**SYLLABUS**

**FOR**

**TWO-YEAR M.Sc. PROGRAMME**

**IN**

**APPLIED CHEMISTRY**



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| **NAAC – A Grade** |

**DEPARTMENT OF CHEMISTRY**

**COLLEGE OF ENGINEERING & TECHNOLOGY**

**(An Autonomous and Constituent College of BPUT, Odisha)**

**Techno Campus, Mahalaxmi Vihar, Ghatikia,**

**Bhubaneswar-751029, Odisha, INDIA**

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**Semester-1**

**Core 1: Inorganic Chemistry-I (PPCCH101)**

**Prerequisite:** Nil

**Purpose:**

**Course Objectives:**

1. To understand the structure and bonding of compounds involving main group elements.
2. To be able to use crystal field theory to understand the spectral properties of coordination compounds.
3. To be able to describe the stability of metal complexes by the use of formation constants and to calculate thermodynamic parameters from them.
4. To understand the reaction and mechanism of co-ordination compounds.

**Syllabus**

**Module I**

***Stereochemistry and Bonding in Main Group Compounds***

Wade’s rule, STYX method, application to boron compounds and carboranes.

Structure and bonding in condensed phosphates, silicates, cyclophosphazenes and S-N cyclic compounds.

***Metal - Ligand Bonding***

Limitation of CFT, MOT: energy level diagram of sigma and pi bonding in octahedral, tetrahedral and square planar complexes.

**Module II**

***Electronic Spectra of Coordination Compounds***

Spectroscopic ground states, term symbols for dn ions, Racah parameters, selection rules and intensities of bands, Orgel diagram, correlation and Tanaube-Sugano diagrams, spectra of 3d metal-aqua complexes of trivalent metal ions (d1-d6), divalent (Mn, Co and Ni), Calculation of Dq, B and β parameters for tetrahedral and octahedral complexes, CT spectra. Spectral properties of lanthanide and actinide metal complexes.

**Module III**

***Metal-ligand Equilibria in Solution***

Stability of metal complexes, compositions of metal complexes by Job’s method. Stepwise and overall stability constant, factors affecting the stability constant, Determination of stability constants by (pH metry and spectroscopic methods) and their applications.

**Module IV**

***Inorganic Reaction Mechanism***

Inert and labile complexes, factors affecting the reactivity of complexes, mechanisms of substitution (acid, base hydrolysis and anation) reactions of octahedral complexes, substitution reactions of square planar complexes, trans-effect – theories and applications in synthesis of metal complexes, redox reactions: mechanism of one election transfer reaction (inner sphere and outer-sphere), Marcus theory for outer-sphere reactions.

**Essential Readings:**

1. Inorganic Chemistry, D. F. Shriver and P. W. Atkins, Oxford University Press, 3rd Edn, 1999.
2. Chemistry of the Elements, N. N. Greenwood and A. Earnshaw, Pergamon Press, 2nd Edn., 2002.
3. Concepts and Models of Inorganic Chemistry, B. Douglas, D. McDaniel and J. Alexander, John Wiley (New York), 3rd Edn., 1993.
4. Inorganic Chemistry –Principles of Structure and Reactivity, J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, Pearson Education (New Delhi), 1st Impression, 2006.
5. Advanced Inorganic Chemistry, F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, John Wiley, 6th Edn,1999.
6. Reaction Mechanisms of Inorganic and Organometallic Systems, R. B. Jordan, Oxford University Press, 3rd Edn., 1998.
7. Fundamental Concept of Inorganic Chemistry, A. K. Das and M. Das, Vol. 4 and 5, CBS Publisher & Distributor Pvt. Ltd., 2nd Edn., 2014.
8. Mechanisms of Inorganic Reactions: Study of Metal Complexes in Solution, F. Basolo and R. G. Pearson. John Wiley and Sons, 2nd Edn. 1974.
9. Inorganic Chemistry, Gary L. Miessler, Paul J. Fischer and Donald A. Tarr, 5th Edn. 2013.
10. An Introduction to Inorganic Chemistry, Keith F. Purcell and John C. Kotz, Saunders, 1980.

**Course Outcomes**

* Understand structure and bonding of compounds involving main group elements.
* Predict the spectral properties of coordination compounds on the basis of crystal filed theory.
* Describe the stability of metal complexes through formation constants and able to calculate thermodynamic parameters from them.
* Demonstrate the reaction mechanism of selected substitution and electron transfer reaction of co-ordination compounds.

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| **PPCCH101**: **Inorganic Chemistry-I** |
| 1 | Program Outcomes | a | b | c | d | e | f | g | h | i | j | k |
| 2 | Mapping of Course Outcomes with Program Outcomes | \* |  |  |  |  |  |  |  |  |  |  |
| 3 | Category | Core | Allied Elective | Free Elective |
|  | \* |  |  |

**Core 2: Organic Chemistry-I (PPCCH102)**

**Prerequisite:** Nil

**Purpose:**

**Course Objectives:**

* 1. To learn the basic principles that governs the structure of molecules.
	2. To describe the importance of structure, reactivity and rearrangement in organic reaction mechanisms.
	3. To explain the various facets of aromatic electrophilic substitution reactions.

