibuprofen, cimetidine, sulfamethoxazole, ciprofloxacin, chloramphenicol.

Chapter-3 Quality Control and Quality Assurance: Introduction, concepts and significance, Quality control charts, the X-quality control chart, the R-quality control chart and its interpretation, spiked sample control charts, blind samples in control. Establishing Quality assurance programme-management commitment, writing standard operating procedures, topics for standard operating procedures, consolidating the programme, monitoring quality assurance data, reporting quality assurance problems, writing the quality assurance manuals. Good laboratory practices: Organization and personnel, quality programme, instrument and calibration.
Criteria for laboratory accreditation. Benefits of laboratory accreditation. Significance of ISO 9000-2000, 9001-2000, 9003-2000, 9004-2000 series of standards.

Chapter-4 Effluents of Industrial Units and Their Purification: Introduction to industrial effluents. Classification of effluents. Classification of basic methods of purifying effluents. i) Purification of suspended and emulsified impurities by mechanical method. ii) Purification of dissolved impurities- a) from mineral matter by ion exchange, reverse osmosis, electrical and reagent methods. b) From organic matter by destructive methods, biological oxidation, ozonization, chlorination, extraction, adsorption and ion exchange) Purification of gases by desorption method.

Learning Resources:

Text Books:

1. Industrial Chemistry, by B. K. Sharma, Krishna Prakashan Media P. Ltd. 2016.
2. Bulk Drug Manufacture, Profile Bulk Drug Manufacturers Association (India), 2021.
3. Environmental Chemistry by B. K. Sharma, Krishna's Educational Publishers, 2019.

Reference Books:

1. Unit Processes in Chemical Engineering by Groggins, McGraw Hill Inc., US revised, 2015.
2. Dryden's Outlines of Chemical Technology, M. Gopala Rao, Marshall Sittig, East-West Press Pvt Ltd.1997, 3rd Edition.
3. Pharmaceutical Manufacturing Encyclopedia Vol. I&II, William Andrew Publishing, 3rd Edition 2007.

Course Code: CY5105	ORGANIC ANALYSIS LABORATORY	Credits L-T-P: Cr 0-0-3: 1.5

Course Outcomes:

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

CO1	Obtain hands-on experience in determining the purity of compound using volumetric and gravimetric methods.
CO2	Identify the number of hydroxyl group present in a molecule.
CO3	Determine the amount of glucose present in a given sample.
CO4	Estimate the acid, iodine and saponification values of oils.
CO5	Solve the structures of organic compounds using spectral data.

Course Articulation Matrix:

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

Syllabus:

Estimations: Estimation of phenol as tribromophenol, 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, number of hydroxyl groups in phenol or alcohol.

Structural Elucidation of Organic Compounds by Spectroscopic methods: UV, IR, ^{1}H-NMR, ^{13}C-NMR and mass spectrometry, spectroscopy identification of following drugs: paracetamol, benzocaine, 7-hydroxy-4-methyl coumarin.

Learning Resources:

Text Books:

1. Laboratory Manual of Organic Chemistry, R. K. Bansal, New Age International Private Limited, 5th Edition, 2009.
2. Comprehensive Practical Organic Chemistry Qualitative Analysis, V. K. Ahulwalia, Sunita Dhingra, Universities Press, 2008.

Reference Books:

1. Text Book of Practical Organic Chemistry, Vogel A. I., 5th Edition, ELBS, 2004.
2. Experimental Organic Chemistry, Clark, F., Most Jr., John Wiley & Sons, 2002.

Course Code: CY5106	ORGANIC PREPARATIONS LABORATORY	Credits L-T-P: Cr 0-0-3: 1.5

Course Outcomes:

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

CO1	Understand the reactions concepts involved in preparation of organic compounds.
CO2	Obtain the hands-on experiences to carry out organic reactions.
CO3	Apply the MCR approach in the preparation of organic compounds.
CO4	Utilize chromatographic techniques in the purification of organic compounds.
CO5	Adapt green methodologies in the synthesis of organic compounds.

