

NATIONAL INSTITUTE OF TECHNOLOGY DURGAPUR

DEPARTMENT OF CHEMISTRY



Revised Curriculum and Syllabi for the Degree of 2 Yr. M. Sc. in CHEMISTRY

(To be effective from the batches admitted in the Academic Session 2026-2027 Onwards)

Revision Approved in PGAC meeting on: _22.05.2026_____

Date: 16.07.2026

DEPARTMENT OF CHEMISTRY
NATIONAL INSTITUTE OF CHEMISTRY

Vision and Mission of the Department:

Vision

To be a globally recognized department in scientific and technical education through value-added teaching, research and innovation and producing quality human resources who can meet the challenges of the ever-changing, technology-based society.

Mission

Producing highly qualified, well- rounded, motivated and technologically sound students possessing fundamental understanding and knowledge in chemical science and technology, who will deliver service and leadership to the ever-changing chemical world and can fulfil the technological and socio- economic need of industry, government, and society.

Programme: 2 yrs. M. Sc. in Chemistry

Programme Educational Objectives (PEOs):

PEO1	Fundamental understanding in the subject of Chemistry and to emphasize on its interdisciplinary nature
PEO2	Development of fundamental knowledge coupled with experimentation, observation and analytical capability suitable for pursuing higher education and research in the frontiers of chemistry.
PEO3	Grooming students with scientific knowledge and technical knowhow of instrumentation for a successful and productive carrier in Chemistry related industry.
PEO4	Making students aware of our environment and how to protect it for sustainable development.
PEO5	Development of effective communication skills to convey chemical information to all stakeholders in the society and cultivating a sense of togetherness with the whole chemical community.

Programme Outcomes (POs):

PO1	Scientific knowledge: Understanding fundamental theory of the classical subjects in chemistry. It includes various domains in the field of physical, organic, inorganic, biological, environmental, analytical, computational chemistry and material science.
PO2	Understanding chemical methods: To learn modern analytical and spectroscopic tools and their applications to different disciplines of chemistry
PO3	Knowledge on emerging areas in Chemistry: To be acquainted with the latest frontiers in Chemistry and to be able to adapt with the ever-changing chemical world.
PO4	Problem analysis: Applying the fundamental knowledge to identify, formulate, and analyze a chemical problem.
PO5	Design/development of solutions: Providing an effective and environmentally sustainable solution

	to any chemical problem with the help of experimentation and computational modelling.
PO6	Technological knowhow: Understanding the underlying principle of modern scientific instruments and their operational procedure.
PO7	Computational advancement: To get acquainted with modern computational facility to understand and follow various types of chemical reactions and processes.
PO8	Thrive in higher education and research: With a vivid understanding of the present day research frontlines in the field of chemistry, students will be confident and well- motivated to pursue higher education and research as their next goal.
PO9	Carrier in chemical industry: With fundamental and applied knowledge in chemistry, building up a successful carrier in industry related to chemistry.
PO10	Understanding Chemistry of environment: To understand the chemistry responsible for environmental degradation and to formulate its remedy for sustainable development.
PO11	Collaborative mindset: Understanding the interdisciplinary nature of chemistry, students to get trained and motivated towards collaborative teamwork.
PO12	Lifelong learning and ethical application of chemical understanding for inclusive socio-economic development.

Mapping of Departmental mission statements to PEOs:

	PEO1	PEO2	PEO3	PEO4	PEO5
Producing highly qualified, well-rounded, motivated and technologically sound students	3	3	3		3
Imparting fundamental understanding and knowledge in chemical science and technology	3	3	3	3	
Students to deliver service and leadership to the ever changing chemical world	3	3	3	3	3
Students to fulfil the technological and socio-economic need of industry, government and society		3	3	3	3

Mapping of POs to PEOs:

	PEO1	PEO2	PEO3	PEO4	PEO5
PO1	3	3	3	3	-
PO2	3	3	3	3	-
PO3	3	3	3	-	-
PO4	-	-	3	3	-
PO5	-	3	3	3	3
PO6	3	3	3	-	-
PO7	3	3	3	-	-
PO8	3	3	-	2	-
PO9	-	-	3	-	-
PO10	-	-	-	3	2
PO11	3	-	-	-	3
PO12	3	3	2	-	3

Correlation levels 1, 2 or 3 as defined below:

1: Slight (Low)

2: Moderate (Medium)

3: Substantial (High)

Curriculum for 2 yrs. M.Sc. in Chemistry:

Semester – I							
Sl. No.	Code	Subject	L	T	S	C	H
1	CY1101	Quantum chemistry	3	1	0	4	4
2	CY1102	Inorganic reaction mechanisms and magnetochemistry	3	1	0	4	4
3	CY1103	Concept of organic synthesis and asymmetric synthesis	3	1	0	4	4
4	CY1104	Group theory and electronic spectroscopy of transition metal complexes	3	0	0	3	3
5	CY1105	Advanced materials and molecular modelling	3	0	0	3	3
6	CY1151	Spectrophotocatalysis	0	0	3	2	3
7	CY1152	Inorganic quantitative estimation	0	0	3	2	3
8	CY1153	Identification of organic compounds from binary mixture	0	0	4	2	4
		TOTAL	15	3	10	24	28
Semester – II							
Sl. No.	Code	Subject	L	T	S	C	H
1	CY2101	Chemical, statistical thermodynamics and electrochemistry	3	1	0	4	4
2	CY2102	Organometallic compounds and bioinorganic chemistry	3	1	0	4	4
3	CY2103	Pericyclic reactions and organic photochemistry	3	1	0	4	4
4	CY2104	Spectroscopy: Theory and applications	3	1	0	4	4
5	CY2105	Structure and function of biomolecules	3	0	0	3	3
5	CY2151	Advanced practical on physical chemistry	0	0	4	2	4
6	CY2152	Synthesis and characterization of inorganic complexes	0	0	3	2	3
7	CY2153	Chromatographic separation of organic compounds	0	0	3	2	3
		TOTAL	15	4	10	25	29
Semester – III							
Students may choose all four (04) DEPTH elective courses from a particular basket or three (03) from one basket and one (01) from other two baskets							
Sl. No.	Code	Subject	L	T	S	C	H

Physical Chemistry basket							
1	CY9111	Advanced quantum and computational chemistry	3	0	0	3	3
2	CY9112	Basics of non-linear dynamics	3	0	0	3	3
3	CY9113	Advanced spectroscopic techniques and applications of group theory	3	0	0	3	3
4	CY9114	Surface science, electrode kinetics and corrosion science	3	0	0	3	3
OR							
Inorganic Chemistry basket							
1	CY9121	Advanced green chemistry and environmental chemistry	3	0	0	3	3
2	CY9122	Synthetic methodology for metal complexes and supramolecular chemistry	3	0	0	3	3
3	CY9123	Small molecule activation, nuclear chemistry and related spectroscopy	3	0	0	3	3
4	CY9124	Application of group theory and inorganic electrochemistry	3	0	0	3	3
OR							
Organic Chemistry basket							
1	CY9131	Advanced organic synthesis	3	0	0	3	3
2	CY9132	Drug design and biophysical chemistry	3	0	0	3	3
3	CY9133	Bioorganic chemistry and natural products	3	0	0	3	3
4	CY9134	Advanced stereochemistry and structure-reactivity correlation	3	0	0	3	3
5	CY3151	Project-I	0	0	12	6	12
6	CY3152	Non-project seminar/Evaluation of summer internship or training	0	0	0	1	0
TOTAL			12	0	12	19	24
Semester – IV							
Sl. No.	Code	Subject	L	T	S	C	H
1	CY4151	Project – II	0	0	24	12	24
2	CY4152	Project Seminar & Viva voce	0	0	0	2	0
TOTAL			0	0	24	14	24

Credit unit of the programme:

Semester	I	II	III	IV	TOTAL
Credit Unit	24	25	19	14	82

Curricular component:

Category	Credit	Percentage weightage
Core courses	37	45%
Elective courses	12	15%
Laboratory	12	15%
Project work	18	22%
Seminar & viva	3	4%
TOTAL	82	

FIRST SEMESTER

Course Code	Title of the course	Program Core / Electives (PCR) (PEL)	Total Number of contact hours				Credit
			Lecture (L)	Tutorial (T)	Practical (P)	Total Hours	
CY1101	Quantum chemistry	PCR	3	1	0	4	4
Pre-requisites		Course Assessment methods [Continuous assessment (CA), mid-term (MT) and end term (ET)]					
NIL		CA+MT+ET					
Course Outcomes	CO1: To understand the difference between macroscopic (classical) and microscopic (quantum) world, quantization of energy, wave particle duality. CO2: To apply Schrödinger wave equation for one electron system (Hydrogen atom) in spherical polar coordinates. CO3: To analyze the vibrational, rotational spectra of diatomic molecules form quantization of energy concept. CO4: To understand the mathematical background of the concept of electron spin, angular momentum, uncertainty principle, Pauli’s exclusion principle CO5: To apply mathematical concepts (vectors, matrix, differential equations, polynomials etc.) to problems of quantum mechanics						
Topics Covered	Introduction to Quantum Mechanics: The dawn of quantum theory, black body radiation, photoelectric effects, Atomic spectra, vibrations in atomic crystals, wave particle duality, Heisenberg uncertainty principle, Time-independent Schrödinger equation (4 L) Postulates of Quantum Mechanics: Fundamental operations of quantum mechanics, eigenvalue problems, wavefunctions and probabilistic representation, operators, average values, commutation relations, time-dependent Schrodinger equation (4 L) Simple applications (exactly solvable problems): Particle in a 1D & 3D box, particle in a box of finite depth, Tunnelling effect. (3 L) The Harmonic Oscillator: Energy levels, Infrared spectra of diatomic molecules, wavefunctions (2 L) Particle on a sphere (rigid rotator): Rigid rotator model of a diatomic molecule, Energy levels, rotation-vibration spectra, spherical harmonics (3 L)						

	The Hydrogen Atom: The Schrodinger equation for a hydrogen atom, energy levels, H atomic spectra, radial wave equations, atomic orbitals, Magnetic effect on electron movement (4 L) Generalized Uncertainty Principle, Angular Momentum: Angular momentum and its measurements (2 L) Electronic wavefunction with spin-Pauli's exclusion Principle Electron spin, spin-orbit interaction, Atomic Term Symbols, The Schrodinger equation for a Helium atom (3 L) Approximation methods: Basic principles of variation and perturbation methods. (2 L) Mathematical Concepts: Representation of complex number, Euler's formula, series and limits, average values etc. (2 L) Linear algebra in quantum mechanics and symmetry operation: Vector space, Determinants, Matrix and liner transformations, orthogonal transformation, symmetry operations, matrix eigenvalue problem etc. (2 L) Partial differential equation: General solution, separation of variable, particle in a rectangular box, in a circle box, hydrogen atom, vibrating string, normal modes of vibration. (2 L) Polynomials in quantum chemistry: The Legendre equation, Legendre polynomials, associated Legendre polynomial, orthogonality and normalization, Hermite equation, Hermite Polynomials. Laguerre equation, associated Laguerre functions, spherical harmonics. (3 L) Function in three dimensions: Spherical polar coordinates, atomic orbitals, volume integrals, density functions, etc. (2 L)
Textbooks and/or reference materials	1. Quantum Chemistry by Levine 2. Physical Chemistry: A Molecular approach by Donald A. McQuarrie 3. Introductory quantum chemistry by A. K. Chandra 4. Molecular Quantum Mechanics By Atkins and Friedman, Oxford 5. The Chemistry Maths Books, Erich Steiner, Oxford 6. Mathematics for chemistry, Doggett and Suicliff, Logman. 7. Mathematical for Physical chemistry: F. Daniels, Mc. Graw Hill.