**Syllabus**

**Module I**

***Stereochemistry:***

Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity, conformation of sugars, Elements of symmetry, chirality, molecules with more than one chiral center, threo and erythro isomers, methods of resolution. Optical purity, enantiotropic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis.

Optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape.

**Module II**

***Reaction Mechanism (Structure, Reactivity and Rearrangements):***

Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes, benzyne.

Types of mechanisms: SN2, SN1, mixed SN1 and SN2, SN at an allylic, aliphatic trigonal and a vinyl carbon. Reactivity: effects of substrate, structure, attacking nucleophile, leaving group and reaction medium, ambient nucleophile and regioselectivity.

Kinetic and thermodynamic control, Hammond’s postulate, Curtin-Hammett principle, potential energy diagrams, transition states and intermediates.

Methods of determining reaction mechanisms, isotope effects. Quantitative treatment, Hammet equation and linear free energy relationships, substituent and reaction constants, Taft equation.

The NGP mechanism, NGP by π and σ bonds, anchimeric assistance.

Classical and nonclassical carbocations, norbornyl systems.

**Module III**

***Aromatic Electrophilic Substitution Reactions:***

The arenium ion mechanism, orientation and reactivity, energy profile diagrams, the ortho/para ratio, ipso attack, orientation in other ring systems, quantitative treatment of reactivity in substrates and electrophiles, diazonium coupling, Vilsmer reaction, Gattermann-Koch reaction.

The SNAr, SRN1 mechanisms, reactivity effect of substrate structure, leaving group and attacking nucleophile.

Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance, reactivity of aliphatic and aromatic substrates at bridgehead, reactivity in the attacking radicals, effects of solvents on reactivity.

**Module IV**

***Molecular rearrangements***

General mechanistic considerations-nature of migration, Migratory aptitude, A detailed study of the following rearrangements: Pinacol-Pinacolone, Wagner-Meerwein, Demjanov, Benzil-Benzilic acid, Favorskii, Arndt-Ester synthesis, The von Richter, Sommelet-Hauser and Smiles rearrangements, Neber, Beckmann, Hoffman, Curtius, Schmidt, Bayer-Villiger, Fries rearrangement, Shapiro reaction.

**Essential Readings:**

1. Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, Michael B. Smith, Wiley, 7th Edn, 2013.
2. Advanced Organic Chemistry Part A & B: Structure and Mechanisms, F. A. Carey, and R. J. Sundberg, Springer International Edition, 5th Edn., 2007.
3. A Guide Book to Mechanism in Organic Chemistry, P. Sykes, John Wiley & Sons, Inc., 6th Edn., 1985.
4. Modern Organic Reactions, H. O. House, Benjamin-Cummings Publishing Co-Subs. of Addison Wesley Longman, 2nd Edn, 1972.
5. Principles of Organic Synthesis, R. O. C. Norman and J.M. Coxon, Blackie Academic and Professional, 3rd Edn.,1993.
6. Stereochemistry of Organic Compounds. P.S. Kalsi, New Age International, 8th Edn., 2015.
7. Organic Synthesis, J. Clayden, N. Greeves, S. Warren, and Wouthers, Oxford University Press, 2nd Edn., 2000.
8. Organic Chemistry: Structure and Reactivity, Seyhan N. Ege, Hayden-mcneil Macmillan Learning, 5th Edn, 2001.
9. Stereochemistry, D. Nasipuri, New Academic Science, 4th Edition,2012

**Course Outcomes**

* Determine the stereochemistry of organic compounds.
* Deduce the organic reaction mechanism through the knowledge of structure, reactivity and rearrangement in organic molecules.
* Reveal the mechanisms of aromatic electrophilic substitution reactions.

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| **PPCCH102**: **Organic Chemistry-I** |
| 1 | Program Outcomes | a | b | c | d | e | f | g | h | i | j | k |
| 2 | Mapping of Course Outcomes with Program Outcomes | \* |  |  |  |  |  |  |  |  |  |  |
| 3 | Category | Core | Allied Elective | Free Elective |
|  | \* |  |  |

**Core 3: Physical Chemistry-I (PPCCH103)**

**Prerequisite:** Nil

**Purpose:**

**Course Objectives:**

* 1. To learn about the standard states of gases, liquid and solids and thermodynamic functions based on the laws of thermodynamics.
	2. To predict the excess functions based on thermodynamic concepts.
	3. To gain knowledge on distribution laws and derives thermodynamic functions for ideal monoatomic and diatomic gases.
	4. To describe on surface active agents, micelles, their properties and catalytic activities at the surface.