Course Articulation Matrix:

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

Syllabus:

Chapter-1 Tetrahydro carbazole synthesis, Claisen-Schmidt reaction 3,5-diphenylisoxazole from benzaldehyde (via chalcone and bromination), 7-hydroxy-3-methyl Flavone, 3-formylchromone, Beckmann rearrangement: acetophenone to *N*-acetanilide, Hofmann hypobromite and Sandmeyer: phthalic anhydride to *o*-chlorobenzoic acid, preparation of acridone from anthranilic acid (through *o*-chloro benzoic acid, *N*-phenyl anthranilic acid), preparation of symmetrical tribromo benzene (aniline to 2,4,6 tribromo aniline, diazotization followed by deamination).

Chapter-2 Isolation and purification of the following natural products: Caffeine, Piperine, Nicotine, Embelin, Lycopene, Rutin, Lawsone, Curcumin.

Chapter-3 Synthesis of physiologically active compounds: Benzocaine, Paracetamol, Principles of chromatography: separation of leaf pigments-chlorophyll a & b xanthophylls, separation of amino acids by paper chromatography.

Chapter-4 Synthesis of Organic Compounds using modern techniques: Ultrasound, Sonifications, Microwave, Solid State Synthesis, Ball Milling, Flow Chemistry.

Learning Resources:

Text Books:

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

3rd Edition.
3. Comprehensive Practical Organic Chemistry Qualitative Analysis, V. K. Ahulwalia, Sunita Dhingra, Universities Press, 2008.

Reference Books:

1. Text Book of Practical Organic Chemistry, Vogel A. I., ELBS, 2004, 5th Edition.
2. Experimental Organic Chemistry, Clark, F., Most Jr., John Wiley & Sons, 2002.
3. Practical Organic Chemistry F. G. Mann & B. C Saunders, ELBS Edition and Longman Group Limited, 2002.

Course Code: CY5161	DRUG DEVELOPMENT AND DELIVERY SYSTEMS	Credits L-T-P: Cr 3-0-0: 3

Course Outcomes:

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

CO1	Understand the concepts of drug design and drug delivery systems.
CO2	Utilize the knowledge in developing active pharmaceutical ingredients.
CO3	Analyze the knowledge in designing new efficient drug delivery systems.
CO4	Apply the concepts of drug design and delivery in pharmaceutical and biopharmaceutical industry application.
CO5	Design the efficient formulations of drugs.

Course Articulation Matrix:

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

Syllabus:

Chapter-1 Drug Design: Introduction to Drug Design, Concepts of Rational Drug Design with examples, Receptor Based Drug Design: Design of Agonist and Antagonist with examples. Structure based drug design, Pharmacophore based drug design, Drug Design by Variation Method, Improvement of Pharmacokinetics of lead molecule with examples, Computer Aided Drug Design.

Chapter-2 Development of Drugs: Anticancer agents: antimetabolite based approaches, anti-angiogenesis, DNA intercalating agents, those which affect signaling pathways or structural proteins such as tubulin, alpha 5 beta 3 receptor targeting.

Chapter-3 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., Osmotic Oral Drug Delivery Systems, Transdermal Drug Delivery Systems, Implantable Drug Delivery Systems.

Chapter-4 Gene Delivery Systems: Introduction to Gene Therapy, Types of gene delivery systems, Introduction to targeting, Passive and active targeting. Targeting Drug Delivery.

Learning Resources:

Text Books:

1. Medicinal Chemistry by Ashutosh Kar, New Age International Publishers, 2018, 8th Edition.
2. The organic chemistry of Drug Design and Drug Action by Richard B Silverman and Mark W Holladay, Academic Press, 2014, 3rd Edition.

Reference Books:

1. An Introduction to Medicinal Chemistry by Graham L Patrick, Oxford Press, 2013, 5th edition.

2. Advances in Novel and Controlled Drug Delivery, Jain, N. K. CBS Publishers and Distributors Pvt. Ltd, 2011.

Course Code: CY5162	ADVANCES IN THE TOTAL SYNTHESIS OF NATURAL PRODUCTS	Credits L-T-P: Cr 3-0-0: 3

Course Outcomes:

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

CO1	Understand the concepts and tactics used in total synthesis of natural products.
CO2	Illustrate the multistep organic synthesis using different reagents.
CO3	Develop the retrosynthetic analysis for complex natural products.
CO4	Analyze the different concepts and strategies in total synthesis.
CO5	Choose the synthon approach in total synthesis of natural products.

