

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 2020-2021 Onwards)
Revision Approved in PGAC meeting on 28/08/2020**

Date: 28th August, 2020

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 yr M. Sc. course in Chemistry

Programme Educational Objectives:

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 skill to convey chemical information to all stakeholders in the society and cultivating a sense of togetherness with the whole chemical community.

Programme Outcomes:

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 analyse 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 acquaint 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 team work.
PO12	Lifelong learning and ethical application of chemical understanding for inclusive socio-economic development.

Mapping of Departmental mission statements to PEO's:

	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 PO's to PEO's

	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 yr M.Sc. in Chemistry:

Semester – I							
Sl.	Code	Subject	L	T	S	C	H
1	CY1101	Quantum Chemistry and Spectroscopy	3	1	0	4.0	4
2	CY1102	Inorganic Reaction Mechanisms and Magnetochemistry	3	1	0	4.0	4
3	CY1103	Concept of Organic Synthesis and Asymmetric Synthesis	3	1	0	4.0	4
4	CY1104	Group theory and Electronic spectroscopy of transition metal complexes	2	0	0	2.0	2
5	CY1105	Mathematical and Computational Chemistry	3	0	0	3.0	3
6	CY1151	Spectrophotometric Analysis	0	0	3	2.0	3
7	CY1152	Spectrophotometric Estimation of Cations and Anions	0	0	3	2.0	3
8	CY1153	Separation and Identification of Organic Compounds from Binary Mixture	0	0	3	2.0	3
		TOTAL	14	3	9	23.0	26
Semester – II							
Sl.	Code	Subject	L	T	S	C	H
1	CY2101	Chemical, Statistical Thermodynamics and Electrochemistry	3	1	0	4.0	4
2	CY2102	Organometallic Compounds and Bioinorganic Chemistry	3	1	0	4.0	4
3	CY2103	Pericyclic Reactions and Organic Photochemistry	3	1	0	4.0	4
4	CY2104	Structural elucidation by spectroscopic method	3	0	0	3.0	3
5	CY2151	Advanced Physical Chemistry Practical	0	0	3	2.0	3
6	CY2152	Synthesis and Characterisation of Complex Compounds	0	0	3	2.0	3
7	CY2153	Chromatographic Separation of Organic Compounds	0	0	3	2.0	3

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TOTAL			12	3	9	21.0	24
Semester – III							
Sl.	Code	Subject	L	T	S	C	H
1	CY3101	Structure and function of biomolecules	2	0	0	2.0	2
2	CY91--	Departmental elective -1	3	1	0	4.0	4
3	CY91--	Departmental elective -2	3	1	0	4.0	4
4	CY91--	Departmental elective -3	3	1	0	4.0	4
5	CY91--	Departmental elective -4	3	1	0	4.0	4
6	CY915-	Elective Practical	0	0	3	2.0	3
7	CY3151	Project- I	0	0	4	4.0	4
8	CY3152	Comprehensive Viva Voce - I	0	0	0	1.0	0
		TOTAL	14	4	7	25.0	25
		Departmental electives:					
	CY9111	Advanced Quantum Chemistry and Application of Group Theory					
	CY9112	Non-Equilibrium Thermodynamics and Biophysical Chemistry					
	CY9113	Material Chemistry and Advanced Spectroscopy					
	CY9114	Surface chemistry, electrode kinetics and Corrosion Science					
	CY9121	Advanced Green Chemistry and Analytical Chemistry					
	CY9122	Synthetic Methodology for Metal Complexes and Coordination Aggregates					
	CY9123	Small Molecule Activation and Nuclear Chemistry					
	CY9124	Group theory, Applied Electrochemistry and X-ray Structure Analysis					

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	CY9131	Application of some Important Reactions in Synthetic Organic Chemistry					
	CY9132	Natural Products and Drug Design					
	CY9133	Bioorganic Chemistry					
	CY9134	Advanced Stereochemistry and Structure-reactivity Correlation					
		Elective Practical:					
	CY9151	Advanced Physical Chemistry-II Laboratory					
	CY9152	Environmental Sample Analysis					
	CY9153	Multi Step Synthesis and Characterization of Organic Compounds					
Semester – IV							
Sl.	Code	Subject	L	T	S	C	H
1	CY4101	Chromatographic Separation and Instrumental Methods of Analysis	2	0	0	2.0	2
2	CY4102	Modern aspects of environmental chemistry	2	0	0	2.0	2
3	CY4103	Molecular modelling in chemistry	1	1	0	2.0	2
3	CY4151	Project – II	0	0	12	12.0	12
4	CY4152	Seminar & Viva voce-II	0	0	0	2.0	0
		TOTAL	5	1	12	20.0	18

Credit unit of the programme:

Semester	I	II	III	IV	TOTAL
Credit Unit	23	21	25	20	89

Curricular component:

Category	Credit	Percentage weightage
Core courses	40	45%
Elective courses	16	18%
Laboratory	14	16%
Project work	19	21%
Total	89	

FIRST 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	
CY1101	Quantum Chemistry and Spectroscopy	PCR	3	1	0	4	4
Pre-requisites		Course Assessment methods (Continuous (CT) and end assessment (EA))					
NIL		CT+EA					
Course Outcome (The students will master the following)	<ul style="list-style-type: none"> • CO1: Foundation in quantum mechanics to remind the difference between macroscopic (classical) and microscopic (quantum) world. • CO2: Understand the concept of quantization of energy and wave-particle duality • CO3: Solving Schrödinger wave equation for model quantum systems. • CO4: Understand the bases behind interaction of light and matter and account for most common spectroscopic methods. • CO5: Analyzing microscopic intramolecular interactions and properties of molecules 						
Topics Covered	Fundamentals of quantum mechanics: operators, functions, basic postulates 5 Lec Time-independent Schrödinger equation, free particle, particle in a box of various dimensions, 3 Lec Tunnelling effect 2 Lec Rigid rotation in a plane 2 Lec Rotation of diatomic molecule, spherical harmonic functions 3 Lec Harmonic oscillator 2 Lec Electronic wave function of hydrogen and hydrogen like atom 3 Lec Magnetic effect on electron movement 2 Lec Raising and lowering operators 2 Lec Many electron theory, Slater determinant, Pauli exclusion principle 2 Lec						

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	Time-dependent Schrödinger equation	2 Lec
	Atomic and molecular term symbol	2 Lec
	Atomic spectra	2 Lec
	Pure rotational and vibrational spectra of diatomic and polyatomic molecules	3 Lec
	Vibrational-rotational coupling	2 Lec
	Raman spectroscopy of molecules, concept of molecular polarizability	4 Lec
	Electronic spectra of molecules	2 Lec
Text Books, and/or reference material	<ol style="list-style-type: none"> 1. Quantum Chemistry by Levine 2. Physical Chemistry: A Molecular approach by Donald A. McQuarrie 3. Introductory quantum chemistry by A. K. Chandra 4. Chemical applications of Group theory by F. A. Cotton 5. Molecular Quantum Mechanics By Atkins and Friedman, Oxford 6. Fundamentals of molecular spectroscopy By Barnwell and McCash. 	

Mapping of CO (Course outcome) and PO (Programme Outcome)

	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 (CT) and end assessment (EA))					

NIL		CT+EA
Course Outcome (The students will master the following)	<ul style="list-style-type: none"> • 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	<p>(i) Stoichiometric mechanism, second order limiting rate constant, base hydrolysis, Effects of non-leaving ligands, proton exchange, activation parameters 5Lec</p> <p>(ii) Stereochemistry of octahedral substitution reactions, racemisation reaction (Bailar twist and Ray –Dutt twist) 4Lec</p> <p>(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. 4Lec</p> <p>(iv) Electron transfer reaction: Types of electron transfer reaction, outer sphere electron transfer process: electron transfer and reorganisation and chemical activation, potential energy diagram, Marcus theory for outer sphere cross reaction. 5Lec</p> <p>(v) Inner sphere electron transfer process: steps, rate law, types of inner sphere electron transfer process, bridging ligand, remote attack, the chemical mechanism. 4Lec</p> <p>(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 3Lec</p>	

	<p>(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 2Lec</p> <p>(viii) Microstates and derivation of Russel-Saunders Terms for p^2, d^2 and pd configuration, Spin-orbit interaction 2Lec</p> <p>(ix) Lande Interval Rule, Hole formalism and equivalency, Hund's third rule and energies of J levels, Russel-Saunders coupling of d^2 system and j-j coupling 3Lec</p> <p>(x) Thermal energy and magnetic property, Magnetic moments for different multiplet widths i.e for multiplet width large compared to KT, small compared to KT and comparable to KT 3Lec</p> <p>(xi) Magnetic properties of Lanthanides, first transition series metal ions and actinides 2Lec</p> <p>(xii) Determination of magnetic susceptibility: Gouy's method, Faraday's method, NMR method and their advantage and disadvantages, magnetic anisotropy. 3Lec</p> <p>(xiii) 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. 2Lec</p> <p>(xiv) 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. 2Lec</p>
Text Books, and/or reference material	<ol style="list-style-type: none"> 1. Inorganic chemistry, Shriver & Atkins, Oxford. 2. Concept and models of inorganic Chemistry, Douglas, Mcdeniel, Alexander, Wiley. 3. Inorganic Chemistry, Huheey, Keiter, kieter, 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 CO (Course outcome) and PO (Programme Outcome)

	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 (PCR) / 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 (CT) and end assessment (EA))					
NIL		CT+EA					
Course Outcome (The students will master the following)	<ul style="list-style-type: none"> • 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 						