Mapping of COs (Course outcomes) and POs (Programme Outcomes)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
CO1	3	2	3	2	2	2	3	3	2	2	1	1
CO2	3	2	3	2	2	2	3	3	2	2	1	1
CO3	3	2	3	2	2	2	3	3	2	2	1	1
CO4	3	3	3	2	2	3	3	3	2	3	1	1
CO5	3	3	3	2	2	3	3	3	2	3	1	1

Course Code	Title of the course	Program Core (PCR) / Electives (PEL)	Total Number of contact hours				Credit
			Lecture (L)	Tutorial (T)	Practical (P)	Total Hours	
CY1102	Inorganic reaction mechanisms and magnetochemistry	PCR	3	1	0	4	4
Pre-requisites		Course Assessment methods [Continuous assessment (CA), mid-term (MT) and end term (ET)]					
NIL		CA+MT+ET					
Course Outcomes	CO1: Basic concept of inorganic reaction mechanism associated with octahedral and square planar complexes. CO2: Types of electron transfer reactions of the complexes including the detail mechanism CO3: Solving the problems related to Marcus theory. CO4: Types of magnetic substances and their magnetic properties. CO5: Quantum numbers and origin of magnetic moments; microstates and derivation of Russel-Saunders Terms for various electronic configuration, Lande Interval Rule, Hole formalism and equivalency. CO6: Determination methods of magnetic susceptibility of various metal complexes, multiplet widths and derivation of various equations to determine magnetic moments, orbital magnetic moment quenching, concept of high-, low-, intermediate- and admixed-spin state and their interactions.						
Topics Covered	(i) Stoichiometric mechanism, second order limiting rate constant, base hydrolysis, Effects of non-leaving ligands, proton exchange, activation parameters. (5 L) (ii) Stereochemistry of octahedral substitution reactions, racemization reaction (Bailar twist and Ray –Dutt twist). (4 L) (iii) Square planar complexes: Ligands substitution reactions, General features, significance of rate law, effect of entering and leaving ligands, The trans effect, theories of trans effect, grounds state effects, transition effect, steric effects of non-leaving ligands, catalysis of substitution by redox process. (4 L) (iv) Electron transfer reaction: Types of electron transfer reaction, outer sphere electron transfer process: electron transfer and reorganization and chemical activation, potential energy diagram, Marcus theory for outer sphere cross reaction. (5 L) (v) Inner sphere electron transfer process: steps, rate law, types of inner sphere electron transfer process, bridging ligand, remote attack, the chemical mechanism. (4 L) (vi) Definition of magnetic properties, types of magnetic bodies, sources of paramagnetism: orbital and spin effects, Diamagnetism and Pascal’s constant, diamagnetic correction of ligands and metal complexes. (3 L) (vii) Quantum numbers and vectors, Mutual inclination of electron orbits and resultant vectors, Russel-Saunders coupling and j-j coupling, Ground State Term Symbol and Hund’s rules. (2 L) (viii) Microstates and derivation of Russel-Saunders Terms for p², d² and pd configuration, Spin-orbit interaction. (2 L) Lande Interval Rule, Hole formalism and equivalency, Hund’s third rule and energies of J levels, Russel-Saunders coupling of d2 system and j-j coupling. (3 L) (ix) Thermal energy and magnetic property, Magnetic moments for different multiplet						

	widths i.e for multiplet width large compared to Δ_o, small compared to Δ_o and comparable to Δ_o. (3 L) (x) Magnetic properties of Lanthanides, first transition series metal ions and actinides. (2 L) (xi) Determination of magnetic susceptibility: Gouy's method, Faraday's method, NMR method and their advantage and disadvantages, magnetic anisotropy. (3 L) (xii) Magnetic properties of complexes with different geometries based on crystal field model, spin-state equilibrium in octahedral stereochemistry, magnetic properties of high-spin, low-spin, intermediate-spin and admixed-spin state concept. (2 L) (xiii) Quenching of Orbital magnetic moment by crystal field, loss of orbital degeneracy and quenching of orbital magnetic moment, valence bond and crystal field interpretation of magnetic moment, shortcomings of crystal field theory. (2 L)
Textbooks and/or reference materials	1. Inorganic chemistry, Shriver & Atkins, Oxford. 2. Concept and models of inorganic Chemistry, Douglas, McDaniel, Alexander, Wiley. 3. Inorganic Chemistry, Huheey, Keiter, Keiter, Medhi, Pearson education 4. Concise Inorganic chemistry, Lee, Wiley india Pvt. Ltd. 5. Elements of magnetochemistry by Dutta & Shyamal 6. Mechanisms of Inorganic Reactions by Fred Basolo and Ralph Pearson

Mapping of COs (Course outcomes) and POs (Programme Outcomes)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
CO1	3	2	3	3			1	3	3			
CO2	3		3	3				3	1	1	1	1
CO3	3	1	3	3				3			1	1
CO4	3	2	3	2	2	1	3	3	3	3	1	1
CO5	3	2	3	3	2	1	3	3	3	3	1	1
CO6	3	2	3	3	2	3	3	3	3	3	1	1

Course Code	Title of the course	Program Core / Electives (PEL)	Total Number of contact hours				Credit
			Lecture (L)	Tutorial (T)	Practical (P)	Total Hours	
CY1103	Concept of organic synthesis and asymmetric synthesis	PCR	3	1	0	4	4
Pre-requisites		Course Assessment methods [Continuous assessment (CA), mid-term (MT) and end term (ET)]					
NIL		CA+MT+ET					
Course Outcomes	CO1: Understanding the various tactics, strategies and control over chemoselectivity, regioselectivity, stereoselectivity while carrying out organic syntheses. CO2: Foundation in the role of enolates, enol equivalents, organometallic reagents, vinyl anion equivalents, allyl cation equivalents, Palladium catalysed coupling reactions,						

	carbocations, carbenes and radicals in making C-C single bonds. CO3: Understanding the concept of retro synthesis, synthones and synthetic equivalents, functional group interconversions and order of events in organic synthesis. CO4: Concept of classic examples of total synthesis of some natural products. CO5: Concept of various aspects of methodologies used for making chiral organic molecules. This includes asymmetric induction via substrate, reagents and catalysis.
Topics Covered	Planning Organic Syntheses: 1. Tactics, Strategy and Control; Selectivity: chemoselectivity, regioselectivity, stereoselectivity. (2 L) 2. Making Carbon-carbon single and double bonds: Enolates, homoenolates, extended enolates, nitrogen analogues of enols and enolates, acyl anion equivalents, allyl anions, specific enol equivalents, Michael reaction, σ-complexes of metals, organometallic reagents, aldol addition and condensation reactions, Mukaiyama aldol condensation, control of facial reactivity, Claisen and Dieckmann condensation, conjugate addition, ortho-strategy for aromatic compounds, Palladium catalysed coupling reactions. Olefination reactions– Wittig and related reactions, Julia olefination. Sulfonylation and selenenylation, hydroalumination, carboalumination, ROMP and RCMP. (8 L) 3. Functional group interconversion and Retro-synthetic analysis: Synthones and synthetic equivalents, functional group interconversions and order of events in organic synthesis. One group-C-X and two groups C-X disconnections, chemoselectivity, reversal of polarity, cyclisation reactions, amine synthesis. One group C–C and two group C–C disconnections (typical examples), use of acetylenes and aliphatic nitro compounds in organic synthesis. Diels-Alder reactions, 1,3- and 1,5-Difunctionalised compounds, α,β-unsaturated carbonyl compounds, control in carbonyl condensation, Michael addition and Robinson annulation. Ring synthesis: saturated heterocycles synthesis of 3-, 4-, 5-, and 6-membered rings, aromatic heterocycles in organic synthesis. (8 L) 4. Classic total synthesis of some natural products: Strategies and synthesis of some classic examples of total synthesis; L-hexoses, Prostaglandins, Longifolene, penicillin, Periplanone etc. (10 L) 5. Asymmetric synthesis: Control of stereochemistry, chiral pool, asymmetric induction via reagents and catalysts, kinetic resolution, Synthesis of enantiometrically pure compounds. (8 L)
Textbooks and/or reference materials	1. Organic Chemistry : J. Clayden, N. Greeves, S. Warren & P. Wothers, 2. Organic synthesis strategy and control : P. Wyatt & S. Warren 3. Advanced Organic Chemistry : F.A. Carey & R.J. Sundberg 4. Principles of Organic Synthesis : R.O.C. Norman & J.M. Coxon. 5. Organic synthesis : Michael B Smith, 6. Classics in Total Synthesis: Targets, strategies and Methods : K.C. Nicolaou & E.J. Sorensen 7. Modern Methods in Organic Synthesis : W. Carruthers, 8. Protective Groups in Organic Synthesis : T.W. Green & P.G.M. Wuts

Mapping of COs (Course outcomes) and POs (Programme Outcomes)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
CO1	3	3	3	3	2	2	2	3	3	2	3	3
CO2	3	3	3	3	3	2	2	3	3	2	3	3
CO3	3	3	3	3	3	2	3	3	3	3	3	3
CO4	3	3	3	3	3	2	3	3	3	3	3	3
CO5	3	3	3	3	3	2	3	3	3	3	3	3

Course Code	Title of the course	Program Core (PCR)/ Electives (PEL)	Total Number of contact hours				Credit
			Lecture (L)	Tutorial (T)	Practical (P)	Total Hours	
CY1104	Group theory and electronic spectroscopy of transition metal complexes	PCR	3	0	0	3	3
Pre-requisites		Course Assessment methods [Continuous assessment (CA), mid-term (MT) and end term (ET)]					
NIL		CA+MT+ET					
Course Outcomes	CO1: Develop the fundamental concept of symmetry and symmetry operations. CO2: Develop the concept of Group theory and how molecular properties dependent on symmetry. CO3: Learn to construct and know the importance of Character table. CO4: Learn to develop Reducible and Irreducible representation and their importance. CO5: Basic techniques to explain the electronic spectra of transition metal complex using molecular symmetry CO6: Distinction of spectra of d-block and f-block transition metal complexes.						
Topics Covered	Fundamental concept of symmetry and probable application in chemistry						(2 L)
	Different symmetry operations with examples						(3 L)
	Properties of symmetry operations and concept and characteristics of Classes						(4 L)
	Concept of Group and their properties with examples						(2 L)
	Systematic determination of Group for a molecule						(3 L)
	Reducible and Irreducible representation and character table						(4 L)
	Introduction of Electronic spectroscopy of coordination compounds:						(2 L)
	Microstates and free-ion terms for electron configurations						(2 L)
	Selection rule for electronic transition						(2 L)
	Correlation diagrams: Orgel and Tanabe-Sugano diagrams						(3 L)
	Jahn-Teller Distortions and Spectra:						(2 L)
	Symmetry labels for configurations, Charge transfer spectra.						(2 L)

	Electronic spectra of lanthanide and actinide complexes (3 L)
Textbooks and/or reference materials	1. Group theory and chemistry by Bishop 2. Chemical application of group theory by F A Cotton 3. Fundamentals of Symmetry and Group Theory with Applications in Chemistry by S S Panja, PHI 4. Molecular theory and group theory by R. L. Carter 5. Inorganic Chemistry, Huheey, Keiter, Medhi, Pearson education 6. Inorganic chemistry, Shriver & Atkins, Oxford 7. Concept and models of inorganic Chemistry, Douglas, McDaniel, Alexander, Wiley

Mapping of COs (Course outcomes) and POs (Programme Outcomes)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
CO1	3	2	2	3	2	1	3	3	1	2	2	2
CO2	3	2	2	3	2	1	3	3	1	2	2	2
CO3	3	2	2	3	2	1	3	3	1	2	2	2
CO4	3	3	2	3	2	1	3	3	1	3	2	2
CO5	3	2	2	3	2	1	3	3	1		2	2

Course Code	Title of the course	Program Core (PCR)/ Electives (PEL)	Total Number of contact hours				Credit
			Lecture (L)	Tutorial (T)	Practical (P)	Total Hours	
CY1105	Advanced materials and molecular modelling	PCR	3	0	0	3	3
Pre-requisites		Course Assessment methods [Continuous assessment (CA), mid-term (MT) and end term (ET)]					
NIL		CA+MT+ET					
Course Outcomes	CO1: Understanding synthetic methods and characterization techniques of different materials. CO2: Understanding Electrical, Ionic, Magnetic, Optical, Catalytic Properties of different materials CO3: Knowledge on the applications of different materials. CO4: Learning computer programs to solve chemical problems. CO5: Introduction to computational chemistry and modelling software packages for cage, clusters and macromolecules.						