**Syllabus**

**Module I**

***Thermodynamics:*** Laws of thermodynamics, thermodynamic functions, standard states for gases, liquids and solids, internal energy, enthalpy, entropy and free energy and calculations between them. Activity, fugacity and mean activity coefficients, Debye-Huckel Limiting Law, thermodynamics of Mixing and Mixtures of Volatile Liquids– ideal and Real Solutions and Activity-Excess Functions.

**Module II**

***Statistical Thermodynamics:*** Distribution Laws: Maxwell-Boltzmann, Bose-Einstein, Fermi-Dirac model. most probable configuration and concept of entropy. Principle of equipartition of energy, partition functions: Molecular partition functions- translational, rotational, vibrational and electronic partition functions. Derivation of thermodynamic functions (energy, enthalpy, entropy and free energy) for ideal monoatomic and diatomic gases.

**Module III**

***Surface phenomena:*** Surface active agents and their classification, micellization, critical micelle concentration (CMC), Krafft temperature, factors affecting the CMC of surfactants, counterion binding to micelles, thermodynamics of micellization, solubilization, microemulsions, reverse micelles, surface films (electro-kinetic phenomena), catalytic activity at surfaces.

**Essential Readings:**

1. Molecular Thermodynamics, D. A. McQuarrie and J. D. Simon, Viva Student Edition, 1st Edn., 2015.
2. Physical Chemistry, R. S. Berry, S. A. Rice and J. Ross, Oxford Univ. Press, 2nd Edn., 2000.
3. Physical Chemistry: A Molecular Approach, D. A. McQuarrie and J. D. Simon, Viva Student Edition, 1st Edn., 2015.
4. Physical Chemistry, R. J. Silbey, R. A. Alberty, M. G. Bawendi, Wiley, 4th Edn., 2005.
5. Physical Chemistry, P.W. Atkins, Oxford University Press, 8th Edn. 1998.
6. Physical Chemistry of Surfaces, A. W. Adamson, Wiley India Edition, 2012
7. Statistical Mechanics, D. A. Mc Quarrie, University Science Books, 2nd Edn., 2000.

**Course Outcomes**

* Understand standard states of gases, liquid and solids.
* Able to determine the excess functions based on thermodynamic concepts.
* Acquired knowledge on distribution laws and able to derive the thermodynamic functions for ideal monoatomic and diatomic gases.
* Get preliminary understanding on surface active agents, micelles, their properties and catalytic activities at the surface.

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| **PPCCH103**: **Physical Chemistry-I** |
| 1 | Program Outcomes | a | b | c | d | e | f | g | h | i | j | k |
| 2 | Mapping of Course Outcomes with Program Outcomes | \* |  |  |  |  |  |  |  |  |  |  |
| 3 | Category | Core | Allied Elective | Free Elective |
|  | \* |  |  |

**AE 1: Quantum Chemistry (PPECH101)**

**Prerequisite:** Nil

**Purpose:**

**Course Objectives:**

* 1. To learn basic mathematical methods in chemistry and their applications in quantum chemistry.
	2. To learn on basis postulates of quantum mechanics and to derive the selection rules for electronic transitions based on the concept of the Schrodinger equation and particle in one-dimensional box.
	3. To predict the solutions of Shrodinger equation for hydrogen and hydrogen like atoms and importance of quantum numbers.
	4. To predict the molecular properties of small molecules based on quantum mechanical concepts of molecular theories.

**Syllabus**

**Module-I**

***Matrix Algebra:*** Matrices, determinants, matrix rank, orthogonal and unitary transformations, eigenvalues and eigenvectors, diagonalization of matrices, spectral theorem, few applications.

Vectors and Tensors: Introduction to vectors; vector operations; coordinate system transformation; covariant and contravariant vector components; few applications; Vector spaces, inner products, linear independence, bases.

Ordinary Differential Equations: Linear first and second order ODEs, homogeneous and inhomogeneous ODEs with constant coefficients, system of linear ODEs, power series solution of differential equations and special functions.

Operators in Quantum mechanics: Linear, Hermitian and Angular Momentum operators, Eigenvalue problem.

**Module-II**

Basic postulates of quantum mechanics. The Schrodinger equation, particle in 1, 2 and 3-dimensional boxes, degeneracy and tunneling. Derivation of selection rules for electronic transitions, harmonic oscillator, spherical coordinates: rigid rotator.

**Module-III**

Solution of the Schrodinger equation for hydrogen and hydrogen-like atoms, significance of n, l and m quantum numbers. variation and perturbation methods. multielectron atoms (helium and Li+ ion), spin quantum number, ground and excited state of helium atom.

LCAO-MO approximation: Hydrogen Molecule ion, Born-Oppenheimer approximation, Hydrogen Molecule, Valence Bond and Molecular Orbital Theory. Homonuclear and heteronuclear diatomic molecules (HF, CO, NO).

