NATIONAL INSTITUTE OF TECHNOLOGY WARANGAL

SCHEME OF INSTRUCTION AND SYLLABI

for M.Sc. Analytical 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. Program 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. – Analytical 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. – Analytical 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. Analytical 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. Analytical Chemistry – Course Structure

II - Year, I – Semester

S. No.	Course Code	Course Name	L	T	P	Credits	Cat. Code
1	CY5201	X-Ray and Microscopic Methods of Analysis	3	0	0	3	PCC
2	CY5202	Physical Methods of Chemical Analysis	3	0	0	3	PCC
3	CY5203	Advanced Chromatographic Methods	3	0	0	3	PCC
4	CY5204	Nanomaterials	3	0	0	3	PCC
5	CY521X	Elective-2	3	0	0	3	PEC
6	CY522X	Elective-3	3	0	0	3	PEC
7	CY5205	Instrumental Methods of Chemical Analysis Laboratory-I	0	0	3	1.5	PCC
8	CY5206	Instrumental Methods of Chemical Analysis Laboratory-II	0	0	3	1.5	PCC
9	CY5248	Seminar-2	0	0	2	1	SEM
		Total				**22**	

Elective-2 (II Year, I Semester)		
S. No.	**Course Code**	**Course**
1	CY5211	Environmental Pollution and Waste Management
2	CY5212	Statistics and Quality Control in Analytical Chemistry
3	CY5213	Chemical, Electrochemical and Biosensors
Elective-3 (II Year, I Semester)		
S. No.	**Course Code**	**Course**
1	CY5221	Bioinorganic Chemistry
2	CY5222	Polymer Chemistry
3	CY5223	Advances in Industrial Catalysis

II - Year, II – Semester

S. No.	Course Code	Course Name	L	T	P	Credits	Cat. Code
1	CY526X	Elective-4	3	0	0	3	PEC
2	CY517X	Elective-5	3	0	0	3	PEC
3	CY5297	Comprehensive Viva-Voce				2	CVV
4	CY5299	Dissertation Work				10	DW
		Total				**18**	

Elective-4 (II Year, II Semester)		
S. No.	**Course Code**	**Course**
1	CY5261	Chemical and Electrochemical Energy Systems
2	CY5262	Surface Analytical Techniques
3	CY5263	Advanced Electroanalytical Methods

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. – Analytical 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 oxime 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 Tunneling; Quantum Dots; Tunneling 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: CY 5201	X-RAY AND MICROSCOPIC METHODS OF ANALYSIS	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 X-ray spectroscopy and electron microscopy for qualitative and quantitative analysis of solid samples
CO2	Interpret X-ray and particle diffraction pattern in assigning the crystallographic aspects of materials
CO3	Analyze electron microscopic images for morphological and in-depth material characteristics
CO4	Evaluate atomic arrangements and interatomic forces in solid materials
CO5	Choose appropriate microscopic technique along with sample preparation methodology for analysis of materials

Course Articulation Matrix:

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

Syllabus:

Chapter-1 X-ray absorption and fluorescence spectroscopy: Principles, Duane-Hunt law, Continuum and Line Spectra, Chemical analysis, Wavelength dispersive and energy dispersive instruments, qualitative and quantitative analysis, Applications.

Chapter-2 Diffraction methods: Introduction, Reflection high energy electron diffraction (RHEED), Neutron diffraction, small angle neutron diffraction (SANS) analysis, Principle, Instrumentation and applications. Small angle X-ray diffraction.

Chapter-3 Electron microscopy: Scanning electron microscopy, instrumentation, electron sources and lenses, resolution and contrast, environmental SEM, FE-SEM, Energy dispersive X-ray spectrometry (EDX), Applications. Transmission electron microscopy (TEM): Principle, instrumentation, imaging, electron diffraction, reflection electron microscopy, applications.

Chapter-4 Probe microscopy methods: Scanning tunneling microscopy (STM), principles, basic parameters, atomic resolution, surface imaging, lithography. Atomic force microscopy: Principles, Chemical force microscopy, AFM Lithography, applications.

Learning Resources:

Text Books:

1. Principles of Instrumental Analysis, Skoog, Holler, Crouch, Cengage Learning, 2020 and 7th Edition (India reprint edition)
2. Physical principles of electron microscopy: an introduction to TEM, SEM and AEM, R F Egerton, Springer, 2016, 2nd Edition.
3. Transmission electron microscopy: A Textbook for materials science, David B Williams, C Barry Carter, Springer, 2009, 2nd edition.

4. Instrumental Methods of Chemical Analysis, Chatwal & Anand, Himalaya, 2014 and 5th Edition.

Reference Books:

1. Surface Analysis: The Principal Techniques, John C Vikerman, Ian Gilmore (Eds.), Wiley 2009, 2nd Edition.
2. Scanning electron microscopy and X-ray microanalysis, J Goldstein, D Newbury, D Joy, C Lyman, P Echlin, E Lifshin, L Sawyer, J R Michael, Springer, 2003 and 3rd Edition.
3. Chemical Analysis – Modern Instrumentation Methods and Techniques, Rouessac and Rouessac, John Wiley, 2010, 6th edition.