Topics Covered	Advanced materials: Amorphous and crystalline materials. (2 L) Symmetry and structure: point groups and space groups, crystal lattices, unit cell. (3 L) Synthesis of materials: high temperature ceramic techniques, solution combustion technique, sol-gel, inorganic metathesis route, hydrothermal techniques, pyrolysis, air sensitive synthesis, bulk materials and nano-materials, porous materials. (2 L) Characterization, properties and Applications: Powder and single crystals X-ray diffraction, visualization and drawing of crystal structure. photoelectron spectroscopy (XPS). X-ray and XPS data analysis. (5 L) Electron microscopy, thermal analysis. (2 L) Defects and non-stoichiometry (2 L) Metal and alloys, Semiconductor, Polymer, metal oxides, Nano-materials, Composites, Porous materials (MOFs, COFs, cages and clusters), Catalytic Properties and Applications. (4 L) ----- Introduction to Fortran/Python language: data types, integer, complex, character, logical constants and variables. Arithmetic statements, expressions, library functions, relational operators. (2 L) Programming exercises to chemical problems (3 L) Application of Density Functional Theory using Materials studio/VASP (or similar) software in chemistry. (4 L) Basic concept on molecular modelling software: application in cage and cluster, macromolecules. (4 L)
Textbooks and/or reference materials	1. A.R. West, Solid State Chemistry and its applications. 2. L.E. Smart and Moore, Solid State Chemistry An Introduction. 3. C.N.R. Rao and J. Gopalakrishnan, New directions in solid state chemistry 4. G.H. Stout and L.H. Jensen, X-ray structure determination: A practical guide 5. Chapman, Fortran 95/2003 for Scientists and Engineers, McGraw-Hill International Edition, New York (2006). 6. W. H. Press, S. A. Teukolsky, W. H. Vetterling, B. P. Flannery, Fortran Numerical Recipes (Fortran 90), Cambridge University Press (1996) 7. User Reference Manual for Gaussian 09 software and Materials Studio 2020 software

Mapping of COs (Course outcomes) and POs (Programme Outcomes)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
CO1	3	3	3	2	2	3	3	3	2	1	2	3
CO2	3	3	3	2	2	3	3	3	2	1	2	3
CO3	3	3	3	2	3	3	3	3	2	1	2	2
CO4	3	3	3	2	3	3	3	3	2	1	2	2
CO5	3	3	3	2	3	3	3	3	2	1	2	2

Course Code	Title of the course	Program Core (PCR)/ Electives (PEL)	Total Number of contact hours				Credit
			Lecture (L)	Tutorial (T)	Practical (P)	Total Hours	
CY1151	Spectrophotocchemical analysis	PCR (Practical)	0	0	3	3	2
Pre-requisites		Course Assessment methods: [Continuous evaluation (CE) and end assessment (EA)]					
NIL		CE+EA					
Course Outcomes	CO1: Basic concepts of spectrophotometric estimation. CO2: Learning about handling of spectrophotometer and fluorescence spectrometer and their basic theory. CO3: To develop laboratory skills and the ability to work independently as well as in a group. CO4: Knowing presentation, analysis and interpretation of data, source of error and error analysis. CO5: To understand the interconnection between experimental foundation and underlying theoretical principles. CO6: To develop the ability of scientific communications through oral quizzes, written reports and presentations.						
Topics Covered	1. Determination of stoichiometry of Ferric salicylic acid complex by Job’s method 2. Determination of indicator constant of methyl orange 3. Determination of concentration of Cu ²⁺ and Fe ³⁺ photometrically by titrating with EDTA 4. Determination of arsenic(III) and antimony(IV) simultaneously in a mixture spectrophotometrically. 5. Determination of molar extinction coefficient 6. Determination of fluorescence quantum yield. 7. Fluorescence quenching experiment. 8. Ag nanoparticle synthesis and spectroscopy Some additional experiments as decided by the Instructor.						
Textbooks and/or reference materials	1. Instruction manual provided by the Instructor 2. Experiments in Physical Chemistry by Carl Garland, Joseph Nibler, David Shoemaker 3. Practicals in Physical Chemistry by P S Sandhu 4. Practical Physical Chemistry by Viswanathan and Raghavan						

Mapping of COs (Course outcomes) and POs (Programme Outcomes)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
CO1	3	3	2									
CO2	3	3		2	2	3		2	2		1	
CO3						2		2	2		3	3
CO4	3	3		3	3		1	3				
CO5								3	3			
CO6								3	3		2	2

Course Code	Title of the course	Program Core (PCR)/ Electives (PEL)	Total Number of contact hours				Credit
			Lecture (L)	Tutorial (T)	Practical (P)	Total Hours	
CY1152	Inorganic quantitative estimation	PCR (Practical)	0	0	3	3	2
Pre-requisites		Course Assessment methods: [Continuous evaluation (CE) and end assessment (EA)]					
NIL		CE+EA					
Course Outcomes	CO1: Basic concepts of spectrophotometric estimation. CO2: Understand to evaluate the estimation of ion mixture. CO3: Learning about handling of spectrophotometer. CO4: Understand the fundamental, scientific basis, preparation of sample, sampling method and analytical methods for water and waste water samples. CO5: Students will also accumulate idea about the permissible limit, present concentration etc. of different environmental impurities.						
Topics Covered	Estimation of $\text{MnO}_4^- - \text{Cr}_2\text{O}_7^{2-}$ in a mixture Estimation of $\text{Cu}^{2+} - \text{Zn}^{2+}$ in a mixture Estimation of $\text{NO}_3^- - \text{PO}_4^{3-}$ in a mixture Estimation of $\text{Ti}^{+4} - \text{V}^{+5}$ in a mixture Estimation of dissolved oxygen and oxygen demands (BOD and COD) of Environmental Samples. Chemical Characterization of soil. Some more experiments from the followings as decided by the Instructor. (i) Determination of Ni in steel (Gravimetrically). (ii) Analysis of Brass and Aluminum in Bronze, (iii) Spectroscopic determination of Iron in Bauxite						
Textbooks and/or reference materials	1. An Advanced Course in Practical Chemistry by Nad, Ghosal and Mohapatra, New Central Book agency. 2. A Manual of Practical Chemistry for Degree Classes (Vol I & II) by R. C. Bhattacharya, 3. College Practical chemistry by Ahluwalia, Dingra and Gulati. 4. Vogels textbook of quantitative chemical analysis By J Mendham, R. C. Denney, M. Thomas and D. J. Barnes, Pearson India. 5. APHA, A, WEF, (1998). Standard Methods for the Examination of Water and Wastewater. American Public Health Association, American Water Works Association, Water Pollution Control Federation, Washington DC.						

Mapping of COs (Course outcomes) and POs (Programme Outcomes)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
CO1	3	3	2	3	3	3		3	2	1	1	
CO2	3	2	1	2	1	2	1	3	2	2	1	1
CO3	3	2	3	2		3	3	3	2	2	1	
CO4	3	3	3	3	3	2	1	3	3	3	2	3
CO5	3	2	3	2	3	2	1	3	3	3	3	3

Course Code	Title of the course	Program Core / Electives (PCR) (PEL)	Total Number of contact hours				Credit
			Lecture (L)	Tutorial (T)	Practical (P)	Total Hours	
CY1153	Identification of organic compounds from binary mixture	PCR (Practical)	0	0	3	3	2
Pre-requisites		Course Assessment methods: [Continuous evaluation (CE) and end assessment (EA)]					
NIL		CE+EA					
Course Outcomes	CO1: Scientific knowledge on principle of separation techniques to reach a targeted pure separate component from a binary mixture, CO2: Become skilled to optimise the uses of solvent obeying the principle of green chemistry. CO3: Separation and purification techniques, like phase transfer, crystallization, GC-Mass and other spectroscopic method will be adopted CO4: Understand the basic concept behind separation process for most common different methodology and their principles like; distillation, sublimation, crystallization and solvent extraction will be adopted. CO5: To reach a maximum yield with minimum uses of solvent, reagents and energy like; heat and electricity (Green chemistry).						
Topics Covered	Separation and identification of individual components, preparation of derivatives of each component, their purification and characterization. 1. Aniline and benzil (Liquid and solid) 2. Ethyl acetoacetate and Benzoic acid (Liquid and solid) 3. Benzil and Benzoic acid (solid and solid) 4. <i>p</i> -chlorobenzoic acid and aniline (solid-liquid) 5. Cyclohexanone/cyclohexanol and <i>N,N</i> dimethyl aniline (liquid and liquid)						
Textbooks and/or reference materials	1. Vogel's Textbook of practical organic chemistry, 5th Edition 2. Advanced practical chemistry, 3rd ed.: Subas C. Das 3. An Advanced Course in Practical Chemistry, New Central Book Agency; 3rd ed.: Nad, Mahapatra and Ghoshal						

Mapping of COs (Course outcomes) and POs (Programme Outcomes)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
CO1	3	2	3	2	2	2	1	3	2	2	1	2
CO2	3	3	2	2	2	2	2	3	2		2	2
CO3	3	2	3	2	2	2	2	2	2		1	2
CO4	3	2	3	2	2	3	1	3	2	3	1	2
CO5	3	3	2	2	2	3	2	3	2		1	2

SECOND SEMESTER

Course Code	Title of the course	Program Core (PCR) / Electives (PEL)	Total Number of contact hours				Credit
			Lecture (L)	Tutorial (T)	Practical (P)	Total Hours	
CY2101	Chemical, statistical thermodynamics and electrochemistry	PCR	3	1	0	4	4
Pre-requisites		Course Assessment methods [Continuous assessment (CA), mid-term (MT) and end term (ET)]					
NIL		CA+MT+ET					
Course Outcomes	CO1: understand the thermodynamics of ideal, non-ideal and multicomponent systems. CO2: understand the concept of entropy of a system at absolute zero and its implication. CO3: account for physical interpretation of partition functions and able to analyse thermodynamic properties of model systems with using Boltzmann, Fermi-Dirac and Bose-Einstein statistics. CO4: understand the ionic properties in solution, like diffusion, migration, conduction and their interrelation. CO5: apply these knowledge to understand principle behind separation of macromolecules, like sedimentation/ultracentrifugation. CO6: account for fundamental ideas of Debye-Huckel theory and its application.						
Topics Covered	Chemical Thermodynamics: Third law of classical thermodynamics and their applications. (2 L) Thermodynamics of ideal and non ideal binary solutions: free energy and entropy of mixing, partial molar quantities and their determination, fugacity and its determination. (4 L) Gibbs-Duhem equation, Duhem- Margules equation, equilibrium constant, temperature dependent equilibrium constant. (3 L) Thermodynamic excess functions. Experimental determination of activity coefficient of electrolytes and non electrolytes. (3 L) Statistical Thermodynamics: Introduction to statistical thermodynamics, probability, ensembles and distribution laws. Partition function. (2 L) Comparison among Maxwell-Boltzmann, Fermi-Dirac and Bose-Einstein Statistics. (2 L) Statistical mechanics on the thermodynamics of mono, diatomic and polyatomic ideal gas-						

	contribution of rotation, vibration and translation to partition function. Concept of residual entropy. (4 L) Electronic contribution to the specific heat of diatomic gases. (1 L) Solids-Vibrational contribution to the specific heat of solids. (1 L) Statistical treatment of Black-body radiation. (1 L) Maxwell-Boltzmann probability distribution of molecular velocities and speeds. (1 L) Dynamics of chemical reaction in solution-transition state theory using partition functions. (1 L) Electrochemistry: Some preliminary concept of electrostatics. (3 L) Ion-solvent interaction: Born equation, Electrostriction and partial molar volume. Solvation number of electrolytes. Dielectric constant of solution. Effect of nonelectrolyte on ion-solvent interaction. Ion-dipole interaction. (4 L) Ion-ion interaction: Debye-Huckel-Onsagar theory of inter-ionic interaction, thickness of ionic atmosphere. Debye-Huckel limiting law. (4 L) Ion transport in solution: Fick's first and second law of diffusion, Molecular interpretation of diffusion, Migration of ion under electric field, Effect of viscosity and diffusion on ionic migration. Relaxation of ionic atmosphere, Effect of high electric field and high frequency of ionic conduction. (4 L) Rate process approach towards ionic migration: Nernst-Planck Flux equation and its application. (2 L) Dielectric relaxation in liquid water. (1 L)
Textbooks and/or reference materials	1. Modern electrochemistry: Ionics (Part 1); and Electrodeics (Part 2) by Bockris and Reddy 2. An introduction to statistical thermodynamics by T. L. Hill 3. Physical Chemistry: Statistical Mechanics by H. Metiu (Taylor and Francis) 4. Physical Chemistry: Thermodynamics by H. Metiu (Taylor and Francis) 5. Chemical Thermodynamics: Principles and Applications; and Advanced Applications by Ott and Goates

Mapping of COs (Course outcomes) and POs (Programme Outcomes)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
CO1	3			2		2	3	3	2	2	1	1
CO2	3			2		2	3	3	2	2	1	1
CO3	3		2	2		2	3	3	2	2	1	1
CO4	3	3	3	2	2	3	3	3	2	3	1	1
CO5	3	3	3	2	3	3	3	3	2	3	1	1
CO6	3			3	1							