	<ul style="list-style-type: none"> CO5: Concept of various aspects of methodologies used for making chiral organic molecules. This includes asymmetric induction via substrate, reagents and catalysis 	
Topics Covered	<p>Planning Organic Syntheses: Tactics, Strategy and Control; Slectivity: chemoselectivity, regioselectivity, streoselectivity</p> <p>Enolates, homoenolates, extenddenolates, nitrogen analogues of enols and enolates, acyl anion equivalents, allyl anions, specific enol equivalents, Michael reaction, σ-complexes of metals, orgnometallic reagents, aldol addition and condensation reactions, Mukaiyama aldol condnsation, control of facial reactivity, Claisen and Dieckmann condensation, conjugate addition, orthostrategy for aromatic compounds, reactions involving carbocation, carbenes and radicals, vinyl anion equivalent, allyl cation equivalent, Palladium catalysed coupling reactions, Olefination reactions – wittig and related reactions, Julia olefination. Sulfenylation and selenenylation, hydroalumination, carboalumination, ROMP and RCMP.</p> <p>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 annealation. Ring synthesis: saturated heterocycles synthesis of 3-, 4-, 5-, and 6-membered rings, aromatic heterocycles in organic synthesis</p> <p>Strategies and synthesis of some classic examples of total synthesis Periplanone B, penicillin V, reserpine, erythronolide B, thienamycin, biotin, menthol, strychnine by Woodward's method.</p>	<p>2 Lec</p> <p>10 Lec</p> <p>8 Lec</p> <p>10 Lec</p>

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	Control of stereochemistry, chiral pool, asymmetric induction via reagents, asymmetric induction via substrate, asymmetric induction via catalysis, kinetic resolution, enantiomerically pure compounds and sophisticated synthesis	8 Lec
Text Books, and/or reference material	<ol style="list-style-type: none"> 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 CO (Course outcome) and PO (Programme Outcome)

	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	2	0	0	2	2

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Pre-requisites	Course Assessment methods (Continuous (CT) and end assessment (EA))																												
NIL	CT+EA																												
Course Outcome (The students will master the following)	<p>CO1: Develop the fundamental concept of symmetry and symmetry operations.</p> <p>CO2: Develop the concept of Group theory and how molecular properties dependent on symmetry.</p> <p>CO3: Learn to construct and know the importance of Character table.</p> <p>CO4: Learn to develop Reducible and Irreducible representation and their importance.</p> <p>CO5: Basic techniques to explain the electronic spectra of transition metal complex using molecular symmetry</p> <p>CO6: Distinction of spectra of d-block and f-block transition complex</p>																												
Topics Covered	<table border="1"> <thead> <tr> <th>Topic</th> <th>Lecture</th> </tr> </thead> <tbody> <tr> <td>Fundamental concept of symmetry and probable application in chemistry</td> <td>01</td> </tr> <tr> <td>Different symmetry operations with examples</td> <td>02</td> </tr> <tr> <td>Properties of symmetry operations and concept and characteristics of Classes</td> <td>04</td> </tr> <tr> <td>Concept of Group and their properties with examples</td> <td>02</td> </tr> <tr> <td>Systematic determination of Group for a molecule</td> <td>01</td> </tr> <tr> <td>Reducible and Irreducible representation and character table</td> <td>04</td> </tr> <tr> <td>Introduction of Electronic spectroscopy of coordination compounds:</td> <td>01</td> </tr> <tr> <td>Microstates and free-ion terms for electron configurations</td> <td>02</td> </tr> <tr> <td>selection rule for electronic transition</td> <td>01</td> </tr> <tr> <td>Correlation diagrams: Orgel and Tanabe-Sugano diagrams</td> <td>02</td> </tr> <tr> <td>Jahn-Teller Distortions and Spectra:</td> <td>02</td> </tr> <tr> <td>Symmetry labels for configurations, Charge transfer spectra.</td> <td>01</td> </tr> <tr> <td>Electronic spectra of lanthanide and actinide complexes</td> <td>03</td> </tr> </tbody> </table>	Topic	Lecture	Fundamental concept of symmetry and probable application in chemistry	01	Different symmetry operations with examples	02	Properties of symmetry operations and concept and characteristics of Classes	04	Concept of Group and their properties with examples	02	Systematic determination of Group for a molecule	01	Reducible and Irreducible representation and character table	04	Introduction of Electronic spectroscopy of coordination compounds:	01	Microstates and free-ion terms for electron configurations	02	selection rule for electronic transition	01	Correlation diagrams: Orgel and Tanabe-Sugano diagrams	02	Jahn-Teller Distortions and Spectra:	02	Symmetry labels for configurations, Charge transfer spectra.	01	Electronic spectra of lanthanide and actinide complexes	03
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Electronic spectra of lanthanide and actinide complexes	03																												
Text Books, and/or reference material	<ol style="list-style-type: none"> 1. Group theory and chemistry by Bishop 2. Chemical application of group theory by F A Cotton 3. Molecular theory and group theory by R. L. Carter 4. Inorganic Chemistry, Huheey, Keiter, Medhi, Pearson education 5. Inorganic chemistry, Shriver & Atkins, Oxford 6. Concept and models of inorganic Chemistry, Douglas, Mcdeniel, Alexander, Wiley 																												

Mapping of CO (Course outcome) and PO (Programme Outcome)

	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	2
CO6	3	3	2	3	2	1	3	3	1	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	
CY1105	Mathematical and computational chemistry	PCR	3	0	0	3	3
Pre-requisites		Course Assessment methods (Continuous (CT) and end assessment (EA))					
NIL		CT+EA					
Course Outcome (The students will master the following)	<ul style="list-style-type: none"> • CO1: Foundation in basic mathematical techniques that are commonly used in chemistry. • CO2: Learn the art of scientific programming to solve chemical problems. • CO3: Write simple programs for matrix diagonalisation, solve numerical differentiation, integration and elementary differential equations. • CO4: Apply computational methods to complex problems of group theory, quantum chemistry, molecular spectroscopy, chemical kinetics and other topics. • CO5: Introduction to computational chemistry software packages for quantum mechanical and macromolecular modelling. 						

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Topics Covered	<p>Complex numbers in chemistry: representation of complex number, Euler's formula, rotational operators, periodicity, periodicity in circle, Periodicity in line, rotation in quantum mechanics. 2 Lec</p> <p>Linear algebra in quantum mechanics and symmetry operation: Vector space, determinants, matrix and linear transformations, orthogonal transformation, symmetry operations, matrix eigenvalue problem etc. 3 Lec</p> <p>Differential equation and chemistry: rate process, harmonic oscillator, wave equation for harmonic oscillator, particle in box, particle in a ring 2 Lec</p> <p>The Legendre equation, Legendre polynomials, associated Legendre polynomial, orthogonality and normalisation, Hermite equation, Laguerre equation, associated Laguerre functions, separable equation in chemical kinetics. 2 Lec</p> <p>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. 3 Lec</p> <p>Function in three dimension: spherical polar coordinates, Density functions, atomic orbitals, volume integrals, average value, Maxwell velocity distribution, Laplacian operator etc. 3 Lec</p> <p>Fourier Transform in IR and NMR spectroscopy and X ray diffraction: orthogonal expansions and Fourier analysis, Fourier series, periodicity, Fourier transforms, Fourier transform pairs and application in IR, NMR and X-rays diffraction. 3 Lec</p> <p>-----</p> <p>Introduction to Fortran/Python language: data types, integer, complex, character, logical constants and variables. Arithmetic statements, expressions, library function, relational operators. 2 Lec</p> <p>Input and output statements, I/O format statements, different types of control statements. 1 Lec</p> <p>Loop structures, subscribed variables and arrays. Writing and executing of simple example programmes. 2 Lec</p> <p>Programming exercises to chemical problems 5 Lec</p> <p>-----</p> <p>Application of Density Functional Theory using Gaussian (or similar) software in chemistry. 5 Lec</p> <p>Basic concept on macromolecule modelling software. 3 Lec</p>
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Text Books, and/or reference material	<ol style="list-style-type: none"> 1. The Chemistry Maths Books, Erich Steiner, Oxford 2. Mathematics for chemistry, Doggett and Suiclific, Logman. 3. Mathematical for Physical chemistry: F. Daniels, Mc. Graw Hill. 4. Chapman, Fortran 95/2003 for Scientists and Engineers, McGraw-Hill International Edition, New York (2006). 5. V. Rajaraman, Computer Programming in Fortran 90 and 95, PHI Learning Pvt. Ltd, New Delhi (1997). 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
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Mapping of CO (Course outcome) and PO (Programme Outcome)

	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	Spectrophotometric Analysis	PCR (Practical)	0	0	3	3	2
Pre-requisites		Course Assessment methods (Continuous (CT) and end assessment (EA) along with Viva-Voce)					
NIL		CT and Viva voce					
Course Outcome	<ul style="list-style-type: none"> • CO1: Basic concepts of spectrophotometric estimation 						

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(The students will master the following)	<ul style="list-style-type: none"> • 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	<ol style="list-style-type: none"> 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: determination of micellar aggregation number. <p>Some additional experiments as decided by the Instructor.</p>
Text Books, and/or reference material	<ol style="list-style-type: none"> 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 Sindhu 4. Practical Physical Chemistry by Viswanathan and Raghavan

Mapping of CO (Course outcome) and PO (Programme Outcome)

	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

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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	Spectrophotometric estimation of cations and anions	PCR (Practical)	0	0	3	3	2
Pre-requisites		Course Assessment methods (Continuous (CT) and end assessment (EA) along with Viva-Voce)					
NIL		CT and Viva voce					
Course Outcome (The students will master the following)	<ul style="list-style-type: none"> • 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 $\text{MnO}_4^- - \text{Cr}_2\text{O}_7^{2-}$ mixture Estimation of $\text{Cu}^{+2} - \text{Zn}^{+2}$ mixture Estimation of $\text{NO}_3^- - \text{PO}_4^{3-}$ mixture Estimation of $\text{Ti}^{+4} - \text{V}^{+5}$ mixture Estimation of dissolved oxygen and oxygen demand (BOD and COD) of Environmental Samples Some more experiments from the followings as decided by the Instructor. <ol style="list-style-type: none"> Determination of Ni in steel (Gravimetrically). Analysis of Brass and Aluminum in Bronze, Spectroscopic determination of Iron in Bauxite 						

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Text Books, and/or reference material	<ol style="list-style-type: none"> 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.
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Mapping of CO (Course outcome) and PO (Programme Outcome)

	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 (PCR) / Electives (PEL)	Total Number of contact hours				Credit
			Lecture (L)	Tutorial (T)	Practical (P)	Total Hours	
CY1153	Separation and Identification of Organic Compounds from Binary Mixture	PCR	0	0	3	3	2
Pre-requisites		Course Assessment methods (Continuous (CT) and end assessment (EA) along with Viva-Voce)					