Course Code: CY 5202	PHYSICAL METHODS OF CHEMICAL ANALYSIS	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 absorption and emission spectrometric methods
CO2	Interpret the results of polarimetry for characterizing chiral compounds
CO3	Apply luminescence methods for studying chemical compounds
CO4	Analyze the results of turbidimetry, nephelometry and refractometry for studying optical properties
CO5	Choose a combination of luminescence, radiometric and refractometric methods for comprehensive analysis

Course Articulation Matrix:

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

Syllabus:

Chapter-1 Atomic Absorption and Atomic Emission Spectrometry; Instrumentation and Application in Trace Metal Analysis; Applications in Ultra Trace Metal Analysis;

Chapter-2 Luminescence Methods; Fluorescence and Phosphorescence and Chemiluminescence; Lazers, Flash Photolysis; Fast reactions; Kinetic Methods of Analysis;

Chapter-3 Polarimetry, Optical Rotatory Dispersion and Circular Dichroism in Qualitative and Quantitative Analysis of Chiral Compounds;

Chapter-4 Turbidimetry and Nephelometry; Scattering of Light by Colloidal and Nanoparticles; Refractometry.

Chapter-5 Mossbauer Spectroscopy: Recoilless Gamma Ray Absorption; Mossbauer Effect; Instrumentation; Chemical Shift (Isomer Shit); Quadrupole Shift; Zeeman Effect; Applications.

Chapter-6 Radiometric and Labeling Methods: Radioactivity as an analytical tool. Neutron activation analysis - Instrumentation and application for trace and ultra-trace analysis, isotope dilution analysis.

Learning Resources:

Text Books:

1. Introduction to Instrumental Analysis, Robert D Braun, McGraw Hill, 2012, 2nd Edition.
2. Principles of Instrumental Analysis, Douglas A. Skoog, F. James Holler, Stanley R. Crouch, Cengage Learning, 2006, 6th Edn.
3. Willard, Merritt, Dean, Settle, Instrumental Methods of Analysis, CBS / Wadsworth Publ. Co., 2004, 7th Edn.
4. Modern Analytical Chemistry, David Harvey, McGraw-Hill International Edition, 2000.

Reference Books:

1. Physical Chemistry, Peter Atkins & Julio de Paula, Oxford University Press, 2016, 10th Edition.
2. Instrumental Methods of Chemical Analysis, Gurdeep R. Chatwal, Sham K. Anand, Himalaya Publishing house, 2012, 5th Edition.

Course Code: CY 5203	ADVANCED CHROMATOGRAPHIC METHODS	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 and instrumentation of liquid and gas chromatography techniques
CO2	Identify strengths of separation and detection techniques for studying sample properties and analytical problems
CO3	Devise optimization methods for achieving better chromatographic separation
CO4	Choose appropriate chromatographic technique for quantifying light-weight analytes from complex matrices
CO5	Develop efficient and eco-friendly analytical methods of separation and quantitation

Course Articulation Matrix:

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

Syllabus:

Chapter-1 Liquid Chromatography: High Performance Liquid Chromatography (HPLC) and Ultra performance liquid chromatography (UPLC): Principle, Modern stationary phases, New detectors, Chiral stationary phases and Chiral mobile phases, Specific applications.

Chapter-2 Supercritical Fluid Chromatography: Supercritical fluids, properties of supercritical fluids, SFC-principle, -instrumentation, detectors, injection techniques, pressure restrictor, specific applications.

Chapter-3 Ion Chromatography and Gel permeation chromatography: Principle, applications in qualitative and quantitative analysis.

Chapter-4 Chromatography with Mass Spectral Detection: Gas Chromatography, GC/MS and LC/MS, Other Hyphenated Methods, Liquid Chromatography/Nuclear Magnetic Resonance: Introduction, principle, instrumentation and applications. Matrix assisted laser desorption ionization-time of flight mass spectrometry (MALDI-TOF MS).

Chapter-5 Multidimensional Chromatography: Gas Chromatography/Gas Chromatography, Liquid Chromatography/Gas Chromatography, Liquid Chromatography/Liquid Chromatography, Other Combinations: Introduction, Principle, Instrumentation and Applications.

Chapter-6 Capillary Electrophoresis and Capillary Electrochromatography: Principles of Electrophoresis, Fundamental Equations, Weak Acids and Bases, Complex Formation, Electrolyte Concentration, Electroosmosis, Diffusion, Adsorption; Zone Electrophoresis, Capillary Electrophoresis, Capillary Zone Electrophoresis, Micellar Electrokinetic

Chromatography, Capillary Electrochromatography: Principle, instrumentation, detectors, applications.

Learning Resources:

Text Books:

1. Chromatographic Methods, A. Braithwaite and F.J. Smith, Blackie Academic & Professional (Chapman & Hall), 2009 and 5th Edition.
2. Hand Book of GC-MS, Fundamentals and Applications, Hans-Joachim Hubschmann, Wiley-VCH, 2015, 3rd edition.
3. Liquid Chromatography-Mass Spectrometry-An Introduction, Robert E. Ardrey, Wiley, 2003 1st edition.
4. Principles of Instrumental Analysis, Skoog, Holler, Crouch, Cengage Learning, 2017, 7th edition.

Reference Books:

1. Chromatography, Concepts & Contrasts, James M. Miller, Jhon Wiley & Sons, 2009, 2nd Edition.
2. Instrumental Methods of Chemical Analysis, Gurdeep R. Chatwal, Sham K. Anand, Himalaya Publishing House, 2012, 5th Edition.

Course Code: CY 5204	NANOMATERIALS	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 history of nanoscience
CO2	Classify nanomaterials based on structural properties
CO3	Model suitable nanomaterials with desired shape, size and structure towards diverse applications
CO4	Select an appropriate technique for characterizing new nanomaterial
CO5	Predict the impact of nanomaterials on the environment

Course Articulation Matrix:

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

Syllabus:

Chapter-1 Introduction: Nanosystems - an overview, Quantum confinement, dimensionality and size dependent phenomena, surface to volume ratio, surface dependent properties at nanoscale.