Course Code	Title of the course	Program Core (PCR) / Electives (PEL)	Total Number of contact hours				Credit
			Lecture (L)	Tutorial (T)	Practical (P)	Total Hours	
CY2102	Organometallic compounds and bioinorganic chemistry	PCR	3	1	0	4	4
Pre-requisites		Course Assessment methods [Continuous assessment (CA), mid-term (MT) and end term (ET)]					
NIL		CA+MT+ET					
Course Outcomes	CO1: knowledge of s, p and d block organometallics in respect of synthesis, structure and bonding in different ligand environment. CO2: knowledge of different types of reactions of organometallics compounds and their role in different catalytic cycles related to industrial processes. CO3: understanding the role of trace elements in health and environment, chemistry of metal cytotoxicity and its remedy. CO4: knowledge the structure and function of metalloenzymes and metalloproteins with special emphasis of iron storage, oxygen transport and photosynthesis. CO5: application of modern spectroscopic tools to elucidate the active sites of metalloenzymes and metalloproteins.						
Topics Covered	Gr. I and Gr. II organometallics: Synthesis, properties and application. (2 L) d-metal organometallics: History, stable electronic configuration, 18 and 16 electronic system, electron count and oxidation state, Nomenclature, π - acid ligands and low oxidation states (3 L) Metal carbonyl: Binary carbonyl: synthesis, bonding, spectroscopic characterization of carbonyl compounds, (4 L) Substituted carbonyl: phosphine, isocyanide, nitrosyl, dinitrogen, carbenes, hydrides, and dihydrogen, η^1 alkyl, alkenyl, alkynyl, aryl, η^2 alkene, alkyne, nonconjugated diene, butadiene, cyclobutadiene, cyclotetracene, allyl ligand, cyclopentadiene, and cycloheptatriene, Metallocenes: synthesis, reactivity and bonding of ferrocene etc. (6 L) Reactions: ligand substitution oxidative addition and reductive elimination, σ -bond metathesis, 1,1 migratory insertion, 1,2 insertion, β -hydride elimination, Homogeneous catalysis: hydrogenation catalyst, hydro formylation, Wacker oxidation of alkenes, asymmetric oxidation, metathesis (5 L) Bio-inorganic: Occurrence and availability of inorganic elements in organisms; essential, beneficial and trace elements, Synergistic and antagonistic relationship of metal ions, Element deficiency and toxicity, Metal poisoning detoxification. (1 L) Biological ligands for metal ions: Nucleobases, nucleotides and nucleic acids (DNA, RNA) as ligands, tetrapyrrole ligands and other macrocycles (chlorin, corrin). (1 L) Concept of protein structures: primary, secondary, tertiary and quaternary; Coordination of proteins and comments on enzymatic catalysis. (1 L) Cobalamins including vitamin and Coenzyme B12: History and structural characterisation; Reactions of the alkylcobalamins (a) One-electron reduction and oxidation, (b) Co-C bond cleavage, (c) Mutase activity of Coenzyme B12 and (d) alkylation reactions of Methylcobalamins; Model systems and the role of the Apoenzyme. (3 L)						

	Metals at the center of photosynthesis: Total efficiency of photosynthesis; Primary processes in photosynthesis such as (a) Light absorption, (b) Exciton Transport, (c) Charge separation and electron transport (Photosystem-I, Photosystem-II, Z- Scheme); Manganese catalysed oxidation of H₂O to O₂ (4 L) The dioxygen molecule, O₂ Uptake, transport and storage: Molecular and chemical properties of O₂, Oxygen transport and storage through Hemoglobin and Myoglobin, Alternative oxygen transport by some lower animals by Hemerythrin and Hemocyanin, Active site structure elucidation using magnetism, light absorption, vibrational spectroscopy and Mössbauer spectroscopy (4 L) Uptake, transport and storage of an essential elements as exemplified by Iron: Iron mobilization problem-----Oxidation states, solubility and medical relevance; Siderophores (Fe uptake by microorganism), Phytosiderophores (Fe uptake by plants), Transport and storage of iron (Transferrin, Ferritin, Hemosiderin). (4 L) Copper containing proteins as an alternative to biological iron: Type 1 blue copper center, Type 2 and Type 3 copper centers in O₂ activating proteins, Copper proteins as Oxidases/Reductases, Cytochrome c Oxidase, Cu-Zn and Ni superoxide dismutases. (4 L)
Textbooks and/or reference materials	1. Concept and models of inorganic Chemistry, Douglas, McDaniel, Alexander, 2. Inorganic chemistry, Shriver & Atkins, Oxford 3. Inorganic Chemistry, Huheey, Keiter, Keiter, Medhi, Pearson education. 4. The Organometallic Chemistry of the Tr. Metals by Robert H. Crabtree. 5. Bioinorganic chemistry by Bertini, Gray, Lippard and Valentine.

Mapping of COs (Course outcomes) and POs (Programme Outcomes)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
CO1	3	2	3	3	2	2	2	3	3	2	1	1
CO2	2	2	3	2	2	2	2	3	3	1	1	1
CO3	2	3	3	2	2	2	2	3	3	3	1	1
CO4	3	3	3	1	2	2	3	3	3	3	1	1
CO5	3	3	3	1	1	3	3	3	3	2	1	1

Course code	Title of the course	Program Core (PCR)/Electives (PEL)	Total number of contact hours				Credit
			Lecture (L)	Tutorial (T)	Practical (P)	Total hours	
CY2103	Pericyclic reactions and organic photochemistry	PCR	3	1	0	4	4
Pre-requisites		Course Assessment methods [Continuous assessment (CA), mid-term (MT) and end term (ET)]					
NIL		CA+MT+ET					

Course outcomes	CO1: To understand the basic principles of pericyclic and their classifications. CO2: To apply the concepts of pericyclic reactions in organic synthesis. CO3: To understand the basic principles of organic photochemical reactions and their classifications. CO4: To learn the concepts of photoredox catalysis. CO5: To apply the concepts of organic photochemistry in organic synthesis. CO6: To analyse the probable mechanism of pericyclic and organic photochemical reactions.
Topics covered	Pericyclic reactions: 22 L Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5- hexatriene and allyl system. (4 L) Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams. FMO & PMO approach. (4 L) Electrocyclic reactions - conrotatory and disrotatory motions. $4n$, $4n+2$ systems. (5 L) Cycloaddition — antarafacial and suprafacial additions, $4n$ and $4n+2$ systems, 2+2 addition of ketenes, 1,3 dipolar cycloadditions and cheletropic reactions.(4 L) Sigmatropic rearrangements –supra-facial and antara-facial shifts of H, Sigmatropic shifts involving carbon moieties, 3,3- and 5,5 sigmatropic rearrangements. Claisen, cope and aza-cope carbon rearrangements. Fluxional tautomerism, Ene reactions. Recent advances from current literature. (9 L) Organic photochemistry: 20 L General information, Photo-chemical energy, effect of light intensity on the rate of photochemical reactions. Jablonski-diagram, photo-sensitisation and quenching. Norrish type-I, type-II processes, Paterno-Buchi reaction, photochemistry of unsaturated compounds. (5 L) Types of photochemical reactions: Photo-dissociation, gas phase photolysis. Photochemistry of alkenes: Intramolecular reactions of the olefinic bond-geometrical isomerism, cyclisation reactions, rearrangement of 1,4- and 1,5-dienes. (3 L) Photochemistry of Carbonyl compounds: Intramolecular reactions of carbonyl compounds saturated, cyclic and acyclic, α,β-unsaturated and β,γ-unsaturated compounds. Cyclohexadienones, Intermolecular cycloaddition reactions, dimerisation and oxetane formation. (5 L) Aromatic compounds: Isomerisations, additions and substitutions. Miscellaneous photochemical reactions: Photo-Fries reactions of anilides, photo-Fries rearrangement, Barton reaction, Singlet molecular oxygen reactions. (2 L) Photo-degradation of polymers, photo-substitution, photo-reduction of ketones, photo-oxidation, di-π methane rearrangement, photochemistry of arenes. (3 L) Organometallic photochemistry, photochemistry of vision. (2 L)
Textbooks and/or reference materials	1. Molecular Orbitals and Organic Chemical Reactions By I. Fleming, Wiley. 2. Pericyclic reaction By S. Sankararaman Wiley VCH, 2005. 3. Photochemistry and Pericyclic Reactions by Jagdamba Singh, New Age Science publisher. 4. Mechanism of Organic Chemistry By Peter Sykes

Mapping of COs (Course outcomes) and POs (Programme Outcomes)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
CO1	3	3	3	2	2	3	1	3	2	1	2	2
CO2	3	3	3	2	2	3	1	3	3	1	1	2
CO3	3	3	3	3	3	3	2	3	3	2	2	3
CO4	3	3	3	3	3	3	2	3	3	3	2	3
CO5	3	3	3	3	3	3	2	3	3	2	2	3
CO6	3	3	3	3	3	3	2	3	3	2	2	3

Course Code	Title of the course	Program Core (PCR) / Electives (PEL)	Total Number of contact hours				Credit
			Lecture (L)	Tutorial (T)	Practical (P)	Total Hours	
CY2104	Spectroscopy: Theory and applications	PCR	3	1	0	4	4
Pre-requisites		Course Assessment methods [Continuous assessment (CA), mid-term (MT) and end term (ET)]					
CY1101		CA+MT+ET					
Course Outcomes	CO1: Understanding the principle and applications of UV-VIS, IR and Raman spectroscopy to elucidate the structure of different organic and inorganic molecules. CO2: Understand the core concept of Mass Spectroscopic techniques and their contribution to the methods of structure elucidation of organic and inorganic species. CO3: Understand the different aspect of Nuclear Magnetic Resonance spectroscopy and its application in the field of structure determination of organic and inorganic species.						
Topics Covered	Theories of Microwave, IR, UV-VIS and Raman spectroscopy and their applications to elucidate the structure of different organic and inorganic molecules. Broadening of spectral lines. Basics of Fourier transform technique. Details of the instrumentation used for these spectroscopic techniques. (16 L) Mössbauer Spectroscopy: Basic principles, spectral parameters and spectrum display. Application of the technique to the studies of (i) bonding and structures of Fe(II), Fe(III) compounds and (ii) detection of oxidation states. (4 L) NMR Spectroscopy: Basic principles, chemical shift, spin-spin interactions and coupling constants, Interpretation of first order NMR spectra; methods for simplification of second order spectra: use of double resonance, Lanthanide shift reagent, spin-tickling, INDOR, NOE, effect of solvents, preliminary idea on ¹⁹ F, ³¹ P, ¹⁴ N, ¹⁵ N, ¹⁷ O, NMR imaging, ¹³ C NMR Spectroscopy: Basic principles, proton decoupled spectra, interpretation and application in organic molecules. (14 L) Mass Spectrometry: Basic principles, soft ionization methods: CI, FD, FAB, plasma desorption; fragmentation pattern in EI, GC-MS, MS-MS, LC-MS. Application of MS in structure elucidation. (8 L)						

Textbooks and/or reference materials	1. NMR spectroscopy (Basic Principles, concepts and application in chemistry): H. Gunther 2. Spectrometric identification of organic compounds: Robert Silverstein 3. Organic spectroscopy: Kemp 4. Structural methods in Inorganic Chemistry : Ebsworth, Rankin and Cradock 5. Fundamentals of Molecular Spectroscopy: Banwell
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Mapping of COs (Course outcomes) and POs (Programme Outcomes)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
CO1	3	3	3	3	3	3	3	3	3	3	3	3
CO2	3	3	3	3	3	3	3	3	3	3	3	3
CO3	3	3	3	3	3	3	3	3	3	3	3	3

Course Code	Title of the course	Program Core (PCR)/ Electives (PEL)	Total Number of contact hours				Credit
			Lecture (L)	Tutorial (T)	Practical (P)	Total Hours	
CY2105	Structure and function of biomolecules	PCR	3	0	0	3	3
Pre-requisites		Course Assessment methods [Continuous assessment (CA), mid-term (MT) and end term (ET)]					
NIL		CA+MT+ET					
Course Outcomes	CO1: Understanding the chemistry behind biological processes CO2: Development of basic knowledge of cell structure and function CO3: Learning of different chemical aspects of biomolecules such as carbohydrates, lipids, proteins, nucleic acids CO4: Generation of concepts on molecular mechanics amongst biomolecules as a stepping stone towards Biophysical Chemistry.						
Topics covered	Carbohydrates : Conformation of monosaccharides, structure and functions of important monosaccharides like glycosides, deoxy sugars, myoinositol amino sugars. N-acetylmuramic acid, sialic acid, disaccharides and polysaccharides. Structural polysaccharides – cellulose and chitin. Storage polysaccharides - starch and glycogen. Structure and biological functions of glucosaminoglycans or mucopolysaccharides. Carbohydrates of glycoproteins and glycolipids. Role of sugars in biological recognition. Blood group substances. Ascorbic acid. Carbohydrate metabolism: Kreb’s cycle, glycolysis, glycogenesis and glycogenolysis, gluconeogenesis, pentose phosphate pathway. (8 L) Lipids: Fatty acids, essential fatty acids, structure and function of triacyl glycerols, glycerophospholipids, sphingolipids, cholesterol, bile acids, prostaglandins. Lipoproteins-composition and function, role in atherosclerosis. Properties of lipid aggregates – micelles, bilayers, liposomes and their possible biological functions. Biological membrane. Fluid mosaic model of membrane structure. Lipid metabolism – oxidation of fatty acids. (8 L)						

	Amino Acids, Peptides and Proteins: Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing. Secondary structure of proteins, forces responsible for holding of secondary structures. α-helix, β-sheets, super secondary structure, triple helix structure of collagen. Tertiary structure of protein – folding and domain structure. Quaternary structure. Structure validation by Ramachandran plot. Metalloprotein. Amino acid metabolism – degradation and biosynthesis of amino acids, sequence determination: chemical/ enzymatic/ mass spectral, racemization/ detection. (8 L) Nucleic Acids: Purine and pyrimidine bases of nucleic acids, base pairing via H-bonding. Structure of RNA and DNA, double helix model of DNA and forces responsible for holding it. Chemical and enzymatic hydrolysis of nucleic acids. The chemical basis of heredity, an overview of replication of DNA, transcription, translation and genetic code. Chemical synthesis of mono and trinucleoside. (8 L)
Textbooks and/or reference materials	1. Principles of Biochemistry by Lehninger 2. Biochemistry by Voet & Voet. 3. Principles of Physical Biochemistry by K. E. van Holde, C. Johnson and P. S. Ho (Pearson).