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NIL		CT and Viva voce
Course Outcome (The students will be enriched with)	<ul style="list-style-type: none"> • 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	<ol style="list-style-type: none"> 1. Aniline and benzil (Liquid and solid) 2. Ethylacetoacetate 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) <p>In each case, separation and identification of individual components, preparation of derivatives of each component, their purification and characterization.</p>	
Text Books, and/or reference material	<ol style="list-style-type: none"> 1. <i>Vogel's</i> Textbook of practical <i>organic</i> chemistry, 5th Edition 2. <i>Advanced practical</i> chemistry, 3rd ed.: Subas C. Das 3. <i>An Advanced Course in Practical Chemistry</i>, New Central Book Agency; 3rd ed.: <u>Nad</u>, <u>Mahapatra</u> and <u>Ghoshal</u> 	

Mapping of CO (Course outcome) and PO (Programme Outcome)

	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	2
CO3	3	2	3	2	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	3	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 (CT) and end assessment (EA))					
NIL		CT+EA					
Course Outcome (The students should be able to)	<ul style="list-style-type: none"> • 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	Third law of classical thermodynamics and their applications.					02 Lec	
	Thermodynamics of ideal and non ideal binary solutions: free energy and entropy of mixing, partial molar quantities and their determination, fugacity and its determination,					04 Lec	

Gibbs-Duhem equation, Duhem- Margules equation, equilibrium constant, temperature dependent equilibrium constant.	03 Lec	
Thermodynamic excess functions. Experimental determination of activity coefficient of electrolytes and non electrolytes.	03 Lec	
Statistical Thermodynamics: Introduction to statistical thermodynamics, probability, ensembles and distribution laws. Partition function.	2 Lec	
Comparison among Maxwell-Boltzmann, Fermi-Dirac and Bose-Einstein Statistics.	2 Lec	
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 Lec	
Electronic contribution to the specific heat of diatomic gases.	1 Lec	
Solids-vibrational contribution to the specific heat of solids.	1 Lec	
Statistical treatment of Black-body radiation.	1 Lec	
Maxwell-Boltzmann probability distribution of molecular velocities and speeds.	1 Lec	
Dynamics of chemical reaction in solution-transition state theory using partition functions.	1 Lec	
Electrochemistry: Some preliminary concept of electrostatics.	3 Lec	
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 Lec	
Ion-ion interaction: Debye-Huckel-Onsagar theory of inter-ionic interaction, thickness of ionic atmosphere. Debye-Huckel limiting law.	4 Lec	
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 Lec	
Rate process approach towards ionic migration: Nernst-Planck Flux equation and its application.	2 Lec	

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	Sedimentation and ultracentrifugation, Transport of ion through membrane: Donan equilibrium Dielectric relaxation in liquid water.	2Lec 1 Lec
Text Books, and/or reference material	<ol style="list-style-type: none"> Modern electrochemistry: Ionics (Part 1); and Electroics (Part 2) by Bockris and Reddy An introduction to statistical thermodynamics by T. L. Hill Physical Chemistry: Statistical Mechanics by H. Metiu (Taylor and Francis) Physical Chemistry: Thermodynamics by H. Metiu (Taylor and Francis) Chemical Thermodynamics: Principles and Applications; and Advanced Applications by Ott and Goates 	

Mapping of CO (Course outcome) and PO (Programme Outcome)

	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 (CT) and end assessment (EA))					
NIL		CT+EA					

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Course Outcome (Students will be enriched by)	<ul style="list-style-type: none"> • 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	<p>Gr. I and Gr. II organometallics: synthesis, properties and application. 2 lec</p> <p>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 lec</p> <p>Metal carbonyl: Binary carbonyl: synthesis, bonding, spectroscopic characterisation of carbonyl compounds, 4 lec</p> <p>Substituted carbonyl: phosphine, isocyanide, nitrosyl, dinitrogen, carbenes, hydrides, and dihydrogen, η^1 alkyl, alkenyl, alkynyl, aryl, η^2 alkene, alkyne, nonconjugated diene, , butadiene, cyclobutadiene, cyclohexatriene, allyl ligand, cyclopentadiene, and cycloheptatriene, Metallocenes: synthesis, reactivity and bonding of ferrocene etc. 6 lec</p> <p>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 lec</p> <p>Cage and metal clusters. 3 lec</p> <p>Bio-inorganic:</p> <p>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 lec</p> <p>Biological ligands for metal ions: Nucleobases, nucleotides and nucleic acids (DNA, RNA) as ligands, tetrapyrrole ligands and other macrocycles (chlorin, corrin),</p>

	<p>Concept of protein structures: primary, secondary, tertiary and quaternary; Coordination of proteins and comments on enzymatic catalysis 1 lec</p> <p>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 lec</p> <p>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 lec</p> <p>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 lec</p> <p>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 lec</p> <p>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 lec</p>
Text Books, and/or reference material	<ol style="list-style-type: none"> 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 CO (Course outcome) and PO (Programme Outcome)

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	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 (CT) and end assessment (EA))					
NIL		CT+EA					
Course Outcome (The students will master the following)	<ul style="list-style-type: none"> • CO1: Understand the basic principles of pericyclic and organic photochemical reactions • CO2: Understand the classification of different types of pericyclic and organic photochemical reactions • CO3: Solving mechanism of pericyclic and organic photochemical reactions • CO4: Understand the application of pericyclic and organic photochemical reactions 						
Topics Covered	Pericyclic Reactions (18L): Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams. FMO & PMO approach. Electrocyclic reactions-conrotatory and disrotatory motions. $4n$, $4n+2$ system,						

	<p>Cycloaddition – antarafacial and suprafacial additions, $4n$ and $4n+2$ systems, $2+2$ addition of ketenes, 1,3 dipolar cycloadditions and cheletropic reactions.</p> <p>Sigmatropic rearrangements-suprafacial and antarafacial 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.</p> <p>Recent advances from current literature.</p> <p>Organic Photochemistry (20L):</p> <p>General information, Photo-chemical energy, effect of light intensity on the rate of photochemical reactions. Jablonski-diagram, photo-sensitisation and quenching.</p> <p>Norrish type-I, type-II processes, Paterno-Buchi reaction, photochemistry of unsaturated compounds.</p> <p>Types of photochemical reactions: Photo-dissociation, gas phase photolysis.</p> <p>Photochemistry of alkenes: Intramolecular reactions of the olefinic bond-geometrical isomerism, cyclisation reactions, rearrangement of 1,4- and 1,5-dienes.</p> <p>Photochemistry of Carbonyl compounds: Intramolecular reactions of carbonyl compounds saturated, cyclic and acyclic, β,γ-unsaturated and α,β-unsaturated compounds. Cyclohexadienones, Intermolecular cycloaddition reactions, dimerisation and oxetane formation.</p> <p>Aromatic compounds: Isomerisations, additions and substitutions. Miscellaneous photochemical reactions: Photo-fries reactions of anilides, photo-fries rearrangement, Barton reaction, Singlet molecular oxygen reactions.</p> <p>Photochemical formation of smog.</p> <p>Photodegradation of polymers, photosubstitution, photoreduction of ketones, photooxidation, di-π methane rearrangement, photochemistry of arenes.</p> <p>Organometallic photochemistry, photochemistry of vision.</p>
Text Books, and/or reference material	<ol style="list-style-type: none"> 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 CO (Course outcome) and PO (Programme Outcome)

	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

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	Structural elucidation by spectroscopic method	PCR	3	0	0	3	3
Pre-requisites		Course Assessment methods (Continuous (CT) and end assessment (EA))					
CY1101		CT+EA					
Course Outcome (The students will master the following)	<ul style="list-style-type: none"> • CO1: Understanding the principle and applications of UV-VIS, IR and Raman spectroscopy to elucidate the structure of different organic and inorganic molecules. • CO2: Understanding the principles of ESR spectroscopy and its application in the structure determination of inorganic complexes and reactive intermediates involved in organic and inorganic reactions. • CO3: Understanding the basic concept of Mössbauer Spectroscopy and usefulness of this technique to the studies of bonding and structures of inorganic compounds. • CO4: Understand the core concept of Mass Spectroscopic techniques and their contribution to the methods of structure elucidation of organic and inorganic species. 						

	<ul style="list-style-type: none"> CO5: 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	<p>Applications of UV-VIS, IR and Raman spectroscopy to elucidate the structure of different organic and inorganic molecules.</p> <p>ESR spectroscopy: Hyperfine coupling, Spin polarization for atoms and transition metal ions, Spin-orbit coupling and significance of g-tensors, application to transition metal complexes including free radicals.</p> <p>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 including those of intermediate- spin, ii) Sn^{II} and Sn^{IV} compounds, nature of M-L bond, coordination number and structure and iii) detection of oxidation states.</p> <p>Mass Spectroscopy Generation of ions and detection; EI, CI, FD, FAB, plasma desorption etc; fragmentation pattern in EI, GC-MS, MS-MS, LC-MS. Application of UV, IR, NMR and MS in structure elucidation.</p> <p>NMR Spectroscopy Long-range spin-spin interaction. Interpretation of non-first order NMR; double resonance, Lanthanide shift reagent, spin-tickling, INDOR, NOE, effect of solvents (aliphatic and aromatic), preliminary idea on ¹⁹F, ³¹P, ¹⁴N, ¹⁵N, ¹⁷O. NMR of solids, NMR imaging. ¹³C NMR Spectroscopy: Introduction, theory, instrumentation, chemical shift, coupling constants, application in organic molecules.</p>	<p>4 Lec</p> <p>4 Lec</p> <p>4 Lec</p> <p>8 Lec</p> <p>15 Lec</p>
Text Books, and/or reference material	<ol style="list-style-type: none"> Elements of magnetochemistry: Dutta and Shyamal Fundamental concept of Inorganic Chemistry (Vol-7): A. K. Das Structural methods in molecular inorganic chemistry: Rankin, Mitzel, Mosrision 	

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	<p>4. NMR spectroscopy (Basic Principles, concepts and application in chemistry): H. Gunther</p> <p>5. Spectrometric identification of organic compounds: Robert Silverstein</p> <p>6. Organic spectroscopy: Kemp</p> <p>7. Structural methods in Inorganic Chemistry : Ebsworth, Rankin and Cradock</p>
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Mapping of CO (Course outcome) and PO (Programme Outcome)

	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
CO4	3	3	3	3	3	3	3	3	3	3	3	3
CO5	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	
CY2151	Advanced Physical Chemistry Practical	PCR			3	3	2
Pre-requisites		Course Assessment methods (Continuous (CT) and end assessment (EA))					
CY1151		CT and viva-voce					
Course Outcome (The students will	<ul style="list-style-type: none"> 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. 						