Chapter-2 Classification of Nanomaterials: Dimensionality based Classification– 0D (quantum dots), 1D (wires), 2D (nanoplate), 3D (nanoparticles); Metal (Copper, silver, gold etc.) and metal oxides; based nanomaterials. Carbon based nanomaterials (buckyballs, nanotubes, graphene), Composite nanomaterials, core-shell nanoparticles, nanoshells, self- assembled monolayers, and magnetic nanoparticles.

Chapter-3 Synthesis: Bottom-up approaches (Chemical Routes): Sol-gel synthesis, microemulsions or reverse micelles, co-precipitation method, solvothermal synthesis, hydrothermal synthesis. Top-down approach (Physical methods): High energy ball milling photolithography, electron-beam lithography (EBL).

Chapter-4 Characterization of nanomaterials: Characterization of nanomaterials using hi-fi instruments - electron spectroscopy and microscopy, probe microscopy, diffraction methods, BET, DLS, electroanalytical techniques and Raman scattering - for the study of nanomaterials,

Chapter-5 Applications:
Solar energy harvesting and storage, catalysis, nanoelectronics, topological insulator, Application of nanomaterials in biology, environmental applications.

Learning Resources:

Text Books:

1. Textbook of Nanoscience and Nanotechnology, B S Murty, P Shankar, Baldev Rai, BB Rath and James Murday, Univ. Press, 2012.
2. Nanomaterials: An Introduction to Synthesis, Properties and Applications, Dieter Vollath, G., Wiley-VCH Verlag GmbH & Co. KGaA, Germany, 2nd Edn., 2013.
3. M. Wilson, K. Kannangara, G. Smith, M. Simmons and B. Raguse, “Nanotechnology: Basic Science and Emerging Technologies”, Overseas Press India Pvt Ltd, New Delhi, 1st Edition, 2002.
4. T. Pradeep, “A Textbook of Nanoscience and Nanotechnology”, Tata McGraw Hill Education Pvt. Ltd, 1st Edition, 2012.

Reference Books:

1. Nanoparticles: From Theory to Application, Schmid, G., Wiley-VCH Verlag GmbH & Co. KGaA, Germany, 2nd Edn., 2010.
2. Concepts of Nanochemistry, Cademartiri L., Ozin G. A., Wiley-VCH Verlag GmbH & Co. KGaA, Germany, 2009.
3. Nanostructures & Nanomaterials; Synthesis, Properties & Applications, Guozhong Cao, Imperial College Press, 2007.
4. Nanotechnology, Fundamentals and Applications: Manasi Karkare, IK International, 2008.
5. Nanomaterials Chemistry, C. N. R. Rao, Achim Muller, K. Cheetham, Wiley-VCH, 2007.

Course Code: CY 5205	INSTRUMENTAL METHODS OF CHEMICAL ANALYSIS 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 and analytical applications of diverse instrumental techniques
CO2	Identify suitable methodologies and instrumental techniques for the study of physical and chemical properties
CO3	Analyze calibration methods of instruments to achieve accuracy and precision
CO4	Select appropriate analytical methods for determining analytes of interest
CO5	Design instrumental methods for quantitation of analytes in domestic and industrial samples

Course Articulation Matrix:

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

Syllabus:

Spectrophotometric detection of phosphate using Molybdenum Blue Method.
Determination of total alkalinity of a given water sample.
Determination of sulphate in a given samples by turbidimetric spectrophotometry.
Determination of dissolved oxygen in the given water sample.
To determine the minimum dose of coagulate required for observing the flocculation in the given water sample.
Determination of Biochemical Oxygen Demand (B.O.D) in the given polluted water sample.
Potentiometric halide titration of Ag^{+}
Determination of acetic acid content in commercially available vinegar using conductometry
Determination of phosphoric acid in Coca-Cola using pH metry.
Flame photometry analysis of a trace metal ion.
Simultaneous determination of two metal ions by spectrophotometry.
Conductometric determination of mixture of acids.
Determination of Copper by spectrophotometry.
Calorimetric determination of Manganese in steel.

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., 2009, 7th Edition.
2. Quantitative Chemical Analysis. Daniel C. Harris, 2015, 9th Edition.

Reference Books:

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

Course Code: CY 5206	INSTRUMENTAL METHODS OF CHEMICAL ANALYSIS LAB-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 differences between titrimetric and instrument-based methods in quantitative analysis
CO2	Apply requisite knowledge for effective quantitative analysis with diverse analytical instruments
CO3	Utilize electrochemical and microscopic analytical methods for characterizing complex analytical samples
CO4	Analyze experimental data of microscopic, diffraction, spin resonance and optical rotatory analyses using software tools
CO5	Design a combination of instrumental methods for comprehensive analysis of pharmaceutical, chemical industry and environmental samples

Course Articulation Matrix:

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

Syllabus:

Titrimetric analysis and Instrumental Methods of Chemical Analysis (only a set of 12 experiments from the designed experiments)

1. Estimation of paracetamol in the given formulation by potentiometry
2. Estimation of equilibrium constant of ethyl acetoacetate by redox titration
3. Estimation of aspirin in pharmaceutical formulation by pH metry
3. Estimation of tolbutamide in pharmaceutical formulation
5. Estimation of ascorbic acid in pharmaceutical formulation by potentiometry
6. Estimation of ibuprofen in the given formulation by titrimetric and conductometric Methods
7. Estimation of isoniazid in the given formulation by redox potentiometric analysis

Modern Instrumental Methods:

1. Hands on Experience on Electrochemical workstation
   -Linear Sweep Voltammetric Estimation of Ascorbic Acid.
2. Cyclic Voltammetric Study of Ferricyanide/ferrocyanide couple.
3. Hands on Experience on Scanning Electron Microscope
   - SEM imaging of metals/polymers/fibers/biopolymers/nanopowders.
4. Hands on experience on Powder X-Ray Diffractometer
   -Analysis of crystalline compounds by XRD-powder method
5. Hands on experience on Electron Spin Resonance (ESR) Spectrometer
   -Analysis of ESR Spectrum
6. Hands-on experience on Nuclear Magnetic Resonance Spectrometer (NMR).
   -Analysis of organic compounds

7. Optical Rotatory Dispersion and Circular Dichroism (ORD CD) analysis of compounds
8. Hands on experience on High-performance liquid chromatography (HPLC) and Gas chromatography (GC)
   -Chromatographic analysis of mixtures by HPLC and GC
9. Hands on experience on thermogravimetric and differential thermal analysis

Learning Resources:

Text Books/Manuals:

1. A Text-book of quantitative chemical analysis of pure salts, alloys, minerals and technical products, John Charles Oslen, Nabu, 2011.
2. Chemical analysis in the laboratory, I M Harvey and R M Baker, RSC, 2019.
3. Quantitative chemical analysis adapted for use in laboratories, Frank Clowes and J B Coleman, Nabu, 2011.
4. Laboratory experiments to accompany general, organic and biological chemistry - An Integrated Approach, D B Macaulay, C Anderson, M M Bloomfield, J M Bauer, Wiley, 2013, 3rd edition.

Reference Books:

1. Practical instrumental analysis - Methods, quality assurance and laboratory management, Sergio Petrozzi, Wiley, 2012, 1st edition.
2. Elements of Chemical Analysis: Inorganic and Organic, E.A. Pamel, Kessinger Pub. Co, 2007.
3. Food analysis laboratory manual, Suzanne Nielsen, Springer, 2015.

Course Code: CY 5211	ENVIRONMENTAL POLLUTION AND WASTE MANAGEMENT	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 causes and effects of environmental pollution for planning mitigation strategies
CO2	Identify relationships between chemical exposure and effects on physiological systems
CO3	Apply basic chemical concepts for probing chemical processes involved in different environmental problems
CO4	Assess water purification and waste treatment processes and the practical chemistry involved
CO5	Discuss local and global environmental issues based on the acquired knowledge

Course Articulation Matrix:

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

Syllabus:

Chapter-1 Air and Noise Pollution: Pollutants Introduction: Definition of pollution; pollutants; classification of pollutants (Physical, chemical and biological), Air borne particles and particulate matters, Temperature inversion, SOX, NOX, Hydrocarbons, Lead & other pollutants; Temperature inversion; photochemical Smog; Health effects of Air pollution; Adverse health effects of tobacco. Measurement of Noise, Health effects of Noise pollution, Control of noise pollution.

Chapter-2 Water pollution: Sources of surface and groundwater pollution; Water quality parameters: COD, BOD, DO, hardness, alkalinity; Biological aspects of water pollution: MPN, Eutrophication; Biological indicator; Arsenic pollution of drinking water and its consequence: An overview. Waste water: Constituents – Microorganisms, Solids, Inorganic constituents, Organic matter, Water Quality requirements, pH values of Wastes and Receiving water, Suspended solids, preliminary, primary, secondary, tertiary treatment, Waste water from some typical industries, sources, characteristics, effect and treatment

Chapter-3 Pollution control and green technologies: Activated Sludge Process (ASP) - Trickling Filters - oxidation ponds, fluidized bed reactors, concept and working of effluent treatment plants (ETPs). Definition and concepts: green technology, Greenhouse Gas (GHG) emissions reduction: carbon capture and storage (CCS) technologies, fuel efficient vehicles, and mass transit, methane emissions reduction and/or reuse; Pollution reduction and removal (Flue Gas Desulfurization (FGD) methods; Rainwater Harvesting; Successful green

technologies: wind turbines, solar panels; 3R's of green technology: recycle, renew and reduce

Chapter-4 Solid Waste: Sources and generation of solid waste; their classification and chemical composition; characterization of municipal solid waste; hazardous waste and biomedical waste. Effect of solid waste disposal on environment: Impact of solid waste on environment, human and plant health; water quality and aquatic life; mining waste and land degradation; effect of landfill leachate on soil characteristics and groundwater pollution.

Chapter-5 Solid waste Management and environmental impact assessment: Different techniques used in collection, storage, transportation and disposal of solid waste (municipal, hazardous and biomedical waste); landfill (traditional and sanitary landfill design); thermal treatment (pyrolysis and incineration) of waste material; drawbacks in waste management techniques; Concept of Integrated waste management. Environmental Impact Assessment, Environmental Impact Assessment process in India-Environmental acts and rules.

Learning Resources:

Text Books:

1. Fundamental Concepts of Environmental Chemistry, G.S. Sodhi, Narosa publishing House, 2005, Second edition.
2. Wastewater treatment, M.N. Rao and A.K. Datta, Oxford Publications, 2013, Third edition.

Reference Books:

1. Environmental Science and Engineering, J. Glynn Henry and Garry W. Heinke, Prentice-Hall, Inc., New Jersey, USA, 1996, Second edition.
2. Environmental and Pollution Science, I. L. Pepper, C. P. Gerba and M. L. Brusseau, Elsevier Academic Press, 2019, Third edition.
3. Design of Landfills and Integrated Solid Waste Management, A. Bagchi, John Wiley & Sons 2004, Third edition.