Course Articulation Matrix:

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

Syllabus:

Chapter-1 Concepts and tactics in organic synthesis, Strategic utilization of name reactions and reagents, Introduction to linear synthesis, Convergent, Divergent and Building block approaches.

Chapter-2 Practical difficulties in large scale synthesis, Construction of 5-membered N and O-containing aliphatic cyclic molecules, heterocycles in natural product synthesis, Symmetry driven total synthesis of Merrilactone A and Resolvin E2.

Chapter-3 Dearomatization strategies in natural product synthesis, protecting group free synthesis, Solid-phase chemistry in the total synthesis of non-peptidic natural products.

Chapter-4 Structure, absolute configuration and total synthesis of natural products: Taxol, Epothilones A, Camptothesin.

Learning Resources:

Text Books:

1. The Total Synthesis of Natural Products, John ApSimon, John Wiley & Sons, 2009.
2. Classics in Stereoselective Synthesis, Erick M. Carreira, Lisbet Kvaerno, WILEY-VCH, 2008.
3. The Logic of Chemical Synthesis, E. J. Corey, Xue-Min Cheng, John Wiley & Sons Inc. 1995.

Reference Books:

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

Wiley-VCH, 2000.
2. Classics in total synthesis-II: More Targets Strategies, Methods, K. C. Nicolaou, Scott A. Snyder, Wiley-VCH, 2003.
3. Classics in total synthesis-III: Further Targets Strategies, Methods, K. C. Nicolaou, Jason S Chen, Wiley-VCH, 2011.

Course Code: CY5163	CARBOHYDRATE CHEMISTRY	Credits L-T-P: Cr 3-0-0: 3

Course Outcomes:

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

CO1	Understand the structure and conformations of carbohydrates.
CO2	Classify the carbohydrates based on structural diversity.
CO3	Apply the knowledge of reaction mechanisms for glycosylation.
CO4	Analyze the importance of carbohydrates and glycolipids in day to day life.
CO5	Discuss the carbohydrate based chiral pool strategies for the synthesis of bioactive molecules.

Course Articulation Matrix:

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

Syllabus:

Chapter-1 Introduction to Carbohydrate Chemistry: Overview of carbohydrates, general properties of carbohydrates; Classification of carbohydrates; Structures and conformational studies of monosaccharides; Reactions of monosaccharides: ring expansions and contractions; reactions at anomeric carbon and epimeric carbons, Oligosaccharides; protecting group methods.

Chapter-2 Polysaccharides: naturally-occurring oligo- and polysaccharides and their conformations; aspects of animal and plant polysaccharides, glycoproteins.

Chapter-3 Glycosylation Methods: Glycosylation, glycosyl donors and acceptors, stereoselective glycosylation, glycosylation strategies – one pot glycosylation, iterative glycosylation; enzymatic glycosylations to oligosaccharides; Glycosidic bond stabilities. Unnatural sugars: Deoxy sugars; synthetic aspects of rare sugars; amino sugars; Carbasugars.

Chapter-4 Glycochemistry: Biological activity of polysaccharides, glycoproteins, proteoglycans, and glycolipids, and the role of glycomics in development and disease; glycotechnology and glycoengineering for the preparation of therapeutic glycans and glycan-coated materials.

Chapter-5 Chiral pool synthesis: Synthesis of carbocycles and heterocycles; proteoglycans and glycosaminoglycans; selected natural product synthesis originating from a sugar scaffold. Fundamentals of glycobiology; tools for glycomics; carbohydrate-based drug discovery.

Learning Resources:

Text Books:

1. Monosaccharides: Their chemistry and their roles in natural products, P. Collins and R. Ferrier, John Wiley & Sons Ltd., Chichester, 1998.
2. Carbohydrates: The essential molecules of life, R. V. Stick, S. J. Williams, Elsevier, Oxford, 2001.