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master the following)	<ul style="list-style-type: none"> • 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	<ol style="list-style-type: none"> 1. Determination of isoelectric pH of gelatin. 2. Rate constant of alkaline hydrolysis of crystal violet 3. Salt effect on the rate of alkaline hydrolysis of crystal violet 4. Solvent effect on the rate of alkaline hydrolysis of crystal violet 5. Micellar effect on the rate of alkaline hydrolysis of crystal violet 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.
Text Books, and/or reference material	<ol style="list-style-type: none"> 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 Sindhu 4. Practical Physical Chemistry by Viswanathan and Raghavan

Mapping of CO (Course outcome) and PO (Programme Outcome)

	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 Characterisation of Complex Compounds	PCR			3	3	2
Pre-requisites		Course Assessment methods (Continuous (CT) and end assessment (EA))					
NIL		CT+ Viva voce					
Course Outcome (The students will master the following)	Course outcome accounts of <ul style="list-style-type: none"> • CO1: Coordination complex synthesis maintaining molarity. • CO2: Crystallization techniques to purify the synthesized materials. • CO3: Decomposition and estimation of metal ion(s) using spectrophotometry. • 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 and their characterization using various spectroscopic methods. Estimation of metal ion of suitable complexes.						
Text Books, and/or reference material	1. Advanced Inorganic Experiments, By G. N. MUKHERJEE.						

Mapping of CO (Course outcome) and PO (Programme Outcome)

	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

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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	0	0	3	2.0	3
Pre-requisites		Course Assessment methods (Continuous (CT) and end assessment (EA))					
NIL		CT+ Viva voce					
Course Outcome (The students will master the following)	<ul style="list-style-type: none"> • 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	<p>Thin Layer Chromatography</p> <p>Determination of R_f values and identification of organic compounds.</p> <p>Preparation and separation of DNP derivatives of carbonyl compounds</p> <p>Separation of a mixture of dyes using cyclohexane and ethyl acetate (8.5:1.5).</p> <p>Paper Chromatography: Ascending and Circular</p> <p>Determination of R_f values and identification of organic compounds.</p> <p>Separation of a mixture of amino acids</p> <p>Separation of sugars</p> <p>Column Chromatography:</p> <p>Separation of Fluorescein and methylene blue</p> <p>Separation of aniline and <i>N,N</i> dimethyl aniline</p> <p>Separation of Lycopene and β-carotene</p>						

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	Demonstration of chromatographic separation by GC & HPLC.
Text Books, and/or reference material	1. Fundamentals of analytical chemistry, Skoog, West, Holler and Crouch, 8th edition, Thomson

Mapping of CO (Course outcome) and PO (Programme Outcome)

	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	
CY3101	Structure and function of biomolecules	PCR	2	0	0	2	2
Pre-requisites		Course Assessment methods (Continuous (CT) and end assessment (EA))					
NIL		CT+EA					
Course Outcome (The students will master the following)	<ul style="list-style-type: none"> • 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	<p>Cell Structure and Functions: Structure of prokaryotic and eukaryotic cells, intracellular organelles and their functions, Overview of metabolic process catabolism and anabolism. ATP – the biological energy currency. Origin of life – chemical evolution and rise of living systems. Introduction to biomolecules, building blocks of biomolecules</p> <p>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,</p>					5 Lec 8 Lec	

	<p>glycolysis, glycogenesis and glycogenolysis, gluconeogenesis, pentose phosphate pathway</p> <p>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.</p> <p>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.</p> <p>Amino acid metabolism – degradation and biosynthesis of amino acids, sequence determination: chemical/ enzymatic/ mass spectral, racemization/ detection.</p> <p>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.</p> <p>Molecular mechanics: Molecular potentials, bonding potentials, non-bonding potentials, electrostatic interactions, dipole-dipole interactions, van der Waal's interaction, hydration and hydrophobic effect. Hydrogen bonds and their effect on stabilizing interactions in macromolecules. Steric interactions, cooperative allosteric effect.</p>	<p>6 Lec</p> <p>8 Lec</p> <p>5 Lec</p> <p>5 Lec</p>
Text Books, and/or reference material	<ol style="list-style-type: none"> 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 CO (Course outcome) and PO (Programme Outcome)

	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	
CY9111	Advanced Quantum Chemistry and Application of Group Theory	PEL	3	1	0	4	4
Pre-requisites		Course Assessment methods (Continuous (CT) and end assessment (EA))					
CY1101, 1104		CT+EA					
Course Outcome (The students will master the following)	CO1: Different time dependent and time independent approximation methods to solve various molecular problems when Schrödinger wave equation cannot be solved exactly. CO2: Born-Oppenheimer approximation to separate nuclear and electronic components from molecular Hamiltonian. CO3: Detailed understanding on the interaction of radiation with matter and selection rules for transition among different molecular energy levels. CO4: Hückel theory in conjugated system and its applications CO5: Development of concept of GOT, SALC from symmetry aspect and their application CO6: Applications of group theory in spectroscopy, chemical bonding						
Topics Covered	Variation and time independent perturbation theory (nondegenerate and degenerate cases): Application towards different systems. 08 lec						

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	<p>Antisymmetric and exclusion principle, Slater determinantal wave function, spin-orbital interaction: LS and JJ coupling, Term symbol and spectroscopic states. 04 lec</p> <p>Molecules and chemical bonding:</p> <p>Born-Oppenheimer approximation: MO and VB treatment of diatomic molecules. 04 lec</p> <p>Directed valence and hybridization in simple polyatomic molecules. Idea of self-consistent field. 04 lec</p> <p>Time dependent perturbation theory: Transition dipole moment. Fermi's Golden rule. Einstein's coefficients for induced and spontaneous emission. 04 lec</p> <p>Hückel theory of conjugated systems. Bond order and charge density calculations. Applications to ethylene, butadiene, cyclopropenyl radical, cyclobutadiene. 06 lec</p> <p>Group theory: GOT, SALC: Their applications: representation of molecular orbitals and shape 04 lec</p> <p>Application of Group theory in developing selection rules in spectroscopy 02 lec</p> <p>Application in crystal field theory and molecular orbital theory 02 lec</p> <p>Concept of orbital symmetry and application in chemical bonding 03 lec</p> <p>Probability and efficiency of transitions in IR and Raman spectroscopy 03 lec</p>
Text Books, and/or reference material	<ol style="list-style-type: none"> 1. Quantum Chemistry by Levine 2. Physical Chemistry: A Molecular approach by Donald A. McQuarrie 3. Introductory quantum chemistry by A. K. Chandra 4. Group theory and chemistry by Bishop 5. Chemical application of group theory by F A Cotton 6. Molecular theory and group theory by R. L. Carter

Mapping of CO (Course outcome) and PO (Programme Outcome)

	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

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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				Credit
			Lecture (L)	Tutorial (T)	Practical (P)	Total Hours	
CY9112	Non-Equilibrium Thermodynamics and Biophysical Chemistry	PEL	3	1	0	4	4
Pre-requisites		Course Assessment methods (Continuous (CT) and end assessment (EA))					
CY2101		CT+EA					
Course Outcome (The students will know:)	<ul style="list-style-type: none"> • CO1: difference between equilibrium and non-equilibrium thermodynamics and the significance of the later. Understanding of different concepts and theories in non-equilibrium thermodynamics. • CO2: Concept on stationary state, coupled transfer (like diffusion and electric charge, heat and electric charge), entropy production and application of these concepts. • CO3: Learning of different biophysical processes inside important biomolecules • CO4: Develop knowledge on various instrumental techniques used in Biophysical Chemistry 						
Topics Covered	<p>Non-equilibrium thermodynamics: 15 Lec</p> <p>Postulates and methodologies, forces and fluxes, linear laws, Gibbs equation, Onsagar reciprocal theory. Curie-Prigogine principle, diffusion, effusion, sedimentation, chemical affinities, membrane properties. Thermoelectric effects.</p> <p>Stationary states: time variation of entropy production, minimum entropy production, stability of stationary state. Fluctuation.</p> <p>Biophysical Chemistry:</p>						

	<p>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, Enzymes as drug targets, pharmacokinetics, pharmacodynamics, ADMET profile, examples of enzyme targeted drug discovery.</p> <p>Nucleic acid structure and therapeutics: Biophysical of nucleic acid, sensing and anti-sensing of nucleotides, interactions between strands of nucleic acid, strand-displacement assay as sensor.</p> <p>Techniques for macromolecular separation: Ion exchange, gel filtration chromatography, sedimentation, electrophoresis and isoelectric focusing,</p> <p>Bio-analytical Chemistry:</p> <p>(i) Applications of X-ray, AFM, UV-Vis, CD, fluorescence, NMR in characterization of biological macromolecules.</p> <p>(ii) Applications of the FRET and AUC to study conformational dynamics of protein and nucleoprotein complexes.</p> <p>(iii) Applications of UV-Vis and ITC to study the kinetics and thermodynamics of protein-ligand binding.</p> <p>(iv) Application of different gel-based assays (SDS-PAGE, Native PAGE, denaturing PAGE, Agarose) to determine nucleic acid stability and DNA repair process.</p> <p>(v) Application of pull-down method and sequencing to analyze protein-DNA interaction.</p>	<p>5 Lec</p> <p>2 Lec</p> <p>3 Lec</p> <p>10 Lec</p>
Text Books, and/or reference material	<ol style="list-style-type: none"> 1. Introduction to Thermodynamics of Irreversible Processes by I. Prigogine 2. Principles of Physical biochemistry by Holde, Johnson and Ho 3. Experimental biophysical Chemistry By Copeland, R. A. 	