Mapping of COs (Course outcomes) and POs (Programme Outcomes)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
CO1	3	1	3	2	2	1	1	3	3	2	3	1
CO2	3	1	2	1	1	1	1	3	2	2	3	1
CO3	3	3	3	2	2	3	1	3	3	2	3	1
CO4	3	3	3	3	2	3	2	2	1	1	2	1

Course Code	Title of the course	Program Core (PCR) / Electives (PEL)	Total Number of contact hours				Credit
			Lecture (L)	Tutorial (T)	Practical (P)	Total Hours	
CY2151	Advanced practical on physical chemistry	PCR (Practical)	0	0	4	4	2
Pre-requisites		Course Assessment methods: [Continuous evaluation (CE) and end assessment (EA)]					
CY1151		CE+EA					
Course Outcomes	CO1: Basic concepts of spectrophotometric estimation and IR spectroscopy. Experimental knowledge on the influence of reaction parameters on the rate of the reaction, and analysis thereon. CO2: Learning about handling of spectrophotometer and IR spectrometer and their basic theory. CO3:To develop laboratory skills and the ability to work independently as well as in a group. CO4: Knowing presentation, analysis and interpretation of data, source of error and error analysis. CO5: To understand the interconnection between experimental foundation and underlying theoretical principles. CO6: To develop the ability of scientific communications through oral quizzes, written						

	reports and presentations
Topics Covered	1. Determination of isoelectric pH of gelatin. 2. Spectroscopic determination of rate constant (alkaline hydrolysis of crystal violet) 3. Salt effect on the rate of an ionic reaction. 4. Solvent effect on the rate of a reaction. 5. Micellar effect on the rate of a reaction. 6. Intermolecular hydrogen bonding in benzyl alcohol using IR spectroscopy 7. Thermodynamics of micellization. 8. Determination of activation parameter of a reaction. 9. Determination of mean ionic activity coefficient of HCl by emf measurement. 10. Determination of viscosity average molecular weight of synthetic polymer.
Textbooks and/or reference materials	1. Instruction manual provided by the Instructor 2. Experiments in Physical Chemistry by Carl Garland, Joseph Nibler, David Shoemaker 3. Practicals in Physical Chemistry by P S Sandhu 4. Practical Physical Chemistry by Viswanathan and Raghavan

Mapping of COs (Course outcomes) and POs (Programme Outcomes)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
CO1	3	3	2									
CO2	3	3		2	2	3		2	2		1	
CO3						2		2	2		3	3
CO4	3	3		3	3		1	3				
CO5								3	3			
CO6								3	3		2	2

Course Code	Title of the course	Program Core (PCR) / Electives (PEL)	Total Number of contact hours				Credit
			Lecture (L)	Tutorial (T)	Practical (P)	Total Hours	
CY2152	Synthesis and characterization of complex compounds	PCR (Practical)			3	3	2
Pre-requisites		Course Assessment methods: [Continuous evaluation (CE) and end assessment (EA)]					
NIL		CE+EA					
Course Outcomes	CO1: Coordination complex synthesis maintaining molarity. CO2: Crystallization techniques to purify the synthesized materials. CO3: Decomposition and estimation of metal ion(s) using spectrophotometry/iodometry. CO4: Characterization of synthesized materials using FTIR, UV-Vis and EPR spectroscopy and CHN analysis. CO5: Spectral data interpretation.						

Topics Covered	Synthesis of a) $[\text{VO}(\text{acac})_2]$; b) $[\text{Co}(\text{NH}_3)_5(\text{N}_3)]$; c) $[\text{Mn}(\text{acac})_3]$; d) $(\text{NH}_4)_2[\text{MnF}_5]$; e) Mohr's salt and other complexes. Crystallization and their characterization by using various spectroscopic methods like, FTIR, EPR, and UV-Vis. Magnetic moment measurement using Gouy's balance. Estimation of Mn and Cobalt from the synthesized complexes.
Textbooks	1. Advanced Inorganic Experiments, By G. N. Mukherjee.

Mapping of COs (Course outcomes) and POs (Programme Outcomes)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
CO1	1	3	3	3	2	2	1	3	3	3	1	1
CO2	2	2	3	3	2	1	1	3	3	3	1	1
CO3	1	3	3	3	2	2	1	3	3	3	1	1
CO4	3	3	3	3	2	2	1	3	3	3	1	1
CO5	3	2	3	3	2	3	1	3	3	3	1	1

Course Code	Title of the course	Program Core (PCR) / Electives (PEL)	Total Number of contact hours				Credit
			Lecture (L)	Tutorial (T)	Practical (P)	Total Hours	
CY2153	Chromatographic separation of organic compounds	PCR (Practical)	0	0	3	2.0	3
Pre-requisites		Course Assessment methods: [Continuous evaluation (CE) and end assessment (EA)]					
NIL		CE+EA					
Course Outcomes	CO1: Understand the working principles of different types of chromatography. CO2: Learn the sampling method including derivatization for analysis. CO3: Master the techniques and application of thin layer, paper and column chromatography. CO4: Learn to analyze the chromatograms of GC and HPLC.						

Topics Covered	Principle of different chromatographic techniques. Thin Layer Chromatography Determination of R_f values and identification of organic compounds. Preparation and separation of DNP derivatives of carbonyl compounds Separation of a mixture of dyes using cyclohexane and ethyl acetate (8.5:1.5). Paper Chromatography: Determination of R_f values and identification of organic compounds. Separation of a mixture of amino acids. Separation of sugars. Column Chromatography: Separation of Fluorescein and methylene blue Separation of aniline and <i>N,N</i> dimethyl aniline Separation of Lycopene and β-carotene Demonstration of chromatographic separation by GC & HPLC. Monitoring of reactions and purification of product mixtures by chromatography
Textbooks and/or reference materials	1. Fundamentals of analytical chemistry, Skoog, West, Holler and Crouch, 8th edition, Thomson

Mapping of COs (Course outcomes) and POs (Programme Outcomes)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
CO1	3	3	3	3	3	3		3	3	3	3	3
CO2	2	3	3	3	3	3		3	3	3	3	3
CO3	1	3	3	3	3	3		3	3	3	3	3
CO4	3	3	3	3	3	3	3	3	3	3	3	3

THIRD SEMESTER:

Course Code	Title of the course	Program Core (PCR)/ Electives (PEL)	Total Number of contact hours				Credit
			Lecture (L)	Tutorial (T)	Practical (P)	Total Hours	
CY9111	Advanced quantum and computational chemistry	PEL	3	0	0	3	3
Pre-requisites		Course Assessment methods [Continuous assessment (CA), mid-term (MT) and end term (ET)]					
CY1101		CA+MT+ET					

Course Outcomes	CO1: To apply different time dependent and time independent approximation methods to solve various molecular problems CO2: To apply Born-Oppenheimer approximation to separate nuclear and electronic components from molecular Hamiltonian. CO3: To analyze the chemical bonding through MO and VB theory CO4: To understand the interaction of radiation with matter and selection rules for transition among different molecular energy levels. CO5: To apply Hückel theory in conjugated system and its applications CO6: To evaluate the structure, spectroscopy, chemical bonding of small molecules using computational chemistry
Topics Covered	Approximate Methods: The variation method, trial wave functions, introduction to perturbation theory, application to simple problems (Zeeman, Stark effect etc.). (7 L) Many Electron Atoms: Classical Calculations of He atom, Hartree-Fock equations of Helium atoms, anti-symmetry in electron wavefunction, Slater determinants, Hartree-Fock-Roothaan method. (5 L) Spin-orbital interaction: LS and JJ coupling, Term symbol and spectroscopic states. (3L) Molecules and chemical bonding: Born-Oppenheimer approximation, MO treatment of diatomic molecules, Idea of self-consistent field method, molecular electronic configurations. (5L) Time dependent perturbation theory: Transition dipole moment. Fermi's Golden rule. Lamberts Beers law, Einstein's coefficients for induced and spontaneous emission. (5L) Hückel theory of conjugated systems: Bond order and charge density calculations. Applications to ethylene, butadiene, cyclopropenyl radical, cyclobutadiene. (3L) Software Demonstration of HF and DFT calculations (using Gaussian or similar software): Modelling of Single molecules: Geometry optimization, Vibrational frequency calculations, time-dependent DFT calculations, NMR shift, Conformational analysis etc. (5L) Gas phase reactions through DFT calculation: Reaction mechanism through analysis of transition states, determination of activation energy, rate coefficients etc. (3L)
Textbooks and/or reference materials	1. Quantum Chemistry by Levine 2. Physical Chemistry: A Molecular approach by Donald A. McQuarrie 3. Introductory quantum chemistry by A. K. Chandra 4. Molecular theory and group theory by R. L. Carter

Mapping of COs (Course Outcomes) and POs (Programme Outcomes)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
CO1	3	1	3	3	3	1	3	3	3	2	1	1
CO2	3	1	3	3	3	1	3	3	3	2	1	1
CO3	3	1	3	3	3	1	3	3	3	2	1	1
CO4	3	1	3	3	3	1	3	3	3	2	1	1
CO5	3	3	2	3	2	1	3	3	2	1	2	3
CO6	3	3	2	3	2	1	3	3	2	1	2	3

Course Code	Title of the course	Program Core (PCR)/ Electives (PEL)	Total Number of contact hours				Credir
			Lecture (L)	Tutorial (T)	Practical (P)	Total Hours	
CY9112	Basics of nonlinear dynamics	PEL	3	0	0	3	3
Pre-requisites		Course Assessment methods (Continuous assessment (CA), mid-term (MT) and end test (ET))					
CY2101		CA+MT+ET					
Course Outcomes	CO1: The complexities of dealing Nonlinear systems compared to linear systems. CO2: The fundamentals of dynamical system theory such as stability, bifurcation etc. CO3: Numerical programing methods and approximate analytical techniques for various nonlinear problems. CO4: The application and usefulness of nonlinear dynamical theory in multi-disciplinary fields.						
Topics Covered	Introduction: Motivation, scope, dynamical view, importance and application with examples of nonlinear dynamical systems. Autonomous and Non-autonomous dynamical systems and difficulty of solving nonlinear problems. (2 L) Numerical programing: Solving coupled ODE(s), PDEs using Euler, Heun, Runge-Kutta 4 th order method, FTCS, plotting and understanding vector field, bifurcation diagram in Fortran/Matlab/Python/ XPPAUT/ GEOGEBRA/ MATHEMATICA/ GNU PLOT etc. (4L) One Dimensional Flows: fixed point and stability with example such as Logistic equation. Linear stability analysis, basics of existence and uniqueness criteria, impossibility of oscillations in 1D flow, concept of potential well; Bifurcation in 1D: Saddle Node, Transcritical, Pitchfork etc with concept of hysteresis, Imperfect bifurcations and Catastrophes with examples. Flows on the circle: Uniform and non- uniform oscillator. Ghosts and bottlenecks. Overdamped pendulum. (4 L) Two Dimensional Flows: Linear systems with definition and example; Classification of linear systems, classification of fixed points: Saddle node, sink, source, spiral, center, star, degenerate nodes, non-isolated fixed points etc. and phase portrait; fixed point and linearization of nonlinear systems; Conservative systems, reversible systems; Limit Cycles: Van Der Pol oscillator, Lyapunov functions, Dulac’s criterion, Poincare-Bendixson Theorem (quantitative description); Lienard systems, Relaxation Oscillators, weakly nonlinear oscillators: Duffing etc; Solution techniques: Regular perturbation theory and its failure; Multi-scale analysis, Method of Averaging, Renormalization of Group etc.; Revisiting bifurcation in 2D flow: Saddle node, Transcritical, Pitchfork, Hopf, homoclinic and heteroclinic bifurcation. Bifurcation analysis using MATCONT/ XPPAUT software; oscillating chemical reactions. (14 L) Spatial Pattern forming systems: Reaction-Diffusion systems, Dispersion relation, Turing Patterns. (2 L) Chaos: Brief description of Chaos in 3D flow using Lorentz Oscillator, Lyapunov exponent etc. (2 L) Application: Ecology: Romeo-Juliet love affairs/ Insect Outbreak dynamics/ flashing rhythm of fire-flies etc., Rabbit vs Sheep model/ Predator-Prey model, Grazing/ Harvesting model/ Lake-Eutrophication model etc, Critical/Tipping and Non-critical transitions and Early Warning Signals of Tipping.						