**Essential Readings:**

1. Maths for Chemists: G. Doggett, M. Cockett and E. Abel: RSC (Tutorial Chemistry Texts), 2012.
2. Basic Mathematics for Chemists: P. Tebbutt, Wiley-Blackwell, 1998.
3. Physical Chemistry: A Molecular Approach, D.A. McQuarrie and J.D Simon, Viva student Edition, 2nd Edn, 2015.
4. Quantum Chemistry. D.A. McQuarrie and J.D Simon, Viva student Edition, 2nd Edn, 2015.
5. Modern Quantum Chemistry, A. Szabo and N. S. Ostlund, Dover Books on Chemistry,1996
6. Quantum Chemistry, I. N. Levine, Prentice Hall India, 4th Edn., 2000.
7. Introductory Quantum Chemistry, A. K. Chandra, Tata McGraw Hill, 4th Edn., 2009.
8. Molecular Quantum Mechanics, P. W. Atkins and R. S. Friedman, Oxford University Press, 3rd Edn., 1997.

**Course Outcomes**

* Utilize the mathematical methods for quantum mechanical calculations.
* Derive the selection rules of electronic transitions based on postulates of quantum mechanics and particle in one-dimensional box.
* Find out the solutions of the Schrodinger equation for hydrogen and hydrogen-like atoms and understand the significance of quantum numbers.
* Predict the molecular properties of small molecules based on quantum mechanical concepts.

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| **PPECH101**: **Quantum Chemistry** |
| 1 | Program Outcomes | a | b | c | d | e | f | g | h | i | j | k |
| 2 | Mapping of Course Outcomes with Program Outcomes | \* |  | \* |  |  |  |  |  |  |  |  |
| 3 | Category | Core | Allied Elective | Free Elective |
|  |  | \* |  |

**AE 2: Group Theory and Molecular Spectroscopy (PPECH102)**

**Prerequisite:** Nil

**Purpose:**

**Course Objectives:**

* 1. To understand about symmetry, point groups and their properties and generate character tables and their applications.
	2. To know the rotational, vibrational and Raman spectra of complex systems with symmetry considerations.
	3. To understand the theory and applications of magnetic resonances.
	4. To learn about theory of Mossbauer spectra and their application to simple systems.

**Syllabus**

**Module-I**

Symmetry elements and symmetry operation, definitions of group, subgroup, relation between orders of a finite group and its subgroup. conjugacy relation and classes. generators, Point group.

Representations of group operators, The great orthogonality theorem (without proof) and its explanation, irreducible and reducible representation, bases of a representation, character of a representation, character table and its meaning, reduction formula, symmetry and selection rules for transitions between rotational, vibrational and electronic states.

**Module-II**

***Rotational and Infrared Spectroscopy***

Rotational spectra of simple polyatomic molecules (linear, non-linear- symmetric top and spherical top, prolate and oblate types) Stark effects on rotational spectrum

Fundamental and overtone bands. Isotope effects.

Symmetry and normal modes of vibration. Determination of normal modes from Symmetry for AB2, AB3, AB4, AB5 and AB6 systems, symmetry of overtones and combination bands.

Raman Spectroscopy concept of polarizability and Selection rules from symmetry considerations.

**Module-III**

***Nuclear Magnetic Resonance***

Nuclear spin; nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurements, factors influencing chemical shift, deshielding, spin-spin interactions, factors influencing coupling constant ‘J’. Classification (ABX, AMX, ABC, A2B2 etc.), spin decoupling; basic ideas about instrument, 1-D NMR studies of nuclei other than proton–13C, 19F and 31P. FT NMR, advantages of FT NMR, use of NMR in medical diagnostics.

Electron Paramagnetic (Spin) Resonance (EPR or ESR) Spectroscopy

Basic principles, zero field splitting and Kramer’s rule, factors affecting the ‘g’ value. Isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densities and McConnell relationship.

**Module-IV**

Principles of Mossbauer spectroscopy: Basic principles, spectral line shape and natural line width, characteristics of Mossbauer nuclides, Doppler’s effect, parameters to evaluate Mossbauer spectra: chemical shift or isomeric shift, quadruple interaction, Magnetic field interaction. Application of Mossbaur spectra to Fe and Sn system with respect to oxidation states.