Mapping of CO (Course outcome) and PO (Programme Outcome)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
CO1	3		2	2				3	2	1	1	
CO2	3		2	2				3	2	1	1	
CO3	3	3	3	2	2	3	2	3	2	2	2	1
CO4	3	3	3	2	3	2	2	3	2	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	
CY9113	Material chemistry and advanced spectroscopy	PEL	3	1	0	4	4
Pre-requisites		Course Assessment methods (Continuous (CT) and end assessment (EA))					
CY1101, 2101, 2104		CT+EA					
Course Outcome (The students will master the following)	<ul style="list-style-type: none"> • CO1: Fundamentals of laser and application in science and industry • CO2: Properties and applications of semiconductors, superconductors, nanomaterials and many other industrially relevant materials. • CO3: Physical chemistry of polymer. • CO4: science behind many modern spectroscopic methods and applications 						
Topics Covered	Laser: Fundamentals and applications, Time resolved laser spectroscopy (picosecond, femtosecond laser spectroscopy) and its application to investigate different photophysical processes like photo-dissociation, photoisomerization (with a reference to vision process) and related topics. 07 lec Free electron gas theory of solids: Fermi level, density of states. 04 lec Semiconductor and superconductor: properties and applications. 03 lec						

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	<p>Physical Chemistry of polymers: Kinetics of polymerization, thermodynamics of macromolecular systems. Determination of molar masses and studies of conformations and morphologies, thermomechanical properties of polymers. Sedimentation and ultracentrifugation of macromolecules. 07 lec</p> <p>Fluorescence sensor, solar and fuel cell, supercritical fluid, ionic liquids, Nanomaterials. 05 lec</p> <p>Kinetics of diffusion controlled reactions, photophysical quenching processes, excited state pH and acidity constant, Charge-transfer processes (Marcus theory).</p> <p>Experimental methods to observe kinetics of fast reactions in solution: stopped flow and relaxation methods. 06 lec</p> <p>Advanced spectroscopy: NMR, X-ray photoelectron spectroscopy, Auger spectroscopy, Mossbouer spectroscopy, SEM 06 lec</p>
Text Books, and/or reference material	<ol style="list-style-type: none"> 1. Modern spectroscopy by J M Hollas 2. Solid state chemistry and its application by West 3. Chemical Kinetics by K. J. Laidler 4. Organic and physical Chemistry of Polymers by Y Gnanou and M. Fontaanille, Wiley. 5. Atkin's Physical Chemistry by P Atkins and J de Paula (7th ed.) 6. Fundamentals of molecular spectroscopy By Banwell and McCash 7. Fundamentals of photochemistry By Rohatgi and Mukherjee.

Mapping of CO (Course outcome) and PO (Programme Outcome)

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

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	

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CY9114	Surface Chemistry, Electrode kinetics and corrosion science	PEL	3	1	0	4.0	4
Pre-requisites		Course Assessment methods (Continuous (CT) and end assessment (EA))					
CY2101		CT+EA					
Course Outcome (The students will master the following)	<ul style="list-style-type: none"> • 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	<p>Surface Chemistry:</p> <p>BET, Harkins-Jura and Gibbs adsorption isotherms, surface tension and surface pressure, contact angle: interfacial tension, Hysteresis. 4 lec</p> <p>Micelles and microemulsions: Phase diagram of micellar system. Mass action model and pseudophase model for non-ionic and ionic micelles. Relationship between thermodynamic properties for micellization with CMC. 3 lec</p> <p>Estimation of fraction of counter ion, aggregation number and solvation for micelles.</p> <p>Concept of reverse micelle and microemulsion. Packing factor. 4 lec</p> <p>Ion transport across membrane: Donnan effect. 2 lec</p> <p>Electrical double layer, Zeta potential, Stability of colloids, Electrokinetic effect (electroosmosis and electrophoresis) 3 lec</p>						

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	<p>Derivation of Butler-volmer equation, Study of the kinetics of different electrode reactions (including elucidation of reaction mechanism). Numerical problems. 4 lec</p> <p>Different forms of corrosion: properties and remedial methods. 4 lec</p> <p>Tafel relation and mixed potential theory, Concept of exchange and limiting current density. 3 lec</p> <p>Potentiodynamic polarization and electrochemical impedance spectroscopic methods to determine rate of corrosion. 4 lec</p> <p>Corrosion control: Cathodic (impressed current method and metallic coating) and anodic control methods. Numerical problems. 4 lec</p> <p>Application of corrosion inhibitors including green inhibitors 2 lec</p> <p>High temperature corrosion 3 lec</p>
Text Books, and/or reference material	<ol style="list-style-type: none"> 1. Modern Electrochemistry 2A - Fundamentals of Electrodeics 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 CO (Course outcome) and PO (Programme Outcome)

	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	3	2
CO5	3	3	3	2	2	2	1	3	3	3	3	2

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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 chemistry and Analytical Chemistry	PEL	3	1	0	4.0	4
Pre-requisites		Course Assessment methods (Continuous (CT) and end assessment (EA))					
NIL		CT+EA					
Course Outcome (The students will master the following)	<ul style="list-style-type: none"> • 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 Lecture 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 Lecture 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.						

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	<p>Principle of Analysis for Air and Water samples: 10 Lecture</p> <p>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. Measurement of DO, BOD and COD. Pesticides as water pollutants analysis.</p> <p>Monitoring and analysis of air: Monitoring technique through high volume sampler, SPM and RPM sampler. Measurement and analysis of SPM, RPM, SOX and NOX.</p> <p>Air and water pollution laws and standards.</p>
Text Books, and/or reference material	<ol style="list-style-type: none"> Green Chemistry, An Introductory Text By Mike Lancaster, RSC publications. Handbook on Green Analytical Chemistry By Miguel de la Guardia, Salvador Garrigues, Wiley. Innovations in Green Chemistry and Green Engineering By Paul T. Anastas, Julie Beth Zimmerman, Springer publications. Alternative Solvents for Green Chemistry By Francesca M Kerton, Ray Marriott, RSC publications. Environmental Chemistry with Green Chemistry By Asim Kumar Das, Books and Allied (P) Ltd.

Mapping of CO (Course outcome) and PO (Programme Outcome)

	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	3
CO5	3	3	3	2	2	3	1	3	3	3	3	3

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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 Coordination Aggregates	PEL	3	1	0	4	4
Pre-requisites		Course Assessment methods (Continuous (CT) and end assessment (EA))					
CY2102		CT+EA					
Course Outcome (The students will master the following)	<ul style="list-style-type: none"> • 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 Nitrogen Based Ligand: N ₂ as Ligand, Reactivity of Bound N ₂ , Macrocyclic Amines, Polyimines, Porphyrin, Polypyrazolylborate Ligand, Hydroxylamido Ligand, Schiff Base Ligand, Azide and Other Anionic Ligand Phosphorus Based Ligands: Phosphine as Ligand, Monophosphines, Diphosphines, Polydentate Phosphines, Phosphate Ligands, Heterocyclic Phosphorus Ligands, Dialkyl- and Diarylphosphido Ligands 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					6 Lec 5 Lec 4 Lec 5 Lec	

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	<p>Sulphur Based Ligand: Thiolates, Disulphides, Thioethers, Sulphur Oxide, Dithiocarbamates, 1,2-Dithiolenes 3 Lec</p> <p>Metal-Organic Frameworks 2 Lec</p> <p>Supramolecular Chemistry: Introduction, Host-Guest Chemistry, SelfAssembly, Supramolecular Building Blocks and Spacer, Driving Forces for the Formation of Supramolecular Structure 2 Lec</p> <p>Spatial Relationships between Host and Guest, Classification Of Host-Guest Compounds, General Introduction To Podand, Coronand, Spherand, Coronand-Podand Hybrid, Cryptands 2 Lec</p> <p>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 Lec</p> <p>Chiral Crown Ethers, Proton Ionisable Crown Ethers, Diester Crown Ethers, Synthesis of Lariat Ethers 2 Lec</p> <p>Synthesis of Calix[n] Arenes, Chiral Calix[n] Arenes, Introduction of Functional Groups in Calix[n] Arenes, Reactions at Upper Rim of Calixarene 3 Lec</p> <p>Selectivity of Cation Complexation, Cation Binding by Crown Ethers, Cation Binding by Lariat Ethers, Cation Binding by Cryptands, Thermodynamic Effect of Binding 4 Lec</p>
Text Books, and/or reference material	<ol style="list-style-type: none"> 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 CO (Course outcome) and PO (Programme Outcome)

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	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 and Nuclear Chemistry	PEL	3	1	0	4	4
Pre-requisites		Course Assessment methods (Continuous (CT) and end assessment (EA))					
CY1102, 2014		CT+EA					
Course Outcome (The students will master the following)	<p>Course outcome accounts of</p> <ul style="list-style-type: none"> • CO1: Diversified biological roles of Nitric Oxide (NO) and the NO donor drugs. • CO2: Enemark-Feltham {MNO}ⁿ notation of metal nitrosyls and their spectroscopic and structural properties to elucidate structure-function relationship. • CO3: Active site structure and role of denitrifying bacteria responsible for nitrite (NO₂⁻), nitric oxide (NO) and nitrous oxide (N₂O) reduction to N₂ sustaining global N₂ cycle. • CO4: Details of structure function of Metalloenzymes responsible for N₂ fixation, reverse process of denitrification. • CO5: Basics of nuclear chemistry, the nuclear spin (I), quadrupole moment (Q) and ellipticity of the nuclides and numerical problems. 						