	<u>Chemistry</u> : Turing pattern formation: Analysis and generation of spot, stripe, Labyrinth etc. patterns using Gierer Meinhardt/ Gray-Scott/ Belousov-Zhabotinski (BZ)/ Chlorine-dioxide-iodine-malonic acid (CDIMA) chemical reactions etc. <u>Biology</u> : Neuron system: Hodgkin-Huxley models/ FitzHugh-Nagumo model analysis, spike and pattern generation etc./ Circadian rhythm/ Glycolytic oscillator etc.; <u>Disease/Epidemics dynamics</u> : Modelling infectious diseases: SIR, SIS model etc. (6 L)
Textbooks and/or reference materials	1. Strogatz, S. Nonlinear Dynamics and Chaos. Reading, MA: Addison-Wesley, 2007. 2. Nonlinear Ordinary Differential Equations, D. W. Jordan, and P. Smith Oxford University Press 1999 3. Guckenheimer, J., and P. Holmes. Nonlinear Oscillations, Dynamical Systems and Bifurcations of Vector Fields. New York, NY: Springer-Verlag, 2002. 4. Introduction to Perturbation Techniques, Ali Hasan Nayfeh, WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, 2004. 5. Lakshmanan, M and R. Rajasekar, Nonlinear Dynamics: Integrability, Chaos and Patterns, Springer, 2003. 6. Clifford Henry Taubes. Modeling Differential Equations in Biology, Cambridge University Press, Second edition 2008. 7.

Mapping of COs (Course Outcomes) and POs (Programme Outcomes)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
CO1	3	1	3	3	2	1	3	3	2	1	1	1
CO2	3	2	3	3	3	1	3	3	3	3	1	2
CO3	3	2	3	3	3	3	3	3	2	3	1	2
CO4	3	2	3	3	3	3	3	3	3	3	3	3

Course Code	Title of the course	Program Core (PCR)/Electives (PEL)	Total Number of contact hours				Credit
			Lecture (L)	Tutorial (T)	Practical (P)	Total Hours	
CY9113	Advanced spectroscopic techniques and applications of group theory	PEL	3	0	0	3	3
Pre-requisites		Course Assessment methods [Continuous assessment (CA), mid-term (MT) and end term test (ET)]					
CY1101, CY2101		CA+MT+ET					
Course Outcomes	CO1: Fundamentals of laser and application in science and industry CO2: Photoelectron spectroscopy, Mossbauer spectroscopy CO3: Modern techniques of fluorescence spectroscopy, CO4: Different aspects of fluorescence process CO5: GOT, SALC and Projection operator CO6: Different Applications of group theory in chemical bonding, IR and Raman spectroscopy, Electronic spectroscopy						

Topics Covered	1. Laser: Fundamentals, Characteristics, Continuous vs. pulsed laser: Q-switching, Mode-locking. (4 L) 2. Time resolved laser spectroscopy (picosecond, femtosecond laser spectroscopy) and its application. (6 L) 3. Laser induced fluorescence spectroscopy and its application. (3 L) 4. Different photophysical processes, photophysical quenching processes and its mechanism, Charge-transfer processes (Marcus theory). Excited state life-time, Fluorescence sensors and different mechanisms, Solvent effect on fluorescence, Lippert-Mataga equation, Excited state pH and dipole moment. (8 L) 5. X-ray photoelectron spectroscopy, Mossbauer spectroscopy. (4 L) 6. Consequences of GOT and development of SALCs. (4 L) 7. Applications of group theory in chemical bonding, IR and Raman spectroscopy, Electronic spectroscopy. (8 L)
Textbooks and/or reference materials	1. Modern spectroscopy by J.M. Hollas 2. Lasers: Fundamentals and Applications by Ajoy Ghatak and K. Thyagarajan 3. Atkin's Physical Chemistry by P. Atkins and J. dePaula (7 th ed.) 4. Fundamentals of molecular spectroscopy By Banwell and McCash 5. Fundamentals of photochemistry By Rohatgi and Mukherjee. 6. Molecular symmetry and group theory by R. L. Carter 7. Fundamentals of Symmetry and Group Theory with Applications in Chemistry by S S Panja, PHI

Mapping of COs (Course Outcomes) and POs (Programme Outcomes)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
CO1	3	3	3	2	2	3	1	3	3	1	2	2
CO2	3	3	3	2	2	2	1	3	3	2	2	1
CO3	3	3	3	2	2	2	1	3	3	2	2	1
CO4	3	3	3	2	2	2	1	3	3	2	2	1
CO5	3	3	3	2	2	2	1	3	3	2	2	1
CO6	3	3	3	2	2	2	1	3	3	2	2	1

Course Code	Title of the course	Program Core (PCR)/Electives (PEL)	Total Number of contact hours				Credit
			Lecture (L)	Tutorial (T)	Practical (P)	Total Hours	
CY9114	Surface science, electrode kinetics and corrosion science	PEL	3	0	0	3	3
Pre-requisites		Course Assessment methods [Continuous assessment (CA), mid- term (MT) and end term test (ET)]					
CY2101		CA+MT+ET					

Course Outcome	CO1: process of adsorption and various adsorption isotherms involving different types of adsorbate-adsorbent combination. Application of adsorption isotherm to determine catalytic efficiency. CO2: basics of surfactants and micelles and their application in science and technology. CO3: concept of electrical double layer, zeta potential and its role for colloidal stability. CO4: kinetics of reaction at the electrode surface and its relevance towards industrially important hydrogen evolution from dissociation of water. CO5: corrosion of various metals under different environmental conditions and mitigation methods.
Topics Covered	Adsorption on solid: BET, Harkins- Jura and Gibbs adsorption isotherms, surface tension and surface pressure, contact angle: interfacial tension, temporary and permanent Hysteresis. (4 L) Micelles and microemulsions: Phase diagram of micellar system. Hydrophilic- Lipophilic balance and application, Mass action model and pseudo-phase model for non- ionic and ionic micelles. Relationship between thermodynamic properties for micellization with CMC. Estimation of fraction of counter ion binding, aggregation number and solvation for micelles Phase diagram of microemulsions. Packing factor and micellar stability. (5 L) Nanoparticles: Optical properties of nanoparticles. (1 L) Electrical double layer and Electrokinetic effects: Electrical double layer, Zeta potential, Stability of colloids, electroosmosis, electrophoresis, streaming potential etc., Ion transport across membrane. (3 L) Electrode kinetics: Derivation of Butler-Volmer equation, Study of the kinetics of different electrode reactions (including elucidation of reaction mechanism). Polarizable and non- polarizable electrodes. Numerical problems. (4 L) Corrosion science: Different forms of corrosion: properties and remedial methods. (2 L) Tafel relation and mixed potential theory, Concept of exchange and limiting current density. (2 L) Potentiodynamic polarization and electrochemical impedance spectroscopic methods to determine rate of corrosion. (3 L) Corrosion control: Cathodic (impressed sacrificial metal, current method and metallic coating) and anodic control methods. Numerical problems. (4 L) Application of corrosion inhibitors including green inhibitors. (2 L) High temperature corrosion: mechanism, kinetics and remedial measures. (2 L)
Textbooks and/or reference materials	1. Modern Electrochemistry 2A - Fundamentals of Electrode Processes by Bockris and Reddy 2. Corrosion Engineering by M G Fontana 3. Corrosion Engineering by B N Popov 4. Surfactant science and Technology (3rd ed.) by D. Myers. 5. Principles of colloid and surface chemistry (3rd ed) by P C Hiemenz and R Rajgopalan

Mapping of COs (Course outcomes) and POs (Programme Outcomes)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
CO1	3	3	3	2	2	2	1	3	3	3	3	1
CO2	3	3	3	2	2	2	1	3	3	3	3	1
CO3	3	3	3	2	2	2	1	3	3	3	3	1
CO4	3	3	3	2	2	2	1	3	3		3	2
CO5	3	3	3	2	2	2	1	3	3		3	2

Course Code	Title of the course	Program Core (PCR)/Electives (PEL)	Total Number of contact hours				Credit
			Lecture (L)	Tutorial (T)	Practical (P)	Total Hours	
CY9121	Advanced green and environmental chemistry	PEL	3	0	0	3	3
Pre-requisites		Course Assessment methods [Continuous (CT), mid-term (MT) and end assessment (EA)]					
NIL		CT+MT+EA					
Course Outcomes	CO1: Students will be given an introduction to green chemistry and learn about its basic concepts. CO2: Students will learn the application of green chemistry. CO3: Demonstrate the design for safer, energy efficient technology and process optimization for cleaner industrial processes. CO4: Understand the fundamentals of pollution prevention technique with respect to health significance. CO5: Fundamental understanding of monitoring and analysis of air and water.						
Topics Covered	Introduction to Green Chemistry: (15 L) Definition and strategic of green chemistry. Why Green Chemistry? Prevention, Atom Economy, Less Hazardous Chemical Syntheses, Designing Safer Chemicals, Safer Solvents and Auxiliaries, Design for Energy Efficiency, Use of Renewable, Feedstocks, Reduce Derivatives, Catalysis, Design for Degradation, Real-time analysis for Pollution Prevention, Inherently Safer Chemistry for Accident Prevention, Laboratory pollution prevention. Application of Green Chemistry: (10 L) Applications and benefits of green chemistry: Production of new chemicals, materials, and products. Examples of successful green technologies; Alternative synthetic routes, new separation processes, new methods for delivery or product application (Alternative solvents, Energy vs. material activity). Importance of pollution and wastefulness in modern cultures by reflecting on the green chemistry.						

	Principle of Analysis for Air and Water samples: (11 L) Objectives of chemical analysis of air and water. Analysis of water: colour, turbidity, total solid, conductivity, acidity, alkalinity, hardness, chloride, sulfate, fluoride, phosphates, and different forms of nitrogen. Heavy metal analysis with respect to health significance. Chemical speciation study. Measurement of DO, BOD and COD. Pesticides as water pollutants analysis. Brief concept of hazardous, biomedical and electronic wastes. Monitoring and analysis of air: Monitoring technique through high volume sampler, SPM and RPM sampler. Measurement and analysis of SPM, RPM, SOX and NOX.
Textbooks and/or reference materials	1. Green Chemistry, An Introductory Text By Mike Lancaster, RSC publications. 2. Handbook on Green Analytical Chemistry By Miguel de la Guardia, Salvador Garrigues, Wiley. 3. Innovations in Green Chemistry and Green Engineering By Paul T. Anastas, Julie Beth Zimmerman, Springer publications. 4. Alternative Solvents for Green Chemistry By Francesca M Kerton, Ray Marriott, RSC publications. 5. Environmental Chemistry with Green Chemistry By Asim Kumar Das, Books and Allied (P) Ltd.