**Essential Readings:**

1. Fundamentals of Molecular Spectroscopy, C. N. Banwell and E. M. McCash, Tata McGraw Hill, 4th Edn., 1995.
2. Molecular Spectroscopy, G. M. Barrow, McGraw Hill, 4th Edn., 1995.
3. Spectra of Atoms and Molecules, P. F. Bernath, Oxford Univ. Press, 2nd Edn., 2005.
4. Chemical Applications of Group Theory, F. A. Cotton, John Wiley, 3rd Edn., 2003.
5. Introduction to Symmetry and Group Theory for Chemists, A. M. Lesk, Springer, 1st Edn., 2004.
6. Molecular Symmetry and Group Theory, A Programmed Introduction to Chemical Applications, A. Vincent, Wiley, 2nd Edn., 2013.
7. Molecular Symmetry and Group Theory, R. L. Carter, Wiley, 2nd Edn., 1997.
8. Basic One and Two Dimensional NMR Spectroscopy, H.Friebolin, Wiley VCH, 1991
9. Symmetry and Spectroscopy of Molecules, K. V. Reddy, New Age International, 2nd Edn., 2009.
10. Molecular Spectra, I. A. Levine, Wiley, 1st Edn., 1975.
11. Physical Methods in Inorganic Chemistry, R. S. Drago, Saunders,2nd edn., 1992.
12. Modern Spectroscopy, J. M. Hollas, John Wiley, 4th Edn., 2004.
13. Symmetry and Spectroscopy: An Introduction to Vibrational and Electronic Spectroscopy, D.C.Haris and M.D. Bertolucci, Dover Publications, Inc., Newyork, 1989
14. Electron Paramagnetic Resonance: Elementary Theory and Practical Applications, J. A. Weil, J. R. Bolton and J. E. Wertz, Wiley Interscience, New York, 1994.
15. Mossbauer Spectroscopy, N. N. Greenwood and T. C. Gibb, Chapman & Hall, 1971.

**Course Outcomes**

* Acquire the fundamental knowledge on symmetry, point groups and their properties; construct the character tables and predict their applications.
* Predict the rotational, vibrational and Raman spectra of complex systems; apply symmetry considerations to vibrational and Raman spectra.
* Understand the theories of magnetic resonances and apply these to predict the structure of molecules/compounds/ions etc.
* Understand the functioning of Mossbauer spectra and their application to ascertain the oxidation states of Fe and Sn systems.

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| **PPECH102**: **Group Theory and Molecular Spectroscopy** |
| 1 | Program Outcomes | a | b | c | d | e | f | g | h | i | j | k |
| 2 | Mapping of Course Outcomes with Program Outcomes | \* | \* |  |  |  |  |  |  |  |  |  |
| 3 | Category | Core | Allied Elective | Free Elective |
|  |  | \* |  |

**Lab 1: Inorganic Chemistry Laboratory (PLCCH101)**

**Prerequisite:** Nil

**Purpose:**

**Course Objectives:**

* 1. To understand the principles of qualitative analysis of inorganic salts mixture and practice these for identification of radicals.
	2. To carry out synthesis of simple complexes and characterize them by UV-Visible and IR spectroscopy.

**Syllabus**

1. Semi micro qualitative analysis of inorganic mixtures containing anions, common cations, less familiar element (W, Mo, Ce, Th, Zr, V and U), insoluble (sulphate, oxides, halide).
2. Preparation and characterization (UV-Visible and IR spectra) of complexes
* Hexamminenickel(II)chloride
* Sodium tris-(oxalate)iron(III)
* Tris(thiourea) copper(I) complex
* ammonium tetrathiocyanatocobaltate(II)
* Chrome alum

**Essential Readings:**

1. Vogel's Qualitative Inorganic Analysis, G. Svehla, Orient Longman, 6th Edn., l987.
2. Inorganic Semi-micro Qualitative Analysis, V. V. Ramanujam, National Publishing Company, 3rd Edn., 1990.
3. A Collection of Interesting General Chemistry Experiments, Elias, A. J., Universities Press, (India) Pvt. Ltd., 1st Edn., 2002.
4. Experimental Inorganic Chemistry, Palmer
5. Experimental Inorganic/Physical Chemistry, Woodhead Publishing,1st Edn.,1999.

**Course Outcomes**

* Identify the acid and basic radicals in a mixture of inorganic salts based on the principles of qualitative analysis.
* Carry out synthesis of simple inorganic complexes and characterize these by UV-Visible and IR spectroscopy.

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| **PLCCH101**: **Inorganic Chemistry Laboratory** |
| 1 | Program Outcomes | a | b | c | d | e | f | g | h | i | j | k |
| 2 | Mapping of Course Outcomes with Program Outcomes |  | \* |  | \* | \* | \* |  |  |  |  |  |
| 3 | Category | Core | Allied Elective | Free Elective |
|  | \* |  |  |

**Lab 2: Organic Chemistry Laboratory (PLCCH102)**

**Prerequisite:** Nil

**Purpose:**

**Course Objectives:**

* 1. To identify the functional groups in organic compound through qualitative analysis.
	2. To know the procedure of distillation and separation techniques and apply these to organic compounds.
	3. To characterize the functional groups of organic compounds through IR spectra.
	4. To practice standard synthesis procedure for synthesis of some organic compounds.
	5. To estimate organic compounds using standard methods.
	6. To use the ChemDraw software to draw the structure of compounds.