Reference Books:

1. Advanced Organic Chemistry, Bahl B.S, Arun Bahl, Sultan Chand and Co., 1986, 12th Edition.
2. Organic Chemistry, Finar I. L., Addison Wesley Longman Ltd., 1996, 6th Edition.

Online Resources:

1. https://nptel.ac.in/content/storage2/courses/104103071/pdf/mod11.pdf

Course Code: CY5171	ADVANCED TOPICS IN OPTICAL AND RESONANCE TECHNIQUES	Credits L-T-P: Cr 3-0-0: 3

Course Outcomes:

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

CO1	Understand the principles of atomic spectra in chemical analysis
CO2	Interpret molecular interactions by using absorption and emission spectra.
CO3	Apply the nuclear spin relaxation processes for studying the molecular motions
CO4	Analyze spin properties of triplet molecules and transition metal complexes using electron spin resonance
CO5	Choose the multiple spin resonance methods for structural elucidation

Course Articulation Matrix:

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

Syllabus:

Chapter-1 Atomic Spectra: Atomic Absorption, Atomic Fluorescence and Atomic Emission Spectra; Term Symbols; Stark and Zeeman Effects, Isotopic Abundance Evaluation; Stellar Radiation Analysis; Gamma-Ray Absorption Spectra, Recoilless Gamma Ray Absorption Spectroscopy.

Chapter-2 Molecular Absorption and Emission Spectra: Specular and Grazing Angle Reflection Spectra; NIR and Vacuum UV Absorptions; Electronic Spectra of Lanthanide Complexes, Organometallics and Composites; in-situ Spectral Techniques; Surface Enhanced Raman Spectroscopy. Fluorescence LifeTime and Quantum Yields; Photoluminescence, Nonlinear Optical Phenomena; Thermochromic, Mechanochromic and Liochromic Properties and Applications.

Chapter-3 Nuclear Spin Relaxation Processes: Measurement of T1 by Inversion Recovery Method, Measurement of T2 by Spin Echoes Method; Applications of Relaxation Times.

Chapter-4 Multiple Spin Resonance Methods: Internuclear Homo and Heteronuclear Double Resonance; Off-Resonance and Gated Decoupling; Spin Tickling; Nuclear Quadrupole Moment and Electric Field Gradient; Asymmetry Parameter; NQR Transitions in Axially Symmetric and Non-Symmetric Molecules; Instrumentation and Applications.

Chapter-5 EPR Spectra: (a) Triplet Spin Systems: Spin Exchange, Hyperfine and Zero-Field Splitting in Triplet Spin Molecules. (b) Transition Metal Complexes: Russell-Saunders and Spin-Orbit Coupling, Hunds' Rules; EPR Manifestations of Jahn-Teller and Krammers Distortions,

(c) Double Resonance Techniques: ENDOR and EEDOR.

Learning Resources:

Text Books:

1. Modern Molecular Spectroscopy, K. S. Randhawa, McMillan, 2003.
2. Electronic Absorption Spectroscopy, D.N. Satyanarayana, University Press, 2001.
3. Magnetic Resonance Spectroscopy: ESR.NMR NQR, D.N. Satyanarayana, University Press, IK International Publishing House, 2021 and 3rd Edition.

Reference Books:

1. Handbook of Molecular Spectroscopy: From Radiowaves to Gamma Rays, Dreamtech Press, 2020 and 2nd Edition.
2. Molecular Vibrations: The Theory of Infrared and Raman Vibrational Spectra, E.B. Wilson, Dower Publications, Inc, 2003 and New Edition.
3. Molecular Spectroscopy Workbench: Advances, Applications, and Practical Advice on Modern Spectroscopic Analysis, Emil W. Ciurczak, Wiley, 1998 and 1st Edition.

Course Code: CY5172	CHEMISTRY OF BIOMOLECULES	Credits L-T-P: Cr 3-0-0: 3

Course Outcomes:

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

CO1	Understand the importance of biomolecules.
CO2	Illustrate the structure and functions of bioorganic molecules.
CO3	Interpret the physiological role of RNA, DNA and enzymes.
CO4	Utilize the concepts of protein purification and synthesis in bio-pharma industry.
CO5	Apply the concepts of enzyme catalysis for industrial applications.