Mapping of COs (Course outcomes) and POs (Programme Outcomes)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
CO1	3	3	3	3	3	2	1	3	3	3	2	3
CO2	3	2	3	2	3	2	1	3	3	3	3	3
CO3	3	2	2	2	3	2	1	3	3	3	2	3
CO4	3	3	3	2	2	3	1	3	3		3	3
CO5	3	3	3	2	2	3	1	3	3		3	3

Course Code	Title of the course	Program Core (PCR)/ Electives (PEL)	Total Number of contact hours				Credit
			Lecture (L)	Tutorial (T)	Practical (P)	Total Hours	
CY9122	Synthetic methodology for metal complexes and supramolecular chemistry	PEL	3	0	0	3	3
Pre-requisites		Course Assessment methods [Continuous assessment (CA), mid-term (MT) and end term (ET)]					
CY1102		CA+MT+ET					
Course Outcomes	CO1: Understand the importance of transition metal complexes. CO2: Basic knowledge of different types of ligands and their applications. CO3: Primary Concept of designing and synthesis of a ligand. CO4: Learn about the different aspects of supramolecular chemistry. CO5: Clear idea about the synthesis of diversified macrocycles. CO6: Fundamentals of thermodynamic effects upon changing the cavity size of a macrocycle.						

Topics covered	Introduction, Importance of ligand design and their applications in metal-complex formation. (6 L) Nitrogen Based Ligand: N₂ as Ligand, Reactivity of Bound N₂, Macrocyclic Amines, Polyimines, Porphyrin, Polypyrazolylborate Ligand, Hydroxylamido Ligand, Schiff Base Ligand, Azide and Other Anionic Ligand. (5 L) Phosphorus Based Ligands: Phosphine as Ligand, Monophosphines, Diphosphines, Polydentate Phosphines, Phosphate Ligands, Heterocyclic Phosphorus Ligands, Dialkyl- and Diarylphosphido Ligands. (4 L) Oxygen Based Ligand: Dioxygen, Sueroxo and Peroxo Ligand, Alkoxides and Aryloxides, Ketone and Ester, Crown Ethers, β-Ketoenolato and Related Ligands, Carbamates, Oxo Anions as Ligands. (5 L) Sulphur Based Ligand: Thiolates, Disulphides, Thioethers, Sulphur Oxide, Dithiocarbamates, 1,2-Dithiolenes. (3 L) Supramolecular Chemistry: Introduction, Host-Guest Chemistry, Self Assembly, Supramolecular Building Blocks and Spacer, Driving Forces for the Formation of Supramolecular Structure. (2 L) Spatial Relationships between Host and Guest, Classification of Host-Guest Compounds, General Introduction to Podand, Coronand, Spherand, Coronand- Podand Hybrid, Cryptands. (2 L) The Chelate and Macrocyclic Effect on Host-Guest Binding, Synthesis of Crown Ethers, The Template Effect, Synthesis of Cryptands, Recent Developments in the Synthesis of Cryptands, Synthesis of Aza Crown Ethers and Related Compounds. (3 L) Chiral Crown Ethers, Proton Ionisable Crown Ethers, Diester Crown Ethers, Synthesis of Lariat Ethers. (2 L) Synthesis of Calix[n] Arenes, Chiral Calix[n] Arenes, Introduction of Functional Groups in Calix[n] Arenes, Reactions at Upper Rim of Calixarene. (3 L) Selectivity of Cation Complexation, Cation Binding by Crown Ethers, Cation Binding by Lariat Ethers, Cation Binding by Cryptands, Thermodynamic Effect of Binding. (4 L)
Textbooks and/or reference materials	1. An Introduction to Supramolecular Chemistry by Asim K Das and Mahua Das. 2. Analytical Chemistry of Macrocyclic and Supramolecular Compounds by S. M. Khopkar. 3. Advanced Inorganic Chemistry by F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann. 4. Synergy in Supramolecular Chemistry edited by Tatsuya Nabeshima. 5. Concepts and Models of inorganic chemistry by B. E. Douglas, D. H. McDaniel and J. J. Alexander.

Mapping of COs (Course outcomes) and POs (Programme Outcomes)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
CO1	3	3	3	3	2	1		3	3	2		1
CO2	3	3	3	3	1		1	3	3	1	1	1
CO3	3	3	3	3	2	2		3	3	2		1
CO4	3		3	2	2	2	1	3	1	1	1	1
CO5	3	3	3	3	2	2	1	3	3	2	1	1
CO6	3		3	2	2	1	1	3	2	1		1

Course Code	Title of the course	Program Core (PCR)/ Electives (PEL)	Total Number of contact hours				Credit
			Lecture (L)	Tutorial (T)	Practical (P)	Total Hours	
CY9123	Small molecule activation, nuclear chemistry and related spectroscopy	PEL	3	0	0	3	3
Pre-requisites		Course Assessment methods [Continuous assessment (CA), mid-term (MT) and end term (ET)]					
CY1102, 2014		CA+MT+ET					
Course Outcomes	CO1: To understand {MNO} ⁿ notations of metal nitrosyls and their properties. CO2: Elucidating the active site structures and investigating the roles of various enzymes related to nitrogen cycle. CO3: Understanding the basics of nuclear chemistry. CO4: To elucidate the electronic structures using NMR, EPR and Mössbauer spectroscopy.						
Topics Covered	Small Molecule Activation: Importance of NO as ligand and its diverse roles in biology, NO Synthase enzyme and NO donors including metal nitrosyls, MO diagram of NO and its various binding modes, Enemark-Feltham {MNO} ⁿ notation, Spectroscopic and structural properties of various {MNO} ⁿ species (M = Fe and Cu), NO detection methods, Electrophilic and nucleophilic reactivity on metal activated NO moiety. (7 L) Naturally occurring activation of small molecules like nitrate (NO ₃ ⁻), nitrite (NO ₂ ⁻), nitric oxide (NO), nitrous oxide (N ₂ O) and nitrogen (N ₂) related to the Denitrification and N ₂ Fixation pathways of Nitrogen Cycle. Enzymes involved for such activation of small molecules and their active site structures, catalytic activity and impact on Atmospheric Nitrogen Cycle. Organic nitrile (RCN) activation by Nitrile Hydratase enzyme. (9 L) Nuclear Chemistry: Concept of Quarks; Size, shape, stability and classification of nuclides, Nuclear potential diagram, Packing fraction, Mass defect, Binding energy and related numerical problems, Quantum numbers of nucleons and magnetic properties, Nordheim rules, Nuclear magnetic resonance and its application to medical diagnosis such as MRI, Electric quadrupole moment of the nuclides and concept of electric multipoles; Nuclear spin (I), quadrupole moment (Q) and Ellipticity of the nucleus and numerical problems. Nuclear shell model, magic number and periodicity of nuclear properties. (8 L) Spectroscopy related to nuclear spin: Electron Paramagnetic/Spin Resonance (EPR/ESR) Spectroscopy: Interaction between nuclear/electron spin with magnetic field, techniques of EPR spectroscopy, Relaxation time and line width in EPR transition, EPR relaxation and chemical bonding, Interaction of nuclear spin with electron spin (hyperfine, superhyperfine coupling), g values and factors affecting it, determination of g values, Zero field splitting, Kramer’s degeneracy and applications of EPR measurements. (5 L) Nuclear resonance or recoilless absorption and Mössbauer Spectroscopy: Recoiling Frequency shift, Frequency broadening and Doppler effect, Characteristics of Mössbauer nuclides and related Decay schemes, Quadrupole splitting,						

	Isomer shift and its application to assign the oxidation state, spin state, site symmetry and bonding properties of Mossbauer nuclides. (5 L)
Textbooks and/or reference materials	1. Nitric Oxide Research (Eds. M. Feelish, J.S. Stamler) Wiley, Chichester, 1996. 2. Activation of Small Molecules, William B. Tolman, Wiley. 3. Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, Wolfgang Kaim and Brigitte Schwederski, Wiley 4. Essentials of Nuclear Chemistry, H. J. Arnikar, New Age International Publishers, 2009 5. Nuclear Physics, Irving Kaplan, Narosa Publishing House, 2002 6. Modern Nuclear Chemistry, W. D. Loveland, D. J. Morrissey, Glenn T. Seaborg, Wiley. 7. Elements of Magnetochemistry, R. L. Dutta & A. Syamal, East-West Press Pvt. Ltd., New Delhi, India.

Mapping of COs (Course outcomes) and POs (Programme Outcomes)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
CO1	3	3	3	2	2	3	3	3	3	2	1	1
CO2	3	2	3	2	2	2	3	3	3	2	1	1
CO3	3	2	3	2	2	2	1	3	2	2	1	1
CO4	3	3	3	2	2	3	1	3	2	3	1	1

Course code	Title of the course	Program Core (PCR)/Electives (PEL)	Total number of contact hours				Credit
			Lecture (L)	Tutorial (T)	Practical (P)	Total hours	
CY9124	Application of group theory and inorganic electrochemistry	PEL	3	0	0	3	3
Pre-requisites		Course Assessment methods [Continuous assessment (CA), mid-term (MT) and end term (ET)]					
CY1104, CY2101		CA+MT+ET					
Course outcomes	CO1: To know group, examples, vector space, matrix and matrix operator. CO2: To know point group and its representations, reducible and irreducible representation. CO3: To know the significance of character tables of point group and its application in chemical problems. CO4: To get knowledge of thermodynamics and kinetics of electrochemical processes. CO5: To get foundation in different electrochemical methods like cyclic voltammetry coulometry and its applications in inorganic fields.						
Topics covered	Group theory: vector space and matrix , representation of groups, techniques and relationships for chemical applications, symmetry and chemical bonding, equation of wave functions, vibrational spectroscopy, transition metal complexes. (24 L) Inorganic Electrochemistry: fundamental of electrode reaction, basic equipment for electrochemical measurements, voltametric techniques, electrochemical behaviour of transition metal complexes, metal complexes containing redox active ligands. (12 L)						

Textbooks and/or reference materials	1. Chemical applications of Group theory, F.A. Cotton John Wiley & sons Inc. 2. Group Theory and Chemistry, David M Bishop, Dober Publication Inc. 3. Molecular Symmetry and group theory, R.L. Carter, John Wiley & sons Inc. 4. Inorganic electrochemistry: Theory, practice and application; by P. Zanello; RSC
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Mapping of COs (Course Outcomes) and POs (Programme Outcomes)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
CO1	1	3	3	3	2	2	1	3	3	3	1	1
CO2	2	2	3	3	2	1	1	3	3	3	1	1
CO3	1	3	3	3	2	2	1	3	3	3	1	1
CO4	3	3	3	3	2	2	1	3	3	3	1	1
CO5	3	2	3	3	2	3	1	3	3	3	1	1

Course code	Title of the course	Program Core (PCR)/Electives (PEL)	Total number of contact hours				Credit
			Lecture (L)	Tutorial (T)	Practical (P)	Total hours	
CY9131	Advanced organic synthesis	PEL	3	0	0	3	3
Pre-requisites		Course Assessment methods [Continuous assessment (CA), mid-term (MT) and end term (ET)]					
CY1103		CA+MT+ET					
Course outcomes	CO1: Understanding of mechanism of organic specific reactions, their application in different field of synthetic organic chemistry. CO2: Uses of strategy and control of Hydroboration and Wittig reaction for carbon-carbon and other special types of bond formation. CO3: Birch reduction, how the better yield of product could be obtained, their tactics, strategy and control has been highlighted. CO4: Role of specific reagents with related mechanisms in their transformation and their mechanism from substrate to products is included for their step by step synthesis. CO5: Research oriented study with innovative idea.						
Topics covered	1. Hydroboration reaction of alkenes, mechanism and hydrolysis process, Regioselectivity, stereoselectivity and Enantioselective hydroboration reaction, Uses of 9-BBN (in Suzuki Cross coupling reaction and others) and Monoisocamphenylborane (IpcBH ₂), isomerization of alkenes via hydroboration reactions, Carbon-Nitrogen, Carbon-halogen bond formation, synthesis of cyclopropyl, cyclobutyl derivatives and bicyclocompounds. (12 L) 2. Birch Reduction: Mechanism, dependent factors, Application of birch reduction in : aminolysis, hydrogenolysis, Wilds & Nelsen modification for pure products in Birch reduction, Regio-selectivity of Birch reduction. Hine postulates; Reduction of substitute benzenoid systems with EWG and EDG; biphenyl systems, regio-selective reduction of naphthalene and substituted naphthalene; Stereo selective of Birch reduction in naphthalene. Reduction of Anthracene and Phenanthrene systems; application in natural product synthesis. (12 L) 3. Wittig reactions or chemistry of Ylide: synthesis of phosphoylide; Stereochemical outcome of Wittig reactions and their dependent factors. Stereo-selectivity in case of stabilized and non-stabilized ylides. Scholar modifications. Effect of ligands in phosphorous						

	ylide. Advantages of Wittig-Horner reaction over Wittig reaction; Difference in reactivity of phosphorous and sulphonylides; Regioselective and stereo-selective reaction with stabilized and non-stabilized sulphonylides. (12 L)
Textbooks and/or reference materials	1. F.A. Carey & R.J. Sundberg, Advanced Organic Chemistry, Springer, 2007 2. K. C. Nicolaou & E. J. Sorensen, Classics in Total Synthesis: Targets, strategies and Methods, Wiley, 1996. 3. W. Carruthers, Modern Methods in Organic Synthesis, Cambridge University Press, 2004. 4. Principles of Organic Synthesis, R.O.C. Norman & J.M. Coxon, Nelson Thornes, 1993, C R C Press. 5. Organic synthesis by M. Smith, Elsevier, 4th Edition, 2016. 6. Recently published papers in reputed journals on Hydroboration reaction, Wittig reaction and Birch reduction have to follow as advance study for this elective paper.