**Syllabus**

1. Qualitative Analysis: Identification of organic compounds.
2. Separation, purification and identification of compounds of binary mixture using TLC and column chromatography.
3. Preparation of Picric acid.
4. Application of steam distillation in isolation of essential oil (clove) and perfume (rose).
5. Preparation of derivatives of aldehydes and ketones.
6. Estimation of (i) phenol, aniline, ascorbic acid and glucose by Fehling’s method & Bertrand's method.
7. Interpretation of IR spectra for functional group identification.
8. Preparation of (i) o-iodobenzoic acid from anthranilic acid, furoic acid from furfural, (ii) Thiamine catalysed benzoin condensation and (iii) benzil from benzoin.
9. Structure Drawing of various organic building blocks using chemdraw softwares.

**Essential Readings:**

1. Experiments and Techniques in Organic Chemistry, D. J. Pasto, C. R. Johnson & M. J. Miller, Printice Hall, 6th Edn.,1992.
2. Systematic Qualitative Organic Analysis, H. Middleton, Rupa Publishing House, 2nd Edn., 1982.
3. Hand Book of Organic Analysis, Qualitative & Quantitative, M. T. Clarke, E. Arnold (publisher)
4. Text book of Practical Organic Chemistry, A. I. Vogel, ELBS (London), 5th Edn., 1989.
5. Macro-scale and Micro-scale Organic Experiments, K. L. Williamson, D. C. Heath & Co., 2nd Edn., 1994.

**Course Outcomes**

* Identify the functional groups in organic compound through qualitative analysis.
* Separate the organic compounds by distillation and separation techniques.
* Characterize the functional groups of organic compounds by IR spectra.
* Synthesis of some organic compounds following standard procedures.
* Estimate organic compounds using standard methods.
* Draw the structure of organic compounds using Chem-Draw software.

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| **PLCCH102**: **Organic Chemistry Laboratory** |
| 1 | Program Outcomes | a | b | c | d | e | f | g | h | i | j | k |
| 2 | Mapping of Course Outcomes with Program Outcomes |  | \* | \* | \* | \* | \* |  |  |  |  |  |
| 3 | Category | Core | Allied Elective | Free Elective |
|  | \* |  |  |

**Semester-2**

**Core 4: Inorganic Chemistry-II (PPCCH201)**

**Prerequisite:** Nil

**Purpose:**

**Course Objectives:**

* 1. To learn about magnetic properties of coordination, lanthanide and actinide compounds.
	2. To understand the organometallic and fluxional compounds, their classifications, bonding and structures.
	3. To study the reactions and catalytic properties of organometallic compounds.
	4. To learn about magnetic properties of coordination, lanthanide and actinide compounds.

**Syllabus**

**Module-I**

***Magnetic properties of coordination compounds***

Types of magnetic behaviour, magnetic susceptibility and its determination by Gouy, Faraday and VSM method, Pascal's constants and constitutive corrections, paramagnetism, Curie-Weiss law, Van Vleck's equation (derivation excluded) and its applications, spin-orbit coupling, ferro- and anti-ferromagnetism coupling, super paramagnetism, high and low spin equilibria. Anomalous magnetic moments, magnetic exchange coupling and spin crossover. Magnetic properties of Lanthanide and Actinide metal complexes.

**Module-II**

***Organometallic Chemistry-I***

Stability and 18 electron rules (covalent and ionic), Alkyls/aryl and hydrides: alkyls and aryls (metal alkyls stabilized carbanion, β-elimination, stable alkyls, agostic alkyls, reductive elimination, preparation of metal allyls). Metal hydrides: synthesis, characterization, reactions, bridging hydrides. Pi-complexes: Synthesis, bonding, properties and applications of alkenes and alkynes, allyls, diene, cyclopentane, dienyl, arenes. Introductory idea on transition metal-carbon multiple compounds: carbene and carbyne.

**Module-III**

***Organometallic chemistry-II***

Reactivity of organo-transition metal complexes:Coordinative unsaturation, substitution reactions (nucleophilic and electrophilic addition and abstraction), oxidative addition and reductive elimination, insertion reactions (insertion of CO, SO2 and alkenes). Catalysis by organo-transition metal complexes: Alkene isomerisation, hydrogenation and hydroformylation; Zeigler-Natta polymerization of ethylene, reduction of carbon monoxide by hydrogen (Fischer-Tropsch reaction).

**Module-IV**

***Fluxional Organometallic Compounds***

Fluxionality and dynamic equilibria in compounds such as η2\_ olefin, η3\_ allyl and dienyl complexes.