Course Code: CY 5212	STATISTICS AND QUALITY CONTROL IN 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 significance of statistical concepts in chemical analysis
CO2	Identify the type of errors occurring in the measurements and minimize them
CO3	apply appropriate calibration method in achieving results with highest precision
CO4	Evaluate statistical tools for improving the quality of analytical measurements
CO5	Develop a standard method for optimizing experimental procedures in analytical chemistry laboratories

Course Articulation Matrix:

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

Syllabus:

Chapter-1 Quality of Analytical Measurements: Propagation of error, Sampling strategy, Quality control methods-property control charts, precision control charts, collaborative tests and uncertainty of measurements, Numerical calculations.

Chapter-2 Significance tests: Comparison tests, outliers, ANOVA calculations.

Chapter-3 Analytical methods Metrological Quality: Various types of analytical methods, regression analysis, Limit of detection, Limit of quantification, Random error, Calibration of equipment and instruments. Curvilinear and outlier analysis.

Chapter-4 Standard Method Development and Validation: Optimization of experimental procedures in analytical chemistry, Standard addition, External standard, internal standard and dilution methods, response surfaces, specific examples, experimental design-fractional factorial designs. Validation testing parameters and their calculation with numerical examples

Learning Resources:

Text Books:

1. Statistics and chemometrics for Analytical chemistry, James N Miller and Jane C Miller, Pearson, 2005 and 5th Edition.
2. Statistical methods in Analytical chemistry, Peter C Meier, Richard E Zund, John Wiley & Sons, 2000 and 2nd Edition.

Reference Books:

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

3. Modern Analytical Chemistry, David Harvey, McGraw Hill-Education., 2000 and 1st Edition.
4. Quality in the Analytical Chemistry Laboratory, Elizabeth Pricard, Vicki Barwick, John Wiley & Sons, 2007 and 1st Edn.

Course Code: CY 5213	CHEMICAL, ELECTROCHEMICAL AND BIOSENSORS	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 physicochemical transduction mechanisms
CO2	Identify strengths of optical, electro and mass transduction mechanisms for sensor applications
CO3	Analyze the results of optical, electro and mass transductions for qualitative and quantitative outcomes
CO4	Choose appropriate transduction method for sensing analytes in complex sample matrices
CO5	Develop analytical methods for efficient biosensor applications

Course Articulation Matrix:

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

Syllabus:

Chapter-1: Principle of chemical and electrochemical biosensors, Industrial applications, medical diagnosis, implant analysis, remote sensing and control, On-site, portable analysis.

Chapter-2 Transduction methodologies: absorbance and fluorescence methods, microcantilever and microbalance methods, electrochemical, optochemical and surface plasmon resonance techniques. Molecular recognition materials: Biomolecular materials, artificial molecular-recognition materials, biomimic-enzymes and -receptors.

Chapter-3 Electrochemical and biosensors: Microelectrodes, interdigitated array electrodes, self-assemblies, microarray methods, miniaturization, multiplex analysis for electrochemical sensors. Surface plasmon resonance, microcantilever and microbalance sensors.

Chapter-4 Applications of Electrochemical Biosensors: Environmental monitoring, Food and beverage industry - preservatives and mycotoxins, Biomedical diagnosis – cholesterol, cancer marker, genome analysis, defense applications.

Learning Resources:

Text Books:

1. Chemical Sensors and Biosensors, Brian R. Eggins, John Wiley, 2004.
2. Sensors in Biomedical Applications – Fundamentals, Technology and applications, Gabor Harsanyi, CRC Press, 2000.
3. Electrochemical Sensors in Bioanalysis,Raluca-Ioana Stefan, CRC Press, 2001.
4. Analytical Electrochemistry, Joseph Wang, John Wiley, 2006.

Reference Books:

1. Optical Sensors, JorgHaus, Wiley VCH, 2010.

2. Biosensors: Electrochemical and mechanical biosensors, Paul Ed Millner, Scion Publishing, 2008.
3. Optical sensors: Industrial, Environmental and Diagnostic Application (Springer Series), R Narayanaswamy, O.S. Wolfbeis (Eds.), Springer, 2010.
4. Biosensors in Food Processing, Safety and Quality Control – Mehmet Mutlu (Ed.), CRC Press, 2010.

Course Code: CY 5221	BIOINORGANIC 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 role of metal ions in biological processes
CO2	Interpret toxicological mechanisms of metals and the biological defenses against the toxic effects
CO3	Identify metal sites in enzymes involved in the activation of molecules
CO4	List medicinal applications of inorganic compounds
CO4	Evaluate coordination chemistry principles in modulating properties of metal centers in enzymes
CO5	Understand role of metal ions in biological processes

Course Articulation Matrix:

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

Syllabus:

Chapter -1 Introduction: Fundamental concepts in biochemistry and biology: biosphere; living organisms; cells and cell compartments; biomolecules, distribution of elements in the earth's crust, seawater and organisms, inorganic elements in biological systems. Essential and trace metal ions in biology and their distribution, overview of metal ion function in metalloproteins and enzymes, metal ion transport and storage, function of special ligands - porphyrins, chlorin and corrin.

Chapter-2 Principles of coordination chemistry and physical methods in Bioinorganic Chemistry: Overview of thermodynamics and kinetics aspects, electronic and geometrical aspects of metal ions, reactions of coordinated ligands, analysis of biomolecules by physical methods.

Chapter-3 Functions of biomolecules: Sodium and potassium transport**,** dioxygen binding and activation by heme, non-heme and copper proteins, Iron transport and storage proteins in bacterial and mammalian systems, Electron transport–FAD, NAD, FMN, ubiquinone and blue copper proteins, Cytochromes, Iron- sulfur proteins – rubredoxin, ferredoxins, Photosynthesis.