Course Articulation Matrix:

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

Syllabus:

Chapter-1 Amino acids: Amino acids: structure, acid-base chemistry, and chemical synthesis; Asymmetric Synthesis of Amino Acids.

Chapter-2 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.

Chapter-3 Coenzymes: Structure and biological function of coenzyme A, thiamine pyrophosphate (TPP), pyridoxal phosphate (PLP), oxidized and reduced forms of NAD^+, NADH, $NADP^+$, NADPH, ATP.

Chapter-4 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.

Chapter-5 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. Principles of Biochemistry, A.L. Lehninger, Worth Publishers, 2017, 7th Edition.
2. Bioorganic Chemistry, H.B. Dugas, Springer, 1996, 3rd Edition.
3. Biochemistry, L. Stryer, W.H.F. Freeman, 2006, 6th Edition.

Reference Books:

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

Course Code: CY5173	ADVANCES IN QUANTUM CHEMISTRY	Credits L-T-P: Cr 3-0-0: 3

Course Outcomes:

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

CO1	Understand first principles calculation.
CO2	Understand the scope, possibility and limitations of first principles calculation for chemical applications.
CO3	Compare the semiempirical, ab initio and density functional theory.
CO4	Apply first principles calculation to solve chemistry problems.
CO5	Analyze the applications of density functional theory for a wide range of problems in chemistry.

Course Articulation Matrix:

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

Syllabus:

Chapter-1 Computational quantum chemistry: Introduction to quantum chemistry; Molecular Mechanics; Simulations of Molecular Aggregates; Many-Electron Wave Functions; Gaussian Basis Sets, Extended Basis Sets, and Orbital Polarization Terms in Basis Sets.

Chapter-2 Semiempirical Method: AM1, PM6, CNDO, INDO, NDDO Formalism.

Chapter-3 Ab initio Methods: Hartree-Fock Self - Consistent Field Methods; perturbation theory, configuration interaction, and coupled cluster methods.

Chapter-4 Density Functional Theory: Density matrix, Thomas-Fermi model, Hohenber-Kohn theorem, Basic principle of Kohn-Sham Theory.

Chapter-5 Applications: Spectroscopic and Thermodynamic Properties through DFT Approach; Hybrid Quantal and Classical Models; Excited Electronic States; Reaction Dynamics in Concluded Phase; Surface Crossing; Molecular Modeling; Drug Discovery and Design; Molecular and Ion Recognition and Transport**.**

Learning Resources:

Text Books:

1. Szabo, Attila, and Neil S. Ostlund. Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory. New York: McGraw-Hill, Inc., 1989
2. Density-functional theory of atoms and molecules. R.G. Parr and W. Yang, Oxford University Press, New York, Oxford, 1989

Reference Books:

1. Essentials of Computational Chemistry; Theories and Models, Christopher J. Cramer, Wiley; 2004
2. Computational Chemistry: Introduction to the Theory and Applications, Errol G. Lewars, Springer, 2016.

Course Code: CY5174	EMERGING TOPICS IN ORGANIC SYNTHESIS	Credits L-T-P: Cr 3-0-0: 3

Course Outcomes:

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

CO1	Understand the concepts of multicomponent reactions and their mechanisms.
CO2	Understand the tandem reactions in organic synthesis.
CO3	Apply the principles of click chemistry in drug discovery, biology and materials chemistry.
CO4	Utilize the soft metal catalyst in organic synthesis.
CO5	Discuss the flow chemistry, micro reactors, separation techniques and process chemistry in organic synthesis.

Course Articulation Matrix:

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

Syllabus:

Chapter-1 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.

Chapter-2 Click chemistry: Importance of in 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.

Chapter-3 Tandem (cascade/domino) reactions in Organic Synthesis, Metal Carbenes in Organic Synthesis, *N*-heterocyclic carbenes in organic synthesis, Hypervalent iodine reagents in organic synthesis.