**Essential Readings:**

1. The Organometallic Chemistry of the Transition Metals**,** [Robert H. Crabtree](http://www.amazon.in/s/ref%3Ddp_byline_sr_book_1?ie=UTF8&field-author=Robert+H.+Crabtree&search-alias=stripbooks), John Wiley & Sons, 1st Edn., 2014.
2. Organo-transition Metal Chemistry: From Bonding to Catalysis**,** [John F. Hartwig](http://www.bookdepository.com/author/John-F-Hartwig), University Science Books, 1st Edn., 2009.
3. Organo-transition Metal Chemistry, Anthony F. Hill, Royal Society of Chemistry, 1st Edn., 2002.
4. Organometallics: A Concise Introduction, Ch. Elshebroicn and A Salzer, Wiley, 3rd Edn., 2006.
5. Organo-transition Metal Chemistry: Applications to Organic Synthesis, S. G. Davies, Pergamon, 1st Edn., 1982.
6. A.K. Das and M. Das, *Fundamental Concept of Inorganic Chemistry,* Vol. 4 and 5, CBS Publisher & Distributor Pvt. Ltd., 2nd Edn., 2016.
7. *Organometallic Chemistry,* R. C. Mehrotra and A. Singh, New Age International Publishers, 2nd Edn, 2000.
8. Elements of Magnetochemistry, R. L. Dutta and A. Samal, S. Chand & Company Ltd., 2nd Edn., 2004.

**Course Outcomes**

* Derive the magnetic properties of coordination, lanthanide and actinide compounds.
* Get knowledge on organometallic and fluxional compounds, their classifications, bonding and structures.
* Comprehend the reactions and the catalytic properties of organometallic compounds.

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| **PPCCH201**:Inorganic Chemistry-II |
| 1 | Program Outcomes | a | b | c | d | e | f | g | h | i | j | k |
| 2 | Mapping of Course Outcomes with Program Outcomes | \* |  |  |  |  |  |  |  |  |  |  |
| 3 | Category | Core | Allied Elective | Free Elective |
|  | \* |  |  |

**Core 5: Organic Chemistry-II (PPCCH202)**

**Prerequisite:** Nil

**Purpose:**

**Course Objectives:**

* 1. To provide an understanding on various types of redox reactions and interconversions including their mechanisms.
	2. To discuss different types of reactions and their mechanisms those proceed through disconnection approaches.
	3. To explain the coupling reactions and to describe the applications of reversal polarity and protecting groups in synthesis of organic compounds.
	4. To explore the synthetic strategies of some complex organic compounds.

**Syllabus**

**Module I**

Organic transformations and reagents: Functional group interconversion including oxidations and reduction and stereochemistry.

***Reductions***

Catalytic hydrogenation, reduction by dissolving metals, Bio-reduction. Hydride transfer reagents: Sodium borohydride, Sodium cynoborohydride, Lithium aluminium hydride, alkoxy substituted LAH reducing agents, DIBAL, Application of Hydroboration. Diborane, diisoamylborane, 9BBN, isopinocamphenyl and diisopinocamphenyl borane. Homogeneous hydrogenation: Mechanism and applications using Rh, Ru and other metal complexes.

***Oxidations***

Scope of the following oxidizing agents with relevant applications and mechanism: DDQ, DCC, Chromium (VI) oxidants, Osmium tetroxide, Selenium dioxide, KMnO4, tertiary-Butyl hydro peroxide. Manganese (IV) oxidants, Swern oxidation, Oxidation with per-acids. Oxidation with hypervalent Iodines.

**Module II**

***Coupling Reactions:*** Carbon-carbon bond formation through coupling reactions (Heck, Suzuki, Stille and Sonogoshira, Negishi), Carbon-hetero atom bond forming reactions using transition metals (Cu,Pd, Rh, Ru, Ni, Fe etc.), Butchwald- Hartwig reaction C-C bond forming reaction; Wittig reaction, Julia-Kocienski olefination, Peterson olefination, Metathesis reaction (Cross or ring closure)

**Module-III**

***Disconnection Approach:*** An introduction to synthons and synthetic equivalents, disconnection approach, functional group inter conversions, the importance of the order of events in organic synthesis, one group C-X and two group C-X disconnections, chemo-selectivity.

***Reversal polarity & protecting group***

Umpolung approach, cyclisation reactions, amine synthesis. Protecting Groups*:* Principle of protection and deprotection of alcohol, amine, carbonyl and carboxyl groups and their application in organic synthesis.

**Module-IV**

***One Group C-C Disconnection:***

Alcohols and carbonyl compounds, regioselectivity, alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis.

***Two Group C-C Disconnections:***

Diels-Alder reaction, 1,3–difunctionalised compounds, α,β-unsaturated carbonyl compounds, control in carbonyl condensations, 1,5-difunctionalised compounds. Micheal addition and Robinson annulation.

***Ring Synthesis:***

Saturated heterocycles, synthesis of 3, 4, 5 and 6 membered rings, aromatic heterocycles in organic synthesis.

***Synthesis of Some Complex Molecules:***

Application of the above protocols in the synthesis of following compounds. Camphor, Vitamin D and Cortisone.