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	<ul style="list-style-type: none"> • CO6: The concepts and working principle of three spectroscopy such as Nuclear Magnetic Resonance (NMR), Electron Paramagnetic Resonance (EPR) and Mössbauer spectroscopy (specifically the last two) those are related to nuclear spin and the s-electron density of the nuclides.
<p>Topics Covered</p>	<p>Importance of NO as ligand and its diverse roles in biology, NO Synthase enzyme and NO donors including metal nitrosyls, MO diagram of NO, Bonding nature of NO, Enemark-Feltham {MNO}ⁿ notation, Spectroscopic and structural properties of various {MNO}ⁿ species, NO detection methods, Electrophilic and nucleophilic reactivity on metal activated NO moiety 8 Lec</p> <p>Nitrite and Nitrous Oxide Reductase, their active site structures and catalytic activity and impact on Atmospheric Nitrogen Cycle 8 Lec</p> <p>The N₂ fixation, Biological N₂ reduction using FeMo cofactor and Models, Chatt Cycle, Electrocatalytic reduction using low-valent tungsten (W), Mo(III) mediated N₂ reduction system, cleavage of N₂, Mo-N₂ complexes, N₂Redcution Mechanisms, Nitrogenase-related transformations 8 Lec</p> <p>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 nucleon and magnetic properties, Nordheim's rules, Nuclear magnetic resonance (NMR) 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 5 Lec</p> <p>Nuclear resonance or recoilless absorption and Mössbauer Spectroscopy; Recoiling Frequency shift, Frequency broadening and Doppler effect, Characteristics of Mössbauer nuclides and related Decay scheme, Quadrupole splitting, Isomer shift and its application to assign the spin states. 3 Lec</p> <p>Nuclear shell model, magic number and periodicity of nuclear properties, liquid drop model. 1 Lec</p> <p>Detection and measurement of radioactivity, Preparation of radio-isotopes, Cow and milk systems, Applications of radio-isotopes as tracers such as for chemical investigation, physico-chemical applications, age determination, medical applications, agricultural and industrial applications etc. 3 Lec</p>

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Text Books, and/or reference material	<ol style="list-style-type: none"> 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. Arnikaar, 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.
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Mapping of CO (Course outcome) and PO (Programme Outcome)

	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
CO5	3	3	3	2	2	3	1	3	2	3	1	1
CO6	3	3	3	3	2	3	1	3	2	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	
CY9124	Group theory, applied electrochemistry and X-ray structure analysis	PEL	3	1	0	4	4

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Pre-requisites	Course Assessment methods (Continuous (CT) and end assessment (EA))
CY1104, 2101	CT+EA
Course Outcome (The students will master the following)	<ul style="list-style-type: none"> • CO1: matrix representation of operator, formation of character tables of different point group and its application in analyzing vibration and electronic spectroscopy of complex molecules. • CO2: Use of character table, symmetry and projection operator to learn hybridization and formation of SALC and LCAO which enable to understand bonding in molecules. • CO3: foundation in different electrochemical methods like cyclic voltammetry, coulometry and associated techniques to analysis inorganic complexes and evaluating kinetic processes occurring at the electrodes-solution interface. • CO4: knowledge of unit cell, symmetry and space group of different crystal. • CO5: idea of reciprocal lattice and its importance in structure elucidation of inorganic complexes using X-ray diffraction technique. • CO6: understanding of the working principle of various electrochemical instruments as well as X-ray diffractometer.
Topics Covered	<p>Group theory: representation of groups, techniques and relationships for chemical applications, symmetry and chemical bonding, equation of wave functions, vibrational spectroscopy, transition metal complexes 12 lec</p> <p>Electrochemistry: fundamental of electrode reaction, basic equipment for electrochemical measurements, voltammetric techniques, coulometric techniques, electrochemical behaviour of transition metal complexes, metal complexes containing redox active ligands 13 lec</p> <p>X-ray structure determination: Diffraction of X-rays, Lattices, Plane and indices, X-ray diffraction. The reciprocal lattice, Brag's law in reciprocal lattice, crystal symmetry and space group, data collection, Intensity of data collection, theory of structure factors, and Fourier syntheses. 13 lec</p>
Text Books, and/or reference material	<ol style="list-style-type: none"> 1. Electrochemical Methods: Fundamentals and Applications By Bard and Faulkner 2. Chemical applications of Group theory by F. A. Cotton 3. Molecular theory and group theory by R. L. Carter 4. Inorganic Electrochemistry: Theory, practice and application By P Zanello (RSC) 5. X-ray Crystallography By William Clegg (Oxford)

Mapping of CO (Course outcome) and PO (Programme Outcome)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
CO1	3	3	3	3	2	2	2	3	2	2	1	1
CO2	3	3	3	2	2	2	3	3	2	1	1	1
CO3	3	3	3	3	2	3	1	3	3	2	1	1
CO4	3	3	3	3	1	3	3	3	2	1	1	1
CO5	3	3	3	3	1	3	3	3	2	1	1	1
CO6	3	3	3	3	2	3	3	3	2	1	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	Application of some important reactions in synthetic organic chemistry	PEL	3	1	0	4	4
Pre-requisites		Course Assessment methods (Continuous (CT) and end assessment (EA))					
CY1103		CT+EA					
Course Outcome (The students will master the following)	<ul style="list-style-type: none"> • CO1: Understanding the mechanistic details of hydroboration reactions of carbon-carbon double and triple bonds and their application towards the formation of C-C, C-N and C-halogen bonds • CO2: Understanding the dissolving metal reduction method of benzenoid systems using Birch reduction condition and their application in some of the natural product syntheses • CO3: Understanding the method of Carbon-carbon double bond formation via Wittig reaction, its modifications and the factors affecting the stereochemistry of the reactions 						

<p>Topics Covered</p>	<p>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 (IpcBH₂), isomerisation of alkenes via hydroboration reactions, Carbon-Nitrogen, Carbon-halogen bond formation, synthesis of cyclopropyl, cyclobutyl derivatives and bicyclo compounds</p> <p>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; single electron transfer system (SET), application in natural product synthesis with special emphasis on Gibberalic acid.</p> <p>Wittig reactions or chemistry of Ylide: synthesis of phosphoylide; Stereo-chemical outcome of wittig reactions and their dependent factors. Stereo-selectivity in case of stabilised 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 sulphur ylide; Regio selective and stereoselective reaction with stabilized and non-stabilized sulphur ylides</p>	<p>12 Lec</p> <p>12 Lec</p> <p>12 Lec</p>
<p>Text Books, and/or reference material</p>	<ol style="list-style-type: none"> Advanced Organic Chemistry : F.A. Carey & R.J. Sundberg. Classics in Total Synthesis: Targets, strategies and Methods: K.C. Nicolaou & E.J. Sorensen Modern Methods in Organic Synthesis : W. Carruthers Organic Synthesis: Michael B. Smith 	

Mapping of CO (Course outcome) and PO (Programme Outcome)

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	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

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	Natural Products and Drug Design	PEL	3	1	0	4	4
Pre-requisites		Course Assessment methods (Continuous (CT) and end assessment (EA))					
NIL		CT+EA					
Course Outcome (The students will master the following)	<ul style="list-style-type: none"> • CO1: Understanding the importance of natural products • CO2: Learning of the structure, synthesis and uses of different Terpenes • CO3: Know the chemistry of Steroids in hormones • CO4: Develop knowledge on the chemical structure, synthesis of different natural pigments • CO5: Concept generation on rational drug design and drug classification • CO6: Introduction to drug manufacturing done in pharmaceutical industries • CO7: Fundamental use of computer in drug design and discovery 						
Topics Covered	Terpenes: Structural studies on sesquiterpenes, diterpenes, triterpenes and carotenoids; chemistry of carryophyllene, abietic acid, beta-amyrin, alpha and beta-carotenoids					9 Lec	
	Steroids and Prostanoids: Reaction and synthesis of steroids, sources of steroid hormones; diosgenin, hecogenin, etc., structure and synthesis of prostanoids					9 Lec	
	Natural Pigments: General methods of isolation, structure elucidation and synthesis of anthocyanins, flavones, flavones,					9 Lec	

	<p>isoflavones, aurone, chalcone, xanthone and their chemical interconversions</p> <p>Drug Design:</p> <p>Drug definition, Concepts of LD50 and ED50, introduction to rational approach to drug design, physical and chemical factors associated with biological activities, structure-activity relationship, and mechanism of drug action. 9 Lec</p> <p>Classification of drugs: Based on structure or pharmacological basis with examples. Antineoplastic agents, cardiovascular drugs, local anti-infective drugs, psychoactive drugs, antibiotics (including vancomycin).</p> <p>Industrial synthesis of important drugs.</p> <p>Modelling: Molecular modeling, conformational analysis, qualitative and quantitative structure-activity relationship.</p>
Text Books, and/or reference material	<p>7. Medicinal Chemistry: An introduction By Gareth Thomas (Wiley)</p> <p>8. Asymmetric Synthesis of Natural products By Ari M P Koskinen (Wiley)</p> <p>9. Chemistry of Natural products By S B Bhat, B A Nagasampagi, M Sivakumar (Narosa)</p> <p>10. An Introduction to Medicinal Chemistry by G L Patrick (Oxford)</p> <p>11. Bioinformatics and Computational Biology in Drug Discovery and Development by William T. Loging (Cambridge)</p>

Mapping of CO (Course outcome) and PO (Programme Outcome)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
CO1	3	1	1	1	1	2	1	2	3	3	1	1
CO2	3	1	1	1	1	2	1	3	2	2	2	1
CO3	3	2	1	1	1	3	1	3	3	3	1	1
CO4	3	1	1	1	1	2	1	2	2	3	1	1
CO5	3	3	3	3	3	3	1	3	3	1	3	1
CO6	3	3	3	3	3	3	1	3	3	1	3	1
CO7	3	3	3	3	3	3	3	3	3	1	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	
CY9133	Bioorganic Chemistry	PEL	4	0	0	4	4
Pre-requisites		Course Assessment methods (Continuous (CT) and end assessment (EA))					
NIL		CT+EA					
Course Outcome (The students will master the following)	<ul style="list-style-type: none"> • CO1: Generation of concept on the interdisciplinary interface lies within Chemistry and Biology • CO2: Learn the Chemistry of Nucleic acids (DNA, RNA) • CO3: Develop knowledge on the enzyme chemistry • CO4: Introduction of enzyme inhibitors and inhibition kinetics 						
Topics Covered	<p>Nucleoside, nucleotides and Nucleic acids: Basic concept and importance; Bio-synthesis of purine and pyrimidine nucleotides, synthesis of adenosine, Guanosine; Nucleotides: synthesis of adenylytic acid (AMP), Guanylic acid (GMP), uridylic (UMP) acid and cytidilic acid; Cell structure, DNA structure and genetic material, replication and transcription of DNA, RNA and protein synthesis, genetic material and genetic code</p> <p>Enzyme Chemistry:</p> <p>Enzymes: Chemical and biological catalysts. Nomenclature and classification, concept and identification of active sites by use of inhibitors, catalytic power, specificity and regulation. Examples of some typical enzyme mechanisms for chymotripsin, and carboxypeptidase-A.</p> <p>Different types of enzyme catalyzed reactions, Co-enzyme chemistry. Enzyme models: Host-guest chemistry, chiral</p>					<p>8 Lec</p> <p>12 Lec</p>	