Chapter-4 Soft metals in Organic Synthesis: Silver in Organic Synthesis, Indium in Organic Synthesis, Gold in Organic Synthesis. Nanomaterials in catalysis and Organic Synthesis, photo catalysis.

Chapter-5: Recent advances in Flow chemistry and Micro reactors, Separation techniques, process chemistry, Trouble shooting in organic synthesis.

Learning Resources:

Text Books:

1. Multicomponent Reactions: Concepts and Applications for Design and Synthesis, Raquel P. Herrera, Eugenia Marqués-López, John Wiley & Sons. 2015, 1st Edition.
2. Click Reactions in Organic Synthesis, Srinivasan Chandrasekaran, John Wiley & Sons, 2016, 1st Edition.
3. Modern Gold Catalyzed Synthesis, Stephen K. Hashmi, Dean F. Toste, John Wiley & Sons, 2012.
4. Modern Solvents in Organic Synthesis, Paul Knochel, Springer, 2003.
5. Domino Reactions in Organic Synthesis, Lutz F. Tietze, Gordon Brasche, Kersten Gericke, John Wiley & Sons, 2006.

Reference Books:

1. Microreactors in Organic Synthesis and Catalysis, Ed. by Thomas Wirth Title, John Wiley & Sons, 2008.
2. Metal Carbenes in Organic Synthesis, K H Dtz, Springer Science & Business Media, 2004.
3. Nanomaterials in Catalysis, Ed. by Philippe Serp, Karine Philippot, John Wiley & Sons, 2012.
4. Chiral Separation Techniques: A Practical Approach, Ganapathy Subramanian, John Wiley & Sons, 2008.

Course Code: CY5175	INDUSTRIAL CHEMISTRY	Credits L-T-P: Cr 3-0-0: 3

Course Outcomes:

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

CO1	Understand the chemistry of paints, varnishes, surface coating and cleaning agents.
CO2	Summarize the importance of fertilizers, pesticides, insecticides, fungicides and herbicides.
CO3	Examine the basic principles of essential oils.
CO4	Apply the concept of chemical formulation in perfumes and cosmetics production.
CO5	Discuss the basic chemistry involved in smart and soft materials.

Course Articulation Matrix:

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

Syllabus:

Chapter-1 Paints, Varnishes and Soaps: Paints & Varnishes: Primary constituents of paints, Dispersion medium (solvent), binder Pigments, formulation of paints and varnishes. Requirements of a good paint. Soaps: manufacture of soaps by hot and cold process, classification of soap, cleansing of soap and classification of detergents (anionic and cationic).

Chapter-2 Surface Coatings: Objectives of coatings surfaces, preliminary treatment of surface, classification of surface coatings. Paints and pigments-formulation, composition and related properties. Oil paint, Vehicle, modified oils, Pigments, toners and lakes pigments, Fillers, Thinners, Enamels, emulsifying agents. Special paints (Heat retardant, Fire retardant, Eco-friendly paint, Plastic paint), Dyes, Wax polishing, Water and Oil paints, additives.

Chapter-3 Fertilizers: natural fertilizers, nitrogenous fertilizer (NH_4NO_3, urea), phosphatic fertilizer (superphosphate, TSP, polyphosphate), potash fertilizer (KCl, KNO_3, K_2SO_4), bio fertilizers. Pesticides: classification, structure of some important pesticides (DDT, BHC, allethrin and pyrethrin).

Chapter-4 Agrochemicals: Pesticides – classification of Insecticides, fungicides, herbicides as organic and inorganic – general methods of application and toxicity. Safety measures when using pesticides. Insecticides: Plant products – Nicotine, pyrethrin – Inorganic pesticides – borates. Organic pesticides – D.D.T. and BHC. Fungicide: Sulphur compounds, Copper

compounds, Bordeaux mixture. Herbicides: Acaricides – Rodenticides. Attractants – Repellents. Preservation of seeds.