Mapping of COs (Course outcomes) and POs (Programme Outcomes)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
CO1	3	2	3	3	3	2	3	3	3	1	3	1
CO2	3	3	2	3	2	2	3	2	3	3	1	2
CO3	3	2	3	2	1	3	2	2	2	2	2	1
CO4	1	2	1	3	2	2	3	2	1	2	1	2
CO5	3	2	2	1	3	2	2	3	2	1	1	3

Course Code	Title of the course	Program Core (PCR)/ Electives (PEL)	Total Number of contact hours				Credit
			Lecture (L)	Tutorial (T)	Practical (P)	Total Hours	
CY9132	Drug design and biophysical chemistry	PEL	3	0	0	3	3
Pre-requisites		Course Assessment methods: [Continuous assessment (CA), mid-term(MT) and end term (ET)]					
CY1103, CY2105		CA+MT+ET					
Course Outcomes	CO1: Introduction to Medicinal Chemistry and Drug Discovery CO2: Concept generation on drug mechanism, classification, pharmacokinetics/pharmacodynamics CO3: Overview of conventional and advanced methods in rational drug design. CO4: Introduction to different biophysical processes inside important biomolecules. CO5: Learning of techniques used for macromolecular separations. CO4: Develop knowledge on various instrumental techniques used in Biophysical Chemistry						
Topics Covered	Drug Design: Introduction: Definition of drugs, difference between drugs and toxins, molecular targets of drugs, different Intermolecular binding interactions between drug and targets. (3 L) Enzyme inhibitor drugs: Real examples of known drugs (anti-bacterial, anti- cholesterol, anti-obesity, anti-biotic, anti-viral, anti-hypertension) with their mechanism of action. (3 L) Pharmacokinetics and pharmacodynamics in drug action: Median lethal dose LD50, Half maximal effective concentration EC50, Therapeutic index TI, Lipinski’s Rule, ADMET,						

	Bioavailability and Gastrointestinal (GI) absorption of a drug, volume of distribution Vd, Phase-I/Phase-II metabolism of drugs and example of toxicity, Role of CYP enzymes, Drug's half-life and steady-state concentration. (3 L) Rational design of drugs: Mechanism based drug design, lead compound, purpose of drug design (improvement of selectivity, improvement of ADMET profiles) with examples of real drugs, Molecular modification (Molecular association and dissociation) in drug design, High-throughput screening (HTS) method. (3 L) Computer-aided drug design: Role of computer in drug design, Basic modeling strategy, Virtual screening, homology modeling, Structure-based drug design, Molecular docking, Ligand-based drug design, 3D-QSAR, 3D-pharmacophore, Database screening, De novo drug design. (4 L) Biophysical Chemistry: Enzyme kinetics and Enzyme inhibition: Introduction of Enzyme, Enzyme-substrate Kinetics, Enzyme inhibition, Reversible inhibition, Irreversible inhibition, Competitive Inhibitor, Allosteric Inhibitor, Non-Competitive Inhibitor, Biophysical and kinetics studies of enzyme-inhibitor complex. (4 L) Molecular Forces in Biological Structures: Electrostatic interactions, hydrophobic and hydrophilic forces, hydrogen bonding interactions, ionic interactions, stabilizing forces in proteins and nucleic acids, steric interactions. (4 L) Techniques for macromolecular separation: Ion exchange, Salting-in and salting-out, dialysis, sedimentation, electrophoresis and isoelectric focusing, gel filtration and ion-exchange chromatography, HPLC. (4 L) Concept generation and applications of biophysical instruments to study the Structure-Function Inter-relationships of biomolecules: Application of spectroscopy instruments (UV-VIS, NMR, CD, Mass) in characterization of biomolecules, Application of protein crystallography and XRD in understanding the structure of proteins, Application of Isothermal Titration Calorimetry (ITC) in analyzing protein-ligand binding, Application of different gel-based assays (SDS-PAGE, Native PAGE, denaturing PAGE, Agarose), Application of multimode plate reader. (8 L)
Textbooks and/or reference materials	1. An Introduction to Medicinal Chemistry by G L Patrick (Oxford) 2. Bioinformatics and Computational Biology in Drug Discovery and Development by William T. Loging (Cambridge) 3. The organic chemistry of drug design and drug action by Richard Bruce Silverman 4. Principles of Physical biochemistry by Holde, Johnson and Ho 5. Experimental biophysical Chemistry By Copeland, R. A.

Mapping of COs (Course Outcomes) and POs (Programme Outcomes)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
CO1	3	3	3	1	1	2	1	2	3	3	3	1
CO2	3	3	3	1	1	2	1	3	2	2	2	2
CO3	3	2	3	1	1	3	3	3	3	3	3	1
CO4	3	1	3	1	1	2	1	2	2	3	1	1

Course Code	Title of the course	Program Core (PCR) /Electives (PEL)	Total Number of contact hours				Credit
			Lecture (L)	Tutorial (T)	Practical (P)	Total hours	
CY9133	Bioorganic chemistry & natural products	PEL	3	0	0	3	3
Pre-requisites		Course Assessment methods: [Continuous assessment (CA), mid- term (MT) and end term (ET)]					
CY1101, CY2105		CA+MT+ET					
Course Outcomes	CO1: To generate concept on the interdisciplinary interface lies within Chemistry and Biology. CO2: To develop knowledge on the enzyme chemistry. CO3: To understand the enzyme inhibitors and inhibition kinetics. CO4: To learn the structures, synthesis and uses of different terpenes. CO5: To know the chemistry of alkaloids. CO6: To know the chemistry of Steroids in hormones.						
Topics Covered	Bioorganic Chemistry: 18 L Enzymes: Chemical and biological catalysts. Nomenclature and classification, concept and identification of active sites by use of inhibitors, catalytic power, specificity and regulation. Different types of enzyme catalyzed reactions, Co-enzyme chemistry, Mechanism of enzyme action. <i>Enzyme models:</i> Host-guest chemistry, chiral recognition, molecular asymmetry and prochirality, biomimetic chemistry, crown ether, cryptates, cyclodextrins, calixarin. (8 L) Examples of some typical enzyme mechanisms: chymotrypsin, carboxypeptidase-A, Lysozyme. (3 L) Chemical models and mimics for enzymes, receptors, peptides, carbohydrates and other bioactive molecules, catalytic antibodies. (4 L) Enzyme catalyzed reactions: Carboxylation and decarboxylation. Isomerization and rearrangement. (3 L) Natural Products 18 L Terpenoids: Classification, isoprene rule, general methods of isolation and structure determination. Biogenetic pathway of mono and sesquiterpenes. Synthesis of α -santonin, abietic acid, gibberellic acid, menthol, caryophyllene and longifolene. (6 L) Alkaloids: Extraction, structure determination and chemistry of alkaloids special reference to nicotine, piperine, papaverine, atropine and morphine. (6 L) Steroids: Synthesis, stereochemistry and reactions of steroids. Cholesterol, and its biosynthesis, Sex hormones: Estrogens, androgens and progestin, D-Vitamins and reactions of steroid. (6 L)						

Textbooks and/or reference materials	1. Principles of Biochemistry by Lehninger 2. Biochemistry by Voet & Voet 3. Asymmetric Synthesis of Natural products By Ari M P Koskinen (Wiley) 4. Chemistry of Natural Products By S B Bhat, B. A. Nagasampagi, M. Sivakumar (Narosa). 5. Chemistry of Plant Natural Products by S. K. Talapatra & B. Talapatra (Springer)
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Mapping of COs (Course Outcomes) and POs (Programme Outcomes)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
CO1	3	3	3	3	2	2	1	3	3	1	1	2
CO2	3	3	3	3	2	2	1	3	3	1	1	2
CO3	3	3	3	3	2	2	1	3	3	1	1	2
CO4	3	3	3	2	2	2	1	3	3	2	1	2
CO5	3	3	3	2	2	2	1	3	3	2	1	2
CO6	3	3	3	2	2	2	1	3	3	2	1	2

Course Code	Title of the course	Program Core (PCR)/Electives (PEL)	Total Number of contact hours				Credit
			Lecture (L)	Tutorial (T)	Practical (P)	Total Hours	
CY9134	Advanced stereochemistry and structure-reactivity correlation	PEL	3	0	0	3	3
Pre-requisites	Course Assessment methods: [Continuous assessment (CA), mid-term (MT) and end term (ET)]						
CY1103	CA+MT+ET						
Course Outcomes	CO1: Learn about the three-dimensional structure of organic molecules, which govern their reactivity in different reactions. CO2: Advance stereochemistry helps to synthesize biological active compounds with better yield and minimum by-products. CO3: In the field of drug design & drug delivery, insecticides and pesticides, new bio-active molecules could be synthesized for better utility in field of pharmaceutical science, agriculture and material science. CO4: It helps to understand the basic knowledge in synthesis of organic molecules and to obey the guidelines of green chemistry principles. CO5: With help of knowledge in stereochemistry and structural correlation, the hurdle in stereochemical problem in industries in large scale production of polymer, drug etc. could be solved.						
Topics Covered	1. Advanced stereochemistry: Configurational analysis: Relative and absolute configuration. (4 L) 2. Determination of relative configuration: (i) Chemical correlation not affecting the chiral atom, (ii) Chemical correlation affecting bonds to the chiral atom in a known way (iii) Correlation by asymmetric synthesis: Horeaus rule, Prelog's rule,						

	Cram's rule (Felkin modification), and Sharpless rule (iv) Physical methods: NMR, MS, IR, dipole moment, ORD, CD. (8L) 3. Optical rotation and optical rotatory dispersion: Preliminary concept about linearly polarised light (LP), RCP and LCP; circular birefringence; and circular dichroism and optical rotatory dispersion; Cotton effect; ORD of ketones and Octant rule. (8 L) 4. Conformation of acyclic and cyclic system (3-8 membered rings), decalin, octalene, and bridged bicyclo systems; stability, reactivity and mechanism, Curtin Hammett principle and Winstein-Elieil equation (special emphasis on 5 and 6 membered rings with and without heteroatoms like O, S and N). (2 L) 5. Stereochemical courses of reactions: effects of $A^{1,3}$ strain in pericyclic, epoxidation hydroboration, iodolactonisation, hydrogenation reactions,, reactions of carbonyls with allyl boranes, syn and anti products in aldol condensations, reductions of carbonyl compounds, dynamic stereochemistry involved in the reactions with cyclic and acyclic molecules. (6 L) 6. Quantitative relationship between structure and reactivity: (i) Linear free energy relation: Hammett equation; Equilibrium and rate in organic reactions. (ii) Separation of polar, steric and resonance. (iii) Taft equation; (iv) Grunwald-Winstein equation. Some applications of structure-reactivity correlation study. (8 L)
Textbooks and/or reference materials	1. Stereochemistry of Carbon Compounds. Ernest L. Eliel. McGraw-Hill 2. Basic Stereochemistry of Organic Molecules, Oxford University Press: Subrata Sen Gupta 3. Stereochemistry Of Organic Compound; Principle and Applications by D. Nasipuri. 4. Stereochemistry. Conformation and Mechanism. P. S. Kalsi

Mapping of COs (Course Outcomes) and POs (Programme Outcomes)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
CO1	3	2	3	2	2	2	1	3	2	2	1	2
CO2	3	2	3	2	2	2	2	3	2	2	1	2
CO3	3	2	3	2	2	2	2	3	2	2	1	2
CO4	3	3	3	2	2	3	1	3	2	3	1	2
CO5	3	3	3	2	2	3	2	3	2	3	1	2