Chapter-4 Enzymes: Hydrolytic enzymes, enzymes deal with hydrogen peroxide and dioxygen, cobalt containing enzymes, Nitrogen-cycle enzymes.

Chapter -5 Medicinal applications: metals in medicine, anti-cancer agents–cisplatin and other compounds, radiopharmaceuticals (Tc), diagnostic (Gd in MRI) and therapeutic agents Toxicity of Hg, Cd, Pb and As and chelation therapy.

Learning Resources:

Text Books:

1. Principle of Bioinorganic chemistry, Lippard and Berg, Univ. Science Books, 1994.
2. Biological Inorganic Chemistry – Structure & Reactivity, Ivano Bertini, Harry B. Gray, Edward I. Stiefel, Joan Selverstone Valentine, Univ. Science Books, 2007.

Reference Books:

1. Elements of Bioinorganic Chemistry, G. N. Mukherjee and A. Das, UN Dhur Pvt. Ltd, 1993, Fourth edition.
2. Bioinorganic Chemistry -- Inorganic Elements in the Chemistry of Life: An Introduction and Guide Wolfgang Kaim, Brigitte Schwederski, Axel Klein, Wiley, 2013, Second edition.

Course Code: CY 5222	POLYMER 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 basics of polymers and polymerization mechanism
CO2	Classify the polymerization methods
CO3	Apply the concepts of polymerization to develop advanced polymeric materials
CO4	Determine physical properties of polymers based on molecular packing
CO5	Formulate plastics with desired characteristics

Course Articulation Matrix:

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

Syllabus:

Chapter 1 Introduction: Definitions, origin, nomenclature, classification of macromolecules; molecular weight (MW) and its distribution; thermal transitions; thermodynamics of polymerization. Naturally occurring polymers-Chemical & Physical structure, properties, source, important chemical modifications, applications of polymers such as cellulose, lignin, starch, rosin, shellac, latexes, vegetable oils and gums, proteins etc. polymers from bio/renewable resources.

Chapter 2 Step and Radical Polymerization Methods: Step Polymerization: Reactivity of functional groups; kinetics; molecular weight in open and closed system - Carothers equation; stoichiometric control of MW; cyclization vs. linear polymerization, cross-linking and gel point; process condition; step-copolymerization, examples of step polymers.
Radical Chain Polymerization: Nature of chain polymerization and its comparison; structural arrangements of monomer units; kinetics; molecular weight and its distribution; chain transfer, inhibition, retardation, auto-acceleration; energetic characteristics; Techniques of radical polymerization – bulk, solution, emulsion, suspension polymerization; examples of polymers made by radical chain polymerization.
Living radical polymerization: Theory; nitroxide-mediated polymerization (NMP); atom transfer radical polymerization (ATRP); radical addition-fragmentation transfer (RAFT); others.

Chapter 3 Ionic, Stereo-regular and Other Polymerization Methods: Ionic chain polymerization: Cationic polymerizations - kinetics, mechanism; anionic polymerization - kinetics, mechanism; living anionic polymerization; examples.
Chain co-polymerization: General considerations; types of copolymers, copolymer compositions, reactivity ratio; radical and ionic copolymerization; examples.
Stereoregular polymerization: Origin and types of stereoisomerism in polymers; factors influencing stereo-regulation; properties of stereoregular polymers; stereospecific ionic

polymerizations; coordination polymerization; Ziegler-Natta polymerization, metallocene polymerization; examples
Other polymerization processes: Ring opening polymerization; group transfer polymerization; metathesis polymerization, etc.

Chapter 4 Characterization and properties: Characterization of macromolecules: Determination of molecular weight - methods for measuring number average, weight average, viscosity average MW; gel permeation chromatography; spectroscopic techniques to determine chemical composition and molecular microstructure.
Reaction of macromolecules: Reactions with polyolefins, polyenes, pendant groups; polymer degradation - thermal degradation, degradation by catalyst residues, degradation by end groups; mechanism of stabilization - antioxidants and heat stabilizers, catalyst quenchers, end-capping; Polymer properties and supramolecular structure: Properties of solid polymers, amorphous and crystalline phases of polymers, structure-property relationship

Chapter 5: Plastics, Compounding of plastics; Fabrication techniques – Compression, injection and transfer molding; Preparation and uses of some thermoplastic and thermosetting resins; Foamed, Reinforced and Conducting polymers, biopolymers.

Learning Resources:

Text Books:

1. Principles of Polymer Science, by Bahadur and Sastry, Narosa Publishing House 2002.
2. Polymer Science by Gowarikar, Johan wiley and Sons 1986.

Reference Books:

1. Textbook of Polymer Science and Engg Anilkumar and Gupta, Tata McGraw-Hill Publishing Co, Ltd., 1978.
2. Polymer Science and Technology by J. R. Fried, Prentice-Hall, Inc 1995.
Polymer chemistry, Seymour and Carraher, Marcel Dekker, 2003.

Course Code: CY 5223	ADVANCES IN INDUSTRIAL CATALYSIS	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 synthesis and properties of Molecular sieves
CO2	Classify catalysts based on the properties
CO3	Analyze mechanisms of new catalytic reactions
CO4	Evaluate the mechanisms of enzymatic catalysis
CO5	Modify the catalyst to meet the required industrial applications

Course Articulation Matrix:

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

Syllabus:

Chapter-1 General Introduction to Catalysts and in particular about Molecular sieves: Definition, Theory, Classifications, and Examples. Molecular sieves: Nomenclature, structure, synthesis, characterization and catalytic applications of Zeolites, Aluminophosphates, Mesoporous materials, Aminophosphates, Hydrotalcite, clays, Nanocomposites and Metal organic Frameworks.