Chapter-5 Chemistry of Essential oils, Perfumes and Cosmetics: Essential oil: Definition–occurrences–Methods of production from plants–Steam distillation and expression method. Perfumes: Formulations–Requirements for a good perfume–Compositions of perfumes–classification of perfumery materials–animals-synthetic formulations–manufacturing and packaging process of perfumes. Cosmetics: Face cream–Sun screen lotion–shaving cream–composition and formulation–Uses and hazards, Sprayer–Hand lotion–nail lacquers–nail bleaches–hair oil–hair dyes–composition and formulations–Uses and hazards.

Learning Resources:

Text Books:

1. Handbook of Industrial Chemistry: Organic Chemicals, M. F. Ali, B. M. El Ali and J. G. Speight, McGraw-Hill Education, 2005.
2. Industrial Chemistry, B. K. Sharma, Goel Publishing House, 2003.
3. Tanning Chemistry: The Science of Leather, A. D. Covington and T. Covington, Royal Society of Chemistry, 2009.

Reference Books:

1. Textbook of Chemical Technology, Vol. 1 and 2, G. N. Pandey, Vikas Publishing House, Pvt. Ltd, 1999.
2. Industrial Inorganic Chemistry, W. Buchner, R. Sohliebs, G. Winter, and K. H. Buchel John Wiley and Sons Ltd, 2007.

Course Code: CY5176	SUPRAMOLECULAR CHEMISTRY	Credits L-T-P: Cr 3-0-0: 3

Course Outcomes:

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

CO1	Understand the principle of molecular self-assembly.
CO2	Classify the different components of noncovalent interactions.
CO3	Identify the role of noncovalent interactions in supramolecular chemistry.
CO4	Analyze host-guest and self-assembly concepts for enhancing catalytic activities.
CO5	Develop molecular devices and biological mimics using self-assembly and crystal engineering approaches.

Course Articulation Matrix:

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

Syllabus:

Chapter-1: Definition of supramolecular chemistry. Nature of binding interactions in supramolecular structures: ion-ion, ion-dipole, dipole-dipole, H-bonding, cation-p, anion-p, p-p, and van der Waals interactions.

Chapter-2: Synthesis and structure of crown ethers, lariat ethers, podands, cryptands, spherands, calixarenes, cyclodextrins, cyclophanes, cryptophanes, corands and hemicarcerands., Host-Guest interactions, pre-organization and complementarity, lock and key analogy. Binding of cationic, anionic, ion pair and neutral guest molecules.

Chapter-3 Crystal engineering: Role of H-bonding and other weak interactions.

Chapter-4 Self-assembly molecules: Design, synthesis and properties of the molecules, self-assembling by H-bonding, metal-ligand interactions and other weak interactions, metallomacrocycles, catenanes, rotaxanes and knots.

Chapter-5 Molecular devices: Molecular electronic devices, molecular wires, molecular rectifiers, molecular switches, molecular logic.

Chapter-6 Relevance of supramolecular chemistry to mimic biological systems: Cyclodextrins as enzyme mimics, ion channel mimics, supramolecular catalysis etc. Examples of recent developments in supramolecular chemistry from current literature.

Learning Resources:

Text Books:

1. Supramolecular Chemistry-Concepts and Perspectives, J.-M. Lehn; Wiley-VCH, 1995.

2. Supramolecular Chemistry, P. D. Beer, P. A. Gale, D. K. Smith, Oxford University Press, 1999.
3. Supramolecular Chemistry, J. W. Steed and J. L. Atwood, Wiley, 2000.

Reference Books:

1. Supramolecular Chemistry: Concepts and Perspectives, Jean-Marie Lehn, Wiley-VCH, 1995 and 1st Edition.
2. Modern Supramolecular Chemistry, Francois Diedrich, Peter J. Stang, Rik. R. Tykwinski, Wiley-VCH, 2008 and 1st Edition
3. The Weak Hydrogen Bond: In Structural Chemistry and Biology, G. R. Desiraju, T. Steiner, Oxford University Press, 2001 and 1st Edition.
4. Principles and Methods in Supramolecular Chemistry, H. –J. Schneider, A. Yatsimirsky, Wiley-VCH, 1999 and 1st Edition.
5. Crystal Engineering – A textbook, Gautam R Desiraju, Jagadese J Vittal & Arunachalam Ramanan. World Scientific Publishing, 2011.