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	<p>recognition, molecular asymmetry and prochirality, biomimetic chemistry, crown ether, cryptates, cyclodextrins, calixarin</p> <p>12 Lec</p> <p>Bioorganic Chemistry:</p> <p>Enzyme kinetics: MichaelisMenten and Lineweaver-Burk plots, reversible and irreversible inhibition.</p> <p>Mechanism of enzyme action: Typical enzyme mechanism for ribonuclease, lysozyme. Chemical models and mimics for enzymes, receptors, peptides, carbohydrates and other bioactive molecules, catalytic antibodies- Design, synthesis and evaluation of enzyme inhibitors.</p> <p>Enzyme catalyzed reactions: Carboxylation and decarboxylation. Isomerization and rearrangement.</p>
Text Books, and/or reference material	<ol style="list-style-type: none"> Principles of Biochemistry by Lehninger Biochemistry by Voet & Voet An Introduction to Medicinal Chemistry by G L Patrick (Oxford)

Mapping of CO (Course outcome) and PO (Programme Outcome)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
CO1	3	2	3	3	3	2	2	3	3	1	3	1
CO2	3	3	3	2	3	3	2	3	3	1	2	1
CO3	3	2	2	3	3	3	1	3	3	1	1	1
CO4	3	3	3	3	3	2	2	2	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	
CY9134	Advanced Stereochemistry	PEL	3	1	0	4	4

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	and Structure-reactivity Correlation						
Pre-requisites		Course Assessment methods (Continuous (CT) and end assessment (EA) and Viva-Voce)					
CY1103		CT+EA					
Course Outcome (The students will be enriched with stereochemistry knowledge)		<ul style="list-style-type: none"> • CO1: Learn about the three dimensional structure of organic molecules, which govern their reactivity in different reactions. • CO2: Advance stereochemistry helps to synthesise 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 synthesised 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 guide lines of green chemistry principle. • 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		<p>1. Advanced stereochemistry: Configurational analysis: Relative and absolute configuration. 2 Lec.</p> <p>2. Determination of relative configuration:</p> <p>(i) Chemical correlation not affecting the chiral atom,</p> <p>(ii) Chemical correlation affecting bonds to the chiral atom in a 'known way'</p> <p>(iii) Correlation by asymmetric synthesis: Horeaus rule, Prelog's rule, Cram's rule (Felkin modification), and Sharpless rule,</p> <p>(iv) Physical methods: NMR, MS, IR, dipole moment, ORD, CD. 8 Lec.</p> <p>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 Lec.</p>					

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	<p>4. Conformation of acyclic and cyclic system (3-8 membered rings), decalin, octalene, and bridged bicyclo systems; stability, reactivity and mechanism, Cortin Hammett principle and Winstein-Eliel equation (special emphasis on 5 and 6 membered rings with and without heteroatoms like O, S and N). 8 Lec.</p> <p>5. Quantitative relationship between structure and reactivity</p> <p>(i) Liner free energy relation: Hammett equation; Equilibrium and rate in organic reactions;</p> <p>(ii) Separation of polar, steric and resonance:</p> <p>(iii) Taft equation;</p> <p>(iv) Grunwald-Winstein equation.</p> <p>(v) Some application of structure-reactivity correlation study. 8 Lec.</p>
Text Books, and/or reference material	<p>1. Stereochemistry of Carbon Compounds. Ernest L. Eliel. McGraw-Hill</p> <p>2. A Guidebook to Mechanism in Organic Chemistry 6th Ed, by Peter Sykes</p> <p>3. Basic Stereochemistry of Organic Molecules, Oxford University Press: Subrata Sen Gupta</p> <p>4. Stereochemistry Of Organic Compound; Principle and Applications by D. Nasipuri:</p> <p>5. Stereochemistry. Conformation and Mechanism. P. S. Kalsi</p>

Mapping of CO (Course outcome) and PO (Programme Outcome)

	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

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	

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CY9151	Advanced Physical Chemistry-II Laboratory	PEL (Practical)	0	0	3	2.0	3
Pre-requisites		Course Assessment methods (Continuous (CT) and end assessment (EA) and Viva-Voce)					
CY1151, 2151		CT + Viva voce					
Course Outcome (The students will well-acquainted with)	<ul style="list-style-type: none"> • CO1: basic understanding of various modern electrochemical, surface characterization, spectroscopic techniques. • CO2: knowledge on measuring the rate of corrosion of metals and its mitigation by chemical route. • CO3: basic understanding on the design of solar cell, nanomaterial preparation and characterization. • CO4: development of laboratory skill, data handling and interpretation, error analysis. 						
Topics Covered	<ol style="list-style-type: none"> 1. Determination of rate of corrosion of metal using potentiodynamic polarization method 2. Determination of rate of corrosion of metal using electrochemical impedance method 3. Evaluation of potential at zero charge on a metal surface in presence of an electrolytic solution. 4. Determination of corrosion inhibition efficiency of an organic corrosion inhibitor. 5. Construction of a dye sensitized solar cell 6. Evaluation of excited state proton transfer process in 1-naphthol by excited state life time measurement 7. Synthesis and characterization of nanoparticles 8. Molecular modelling programs <p>Any other practical as assigned by the Instructor</p>						
Reference material	<ol style="list-style-type: none"> 1. Instruction manual provided by the Instructor 2. Selected experiments in Physical Chemistry By N. G. Mukherjee 3. Advanced Physical Chemistry Experiments: By Gurtu & Gurtu 						

Mapping of CO (Course outcome) and PO (Programme Outcome)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
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CO1	3	3	3	3		3		3	3			
CO2	3	3	3	3	3	3		3	3	2	2	1
CO3	3	3	3	3	3	3		3	3	2	3	1
CO4				3	3						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	
CY9152	Environmental Sample Analysis	PEL (Practical)	0	0	3	2.0	3
Pre-requisites		Course Assessment methods (Continuous (CT) and end assessment (EA) and Viva-Voce					
CY1152,2152		CT and Viva voce					
Course Outcome (The students will master the following)	<ul style="list-style-type: none"> • CO1: The course is designed to give the students a broad understanding of the issues related to the basic concepts and principles of analysis of soil and water quality parameters. • CO2: Students will also accumulate idea about the permissible limit, present concentration etc. of different environmental impurities. • CO3: Demonstrate an idea about the soil, water and wastewater quality standards and its regulations. • CO4: Students will also accumulate idea about the soil quality status with respect to nutrients like N, P and K present. 						
Topics Covered	<ol style="list-style-type: none"> 1. pH measurement of soil; 2. Estimation of organic carbon content in soil; 3. Chlorine content in drinking water; 4. Estimation of phenol in industrial waste-water sample 5. N, P and K of soil 6. Cyanide in industrial waste-water sample 						
Text Books, and/or	<ol style="list-style-type: none"> 1. 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. 						

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reference material	<p>2. Practical Environmental Analysis. Miroslav Radojevic & Vladimir N. Bashkin, Publisher: Royal Society of Chemistry; 2nd edition (April 26, 2006), ISBN-10: 0854046798, ISBN-13: 978-0854046799</p> <p>3. Practical Manual of wastewater chemistry. Barbara A. Hauser, Publisher: CRC Press, 1st edition (June 1, 1996). ISBN-10: 1575040123 ISBN-13: 978-1575040127.</p>
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Mapping of CO (Course outcome) and PO (Programme Outcome)

	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	3	3	3	2	1	3	3	3	3	3
CO4	3	3	3	2	3	2	1	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	
CY9153	Multi Step Synthesis and Characterization of Organic Compounds	PEL	0	0	2	3	2
Pre-requisites		Course Assessment methods (Continuous (CT) and end assessment (EA) and Viva-Voce)					
CY1153, 2153		CT and Viva voce					
Course Outcome (The students will be enriched	<ul style="list-style-type: none"> CO1: To reach a targeted product through multistep reaction process using suitable reagents and optimum reaction conditions. CO2: Separation and Purification of products, which will use as starting reagents for the next steps. 						

with practical knowledge of these CO)	<ul style="list-style-type: none"> • CO3: 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 spectroscopic method like; UV-Vis, FT-IR, NMR, ESI-Mass and GC-Mass. • CO5: To reach a maximum yield with minimum uses of solvent, reagents and energy like; heat and electricity (Green chemistry).
Topics Covered	<ol style="list-style-type: none"> 1. Oxidation of Benzoin to benzil followed by rearrangement to benzilic acid <ol style="list-style-type: none"> (i) Discussion, experimental setup, collection of starting reagent and chemicals. 1 hr (ii) 1 st step reaction of benzoin to benzil oxydation reaction. 2 hrs (iii) Separation and purification benzil, determination of yield and melting point 3 hrs (iv) Second step reaction of Benzil to benzylic acid rearrangement, yield and M.P. determination. 3 hrs (v) Analysis of Benzil and Benzylic acid with spectroscopic analysis 3 hrs 2. Preparation of benzophenoneoxime followed by rearrangement to benzanilide <ol style="list-style-type: none"> (i) Discussion, experimental setup, collection of starting reagent and chemicals. 1 hr (ii) 1 st step reaction between cyclohexanone and hydroxylamine to benzophenoneoxime 2 hrs (iii) Separation and purification benzophenoneoxime, determination of yield and melting point and next step reaction from benzophenoneoxime to benzinilide. 3 hrs (iv) Analysis of benzophenoneoxime and benzinilide with spectroscopic analysis. 3 hrs 3. Preparation of 1,3,5tribromobenzene from 2,4,6- tribromoaniline via diazotization <ol style="list-style-type: none"> (i) Discussion, experimental setup, collection of starting reagent and chemicals. 1 hr (ii) 1 st step reaction between 2,4,6-tribromoaniline and diazotising reagents to diazonium salt of 2,4,6-bromo benzene. 2 hrs.