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

Chapter-3 Characterization of Catalysts: Elemental Analysis (Surface and Bulk), Low and Wide angle XRD, SEM – EDAX, TEM, TG/DTA, TPD-NH_3, TG-MS, BET-Surface area, FT-IR, Raman, ESR, UV-Vis., XPS, MASNMR, and Cyclic voltammetry.

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

Chapter-5 Other Industrially important catalysts and processes: Wilkinson catalyst, Zeigler Natta catalyst, Fisher trope synthesis, Heck reaction, Suzuki coupling reaction, Haber process, Bio-diesel production, Dye degradation and Photocatalysis.

Chapter–6 Enzymatic catalysis: Effect of Temperature on Enzymatic catalysis, Kinetics, The Lineweaver – Burk method, The Eadie-Hofstee method, Examples of Enzymatic catalysis, General Mechanism, Elucidating Mechanisms for the Inhibition of Enzyme Catalysis, Advantages, Limitations, and Applications.

Learning Resources:

Text Books:

1. Catalysis: Principles and Applications, B. Viswanathan, S. Sivasanker, A.V. Ramaswamy, Narosa Publishing House, New Delhi 2007.
2. Mesoporous Zeolites, Preparation, Characterization and Applications, Edited by Mark E. Davis, Wiley-VCH, Verlag GmbH & Co. KGaA, 2015.
3. Industrial Catalysis A Practical Approach, Jens Hagen, Wiley-VCH, Verlag GmbH & Co. KGaA, 2006.
4. Modern Analytical Chemistry, David Harvey, McGraw-Hill International Edition, 2000.

Reference Books:

1. Molecular sieves of synthesis and Identification, R. Szostak, Van Nostrand Reinhold catalysis series, New York, 1989.
2. Hand book of molecular sieves, R. Szostak, International zeolite association, 2010.
3. Solid State Chemistry an Introduction, Lesley Smart and Elaine Moore, Stanley Thomes (Publishers) Ltd., 2004, 2nd Edition.

Course Code: CY 5261	CHEMICAL AND ELECTROCHEMICAL ENERGY 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 basic concepts of thermochemistry and chemical kinetics of energy sources.
CO2	Illustrate principles of electrochemical energy storage systems and their applications
CO3	interpret principles of solar energy harnessing for promising applications
CO4	Design new materials based on band gap engineering for energy harvesting
CO5	Develop pilot devices for energy storage applications

Course Articulation Matrix:

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

Syllabus:

Chapter 1 Green Energy Resources: Quality of Chemical Energy Sources; Monitoring of Energy Extraction from Materials; Nanochemical Methods in Energy Extraction; Modeling of Combustion and Other Energy Tapping from Materials.

Chapter 2 Thermochemistry and Chemical Kinetics of Energy Sources: Heats of Combustion of Fuels; Differential Scanning Calorimetry; Ignition Point, Flash Point; Coal Carbonization and Gasification;
Chemical Energy Sources; Chemistry of Conventional and Non-Conventional Energy Materials: Petroleum Products, Petroleum Refinery; Biomass and Gober Gas; Hydrogen as a Fuel.

Chapter 3 Electrochemical Energy Systems: Battery & Supercapacitors: Primary and Secondary batteries, Solid state and molten solvent batteries, Lithium-ion batteries, Electrochemical Supercapacitors, fuel cells.

Chapter 4 Band gap engineering of materials for Solar Energy Harnessing: Concept of metal, semiconductor, insulator and their band structure. P-N junction and its behaviour in forward and reverse biasing, Metal semiconductor junctions, concept of band bending & band gap engineering.

Photovoltaic and Photogalvanic energy storage, Regenerative Photoelectrochemical Cells; Photocorrosion; Electrodes with chemically modified surfaces. Chemically Modified Electrodes for Water Cleavage; E-pH diagram of water, Organic photovoltaic cells.

Learning Resources:

Text Books:

1. Energy Systems Engineering – Evaluation and Implementation, Francis Vanek, Louis Albright, Largus Argenent, Mc Graw-Hill, 2012.
2. Energy Systems and Sustainability: Power for a Sustainable Future, Bob Everett, Godfrey Boyle, Stephen Peake and Janet Ramage, Oxford Uni Press, 2012.
3. Chemical and Electrochemical Energy Systems, R. Narayan and B. Viswanathan, Universities Press, 1998
4. Lithium Ion Batteries – Advances and Applications, Gianfranco Pistoria, Elsevier, 2014.

Reference Books:

1. Dynamic Modeling of Electrochemical Energy Systems, Lucia Gauchia and Javier Sanz; LAP Lambert Academic Publishing, 2010
2. Electrochemical Energy: Advanced Materials and Technologies (Electrochemical Energy Storage and Conversion, Pei Kang Shen Chao-Yang Wang, San Ping Jiang (Ed), CRC, 2016
3. Tomorrow's Energy: Hydrogen, Fuel Cells, and the Prospects for A Cleaner Planet, Peter Hoffmann, Byron Dorgan, MIT Press, 2012
4. Solar Energy Conversion, Yuri V Pleskov, Springer-Verlag, 1990
5. Solar Energy Conversion – Dynamics of Interfacidal Electron and Excitation Transfer, Piotrowiak, Laurie Peter, Heinz Frei and Tim Zhao, RSC, 2013

Course Code: CY 5262	SURFACE ANALYTICAL 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 basic principles and instrumentation of surface analytical techniques
CO2	Illustrate the methodology and applications of surface analytical techniques
CO3	Identify suitable analytical technique for studying surface characteristics of diverse materials
CO4	Analyze the data obtained from the analytical techniques to know the surface properties
CO5	Design appropriate instrumental techniques for analysis of samples

Course Articulation Matrix:

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

Syllabus:

Chapter-1 Surface structural analysis: Introduction to surface structural analysis and surface heterogeneity. Atomic force microscopy.