	<p>(iii) Separation and purification benzophenoneoxime, determination of yield and melting point and next step reaction to obtain 1,3,5-tribromobenzene. 3 hrs</p> <p>(iv) Analysis of product 1,3,5-tribromobenzene with spectroscopic analysis. 3 hrs</p> <p>4. Preparation of Diethyladipate from Cyclohexanol followed by Dickmann cyclisation to 2-carboethoxy cyclopentanone.</p> <p>(i) Discussion, experimental setup, collection of starting reagent and chemicals. 1 hr</p> <p>(ii) 1st step reaction between Cyclohexanol and oxidising agent Conc. HNO₃ oxidation to Adipic acid followed by esterification to Diethyladipate. 2 hrs</p> <p>(iii) Next step Dickmann cyclisation of Diethyladipate to 2-carboethoxy cyclopentanone. 1 hr</p> <p>(iv) Separation and purification of Diethyladipate and 2-carboethoxycyclopentanone, their yield and boiling point determination</p> <p>(v) Analysis of product 1,3,5-tribromobenzene with spectroscopic analysis. 3 hrs</p> <p>5. Preparation of <i>p</i>-nitro aniline from acetanilide</p> <p>(i) Discussion, experimental setup, collection of starting reagent and chemicals. 1 hr</p> <p>(ii) 1st step reaction between acetanilide and nitrating agent Conc. H₂SO₄ & HNO₃ oxidation to P-nitroacetanilide 2 hrs</p> <p>(iii) Hydrolysis of P-nitroacetanilide to P-nitroaniline with H₂SO₄ in aqueous medium 1 hr</p> <p>(iv) Separation and purification of P-nitroacetanilide & P-nitroaniline, their yield and melting point determination 2 hrs</p> <p>(v) Analysis of product 1,3,5-tribromobenzene with spectroscopic analysis. 3 hrs</p>
Text Books, and/or reference material	<ol style="list-style-type: none"> 1. <i>Vogel's Textbook of practical organic chemistry</i>, 5th Edition 2. <i>Advanced practical chemistry</i>, 3rd ed.: Subas C. Das

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3. An Advanced Course in Practical Chemistry, New Central Book Agency; 3rd ed.: Nad, Mahapatra and Ghoshal

Mapping of CO (Course outcome) and PO (Programme Outcome)

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

FOURTH 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	
CY4101	Chromatographic Separation and Instrumental Methods of Analysis	PCR	2	0	0	2	2
Pre-requisites		Course Assessment methods (Continuous (CT) and end assessment (EA))					
NIL		CT+EA					
Course Outcome (The students will master	<ul style="list-style-type: none"> • CO1: Get a comprehensive knowledge about solvent extraction, ion exchange and different chromatographic techniques • CO2: Application of these techniques in practical and industrial capacity • CO3: Working principles and application of some instrumental methods 						

the following)	
Topics Covered	<p>Separation techniques:</p> <p>Solvent extraction, distribution law, distribution constant, extraction of inorganic species, separation of metal ion as chelates, extraction of metal chlorides and nitrates, solid phase extraction 03</p> <p>Ion exchange, ion exchange resin, ion exchange equilibria, application of ion exchange methods, home water softeners 02</p> <p>Chromatography: general description of chromatography, classification of chromatography, elution of column chromatography, migration rates, distribution constants, relation between, volumetric flow rate and linear flow rates, retention factor, selectivity factor, rate theory of chromatography, a quantitative description of column efficiency, thin layer chromatography (TLC) 03</p> <p>Gas chromatography (GC), Instrumentation, Introduction, carrier gas system, sample injection system, column configurations and column oven, detection system, characteristic of ideal detector, FID, TCD, ECD, mass spectroscopy gas chromatography column and stationery phase, capillary, tubular column, packed column, liquid stationery phase, applications 03</p> <p>High performance liquid chromatography: partition or liquid liquid chromatography, adsorption or solid liquid chromatography, ion exchange or ion chromatography, size exclusion chromatography, and chiral chromatography 03</p> <p>Instrumental method:</p> <p>Thermoanalytical Techniques: thermogravimetric analysis (TGA), Introduction, principle, instrumentation, Factors affecting TGA, application, differential thermal analysis, principle, instrumentation, application 03</p> <p>Electroanalytical techniques: electrogravimetry, electrical components, Galvanostat and potentiostat, principle, experiments, coulometry, principle, coulometer, coulometry cell, constant current coulometry 03</p> <p>Polarography: Principal, process of current, polarographic cell, Ilkovic equation, half wave potential, experimental set up, application, quantitative and qualitative analysis, cyclic voltammetry: principal, cell configuration, instrumentation and circuit, application 04</p> <p>Atomic absorption spectroscopy: Principle, Instrumentation, application 02</p>

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Text Books, and/or reference material	<ol style="list-style-type: none"> 1. Fundamentals of analytical chemistry, Skoog, West, Holler and Crouch, 8th edition, Thomson 2. Instrumental methods of analysis, Williard, Merit, Dean, Settle, CBS publishers & distributors 3. Inorganic electrochemistry, theory practice and application, Piero Zanzello, RS.C
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Mapping of CO (Course outcome) and PO (Programme Outcome)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
CO1	3	3	3	3	3	3	3	3	3	3	3	2
CO2	3	3	3	3	3	3	3	3	3	2	1	2
CO3	3	3	3	3	3	3	3	3	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	
CY4102	Modern aspects of environmental chemistry	PCR	2	0	0	2.0	2
Pre-requisites		Course Assessment methods (Continuous (CT) and end assessment (EA))					
NIL		CT+EA					
Course Outcome (The students will master the following)	<ul style="list-style-type: none"> • CO1: The course is designed to give the students a broad understanding of the issues related to the basic concepts of environmental chemistry. • CO2: To understand the chemistry responsible for environmental degradation and to formulate its remedy for sustainable development. • CO3: Students will be given an introduction to green chemistry and learn about its basic concepts for modern techniques using presently. 						
Topics Covered	Modern aspect of environmental chemistry:					16 Lecture	

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	Chemical aspects of air, water and soil pollution, chemistry of photochemical and sulphurous smog, stratosphere-chemistry and pollution, chemical speciation and organometallic compounds in the environment, priority and water pollutants-their effects, chemical analysis and control. Solid wastes from Industries. Radioactive solid waste disposal. Recovery and recycling. Ecological balance and planning of Industrial complexes. Reactions in living systems. Bioreactors. Biochemical process in industries. Biotechnology as low-energy, ecologically safe alternatives. Green chemistry, some recent environment disasters: Bhopal gas tragedy, Chernobyl, Three mile island etc
Text Books, and/or reference material	<ol style="list-style-type: none"> 1. Solutions Manual for Environmental Chemistry, Colin Baird and Michael Cann, Publisher: W. H. Freeman; 5th edition (May 7, 2012), ISBN-10: 1464106460 ISBN-13: 978-1464106460. 2. Chemistry Fundamentals: An Environmental Perspective. Phyllis Buell and James Girard Publisher: Jones & Bartlett Publishers; 2nd edition (April 2002), ISBN-10: 0763710741, ISBN-13: 978-0763710743. 3. Elements of Environmental Chemistry, Ronald A. Hites & Jonathan D. Raff; Publisher: Wiley; 2nd edition (April 24, 2012), ISBN-10: 1118041550, ISBN-13: 978-1118041550 4. L.W. Moore and E. A. Moore, Environmental Chemistry, McGraw Hill Publication, New York, 2002. 5. M. Khopkar, Environmental Pollution Analysis, New Age International (P) Ltd. 6. C. Baird., Environmental Chemistry, W. H. Freeman and Company, 1995.

Mapping of CO (Course outcome) and PO (Programme Outcome)

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

	Title of the course	Total Number of contact hours	Credit
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Course Code		Program Core (PCR) / Electives (PEL)	Lecture (L)	Tutorial (T)	Practical (P)	Total Hours	
CY4103	Molecular modelling in chemistry	PCR	1	1	0	2.0	2
Pre-requisites		Course Assessment methods (Continuous (CT) and end assessment (EA))					
NIL		CT+EA					
Course Outcome (The students will master the following)	<ul style="list-style-type: none"> • CO1: Apply the principles of quantum mechanics to understand molecular interactions, structure and chemical bonding. • CO2: Modelling of large assembly of atoms/molecules using approximate molecular dynamic simulations and Monte Carlo methods. • CO3: Knowledge on commercially available molecular modelling software packages. 						
Topics Covered	<p>Brief review of the basic principles of quantum mechanics of atoms and molecules. Concept of quantum mechanical <i>ab initio</i> calculations within Born-Oppenheimer approximation, density functional theory, semi-empirical and Molecular Mechanics calculations. 3 Lec</p> <p>Potential energy surfaces and intermolecular interactions and modelling of calculated energy by model potentials for simple atoms, ions and molecules. Concept of short range and long range interactions. 2 Lec</p> <p>Study of an assembly of atoms or molecules (cluster and/or bulk phases). Approximation of the total potential energy as the sum of pair potentials. 2 Lec</p> <p>Concept of large number of microstates, averages and basic principles of Monte Carlo and Molecular Dynamics simulations. 3 Lec</p> <p>Flexible models and calculation of force constants. Structural and dielectric properties of a polar medium: Continuum models versus molecular models. Calculation of structure, energy and free energy through simulations using molecular models. 4 Lec</p>						

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	<p>Study of self-organized assemblies, bio-molecules like peptides, proteins, membranes and ion channels through simulations. 3 Lec</p> <p>Concept of hydrophobic and hydrophilic interactions. Use of molecular modelling in drug design. 3 Lec</p>
Text Books, and/or reference material	<p>1. Molecular Modelling: Principles and Applications By A.R. Leach, Longman (1996).</p> <p>2. Molecular Modelling and Simulation By T. Schlick, Springer (2006).</p>

Mapping of CO (Course outcome) and PO (Programme Outcome)

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