Chapter-2 Electron Spectroscopy for Chemical Analysis (ESCA) and Auger Electron Spectroscopy (AES): Principles, Instrumentation, Quantification methods and standards, Analytical Applications. Depth Profile Analysis.

Chapter-3 Secondary Ion Mass Spectrometry (SIMS): Principle, Instrumentation, Specific Applications.

Chapter-4 Surface-Enhanced Raman Spectroscopy (SERS): Principles, Electromagnetic theory of SERS, Sensitivity factor, Quantitative analysis, SERRS of Ag and Au metal colloids.

Chapter-5 Electron Energy Loss Spectroscopy (EELS) and Electron Microprobe Analysis (EMPA): Principle, Instrumentation, Specific Applications.

Chapter-6 Low Energy Ion Scattering Spectroscopy (LEISS): Principle, Instrumentation, Specific Applications.

Learning Resources:

Text Books:

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

3. An introduction to surface analysis by XPS and AES, John F Watts, John Wolstenholme, Wiley, 2019, 3rd edition.
4. Surface enhanced Raman spectroscopy: Analytical, Biophysical and Life Science Applications, Sebastian schlucker, Wolfgang Kiefer (Eds), Wiley VCH, 2011, 1st edition.

Reference Books:

1. Principles of Instrumental Analysis, Skoog, Holler, Crouch, Cengage Learning, 2017, 7th Edition.
2. Instrumental Methods of Analysis, Willard, Merritt, Dean, Settle, CBS / Wadsworth Publ. Co., 1988, 7th Edition.
3. Practical Surface Analysis by Auger and X-ray Photoelectron Spectroscopy, D. Briggs, M.P. Seah, John Wiley, 1990, 2nd edition.
4. Surface and thin film analysis, Gernot Friedbacher, Henning Bubert (Eds), Wiley-VCH, 2011, 2nd Edition.
5. Surface enhanced Raman scattering: Physics and applications, Katrin Kneipp, Martin Moskovits, Harald Kneipp (Eds), Springer, 2006, 2006th edition.

Course Code: CY 5263	ADVANCED ELECTROANALYTICAL METHODS	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 stationary and dynamic electroanalytical methods
CO2	Identify strengths of pulse methods for superior quantitative analysis
CO3	Analyze the results of micro- and rotating disc electrodes for interpreting mechanisms of electrochemical reactions
CO4	Evaluate the efficiency and capacity of electrochemical energy storage materials
CO5	Choose a combination of electroanalytical methods for comprehensive analysis of electrochemical materials and devices

Course Articulation Matrix:

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

Syllabus:

Chapter 1 Introduction, Steady state and potential step techniques: linear sweep voltammetry, Cyclic Voltammetry: principles and applications. Open circuit potential and Stern layer thickness.

Chapter 2: Differential pulse voltammetry, Square wave voltammetry, Stripping voltammetry: anodic stripping and cathodic stripping voltammetry, adsorptive stripping voltammetry, principles and applications. Hydrodynamic measurements, Rotating disk and ring disk electrodes, microelectrodes, and flow-cell analysis, Capillary systems and Lab-on-chip analysis.

Chapter 3: Chronomethods, principles, instrumentation and applications. Electrocatalysis of hydrogen and oxygen evolution reactions. Applications in Electrochemical Sensors and Advantages. Chronopotentiometric analysis, principle, methodology and instrumentation, Applications in the development of Capacitors and electrochemical supercapacitors, Cyclic charging discharging processes, C rate and electrochemical capacitance. Electrochemical supercapacitors: comparison with batteries for energy storage, density and charge-discharge behaviour, energy and power densities of storage devices, Pseudocapacitance, ruthenium and porous materials, applications.

Chapter 4: Electrochemical impedance spectroscopic measurements, principles and applications, Potentiodynamic polarization studies, Tafel methods. Electrochemical quartz crystal microbalance, principle, thin layer coatings, electropolymerization and electrodeposition of metals, adlayer formations, applications.

Chapter 5: Electrochemical scanning tunneling microscopy and Electrochemical atomic force microscopy, principles, instrumentation, Potential-UV-VIS measurements, Potential-

Infrared measurements, applications.

Learning Resources:

Text Books:

1. Electrochemical methods: Fundamentals and applications, Allen J Bard and Larry R Faulkner, John Wiley, 2nd Edn., 2010.
2. Electroanalytical methods: Guide to experiments and applications, Fritz Scholz, Springer, 2nd Edn., 2010.
3. Fundamentals of Electroanalytical Chemistry, P M S Monk, John Wiley, 2003.
4. Electrochemical supercapacitors - Scientific fundamentals and technological applications, B E Conway, Springer, 2014.

Reference Books:

1. Analytical Electrochemistry, Joseph Wang, John Wiley, 3rd Edn., 2006.
2. Electrochemistry of Functional Supramolecular Systems, Paola Ceroni, Alberto Credi and Margherita Venturi (Ed.), John Wiley, 2010.

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 Co-enzymes: Structure and biological function of co enzyme 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 – Repellants. 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. Text Book 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.