**Essential Readings:**

1. Modern Organic Synthesis and Introduction. G.S Zweifel, M. Nantz, P. Somfai, Wiely, 2nd edition, 2014
2. Organic Synthesis: Concepts, Methods and Starting Materials, J. Fuhrhop and G. Penzlin, VCH, Weinheim, Germany,2nd Edn., 1993.
3. Some Modern Methods of Organic Synthesis, W. Carruthers, Cambridge Univ. Press, 4th Edn, 2004.
4. Modern Synthetic Reactions, H. O. House, W. A. Benjamin, 2nd Edn., 1972.
5. Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, Michael B. Smith, 7th Edn., Wiley, 2013.
6. Principles of Organic synthesis, R.O.C. Norman, J. M. Coxon, CRC Press, 3rd Edn., 1993.
7. Advanced Organic Chemistry Part B: Structure and Mechanism, Francis A. **Carey**, Richard J. **Sundberg**, Springer, 5th Edn., 2008.
8. Organic Synthesis: The Disconnection Approach, S. Warren and P. Wyatt, Wiley India Pvt. Ltd, 2nd Edn., 2008.

**Course Outcomes**

* Identify the oxidising and reducing agents and elucidate the mechanisms of redox reactions and interconversions.
* Understand the mechanism of reactions those undergo through disconnection approaches.
* Depict the coupling reactions and demonstrate the applications of reversal polarity and protecting groups in synthesis of organic compounds.
* Describe the synthetic strategies for synthesis of some complex organic compounds.

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| **PPCCH202**:Organic Chemistry-II |
| 1 | Program Outcomes | a | b | c | d | e | f | g | h | i | j | k |
| 2 | Mapping of Course Outcomes with Program Outcomes | \* |  |  |  |  |  |  |  |  |  |  |
| 3 | Category | Core | Allied Elective | Free Elective |
|  | \* |  |  |

**Core 6: Physical Chemistry-II (PPCCH203)**

**Prerequisite:** Nil

**Purpose:**

**Course Objectives:**

* 1. To learn about complex reactions and theories of chemical reactions based on various postulations/mechanisms.
	2. To gain knowledge on kinetics on solution-phase and the factors affecting the reaction rates including diffusion controlled reactions.
	3. To get an idea about transport phenomena and laws governing this.
	4. To study about various laws governing electrochemical reactions and applications of these to garner energy.

**Syllabus**

**Module-I**

***Chemical Kinetics:*** Complex reactions: opposing, parallel and consecutive reactions. Chain reactions (linear), branching chains–explosion limits; Rice Herzfeld scheme for photochemical reactions.

Theories of reaction rates: Collision theory, potential energy surfaces (basic idea). transition state theory (both thermodynamic and statistical mechanics formulations). Theory of unimolecular reactions, Lindemann mechanism, Hinshelwood treatment, RRKM model (qualitative treatment).

**Module-II**

Solution kinetics: Factors affecting reaction rates in solution, effect of solvent and ionic strength (primary salt effect) on the rate constant, secondary salt effect, isotope effect, Kramers theory. Diffusion limited reactions. Study of fast reactions using stopped flow and relaxation techniques (T-jump and P-jump).

***Transport phenomena:*** Diffusion coefficients, Fick's first and second laws, relation between flux and viscosity, relation between diffusion coefficient and mean free path.

**Module III**

***Electrochemistry-I:*** Debye Huckel-Onsager equation for the equivalent conductivity of electrolytes –experimental verification of the equation –conductivity at high field and at high frequency –conductivity of non-aqueous solutions-effect of ion association on conductivity.

***Electrochemistry-II:*** Mechanism of the hydrogen evolution reaction and oxygen evolution reactions. Some electrochemical reactions of technological interest- corrosion and passivity of metals-construction and use of Pourbaix and Evans diagrams- methods of protection of metals from corrosion, Fuel cells - electro deposition. Nernst-Einstein equation, Stokes-Einstein Debye equation (SED), Einstein-Smoluchowski-equation.

**Essential Readings:**

1. Chemical Kinetics, K. J. Laidler, Pearson, 3rd Edn.,2004
2. Physical Chemistry - A Molecular Approach, D. A. McQuarrie and J. D. Simon, Viva Books Private Limited, 1st Edn., 2011.
3. Fundamentals of Photochemistry- K. K. Rohatgi-Mukharjii, New Age International, 3rd Edn., 2017.
4. Elements of Physical Chemistry, P. Atkins and J. de Paula, Oxford Press, 6th Edn., 2015.
5. Physical Chemistry, R. S. Berry, S. A. Rice and J. Ross, Oxford Univ. Press, 2nd Edn., 2000.
6. Chemical Kinetics and Dynamics, J. I. Steinfeld, J. S. Francisco, W. L. Hase, Princtice Hall, 2nd edn., 1999.
7. Modern Electrochemistry, J. O. M. Bockris and A. K. N. reddy, Springer, 2nd edn., 2000.

**Course Outcomes**

* Gain knowledge on complex reactions and theories of chemical reactions based on various postulations/mechanisms.
* Describe the solution-phase kinetics and the factors affecting the reaction rates including diffusion controlled reactions.
* Familiar with the transport phenomena and laws governing this.
* Understand the laws governing electrochemical reactions and their applications to garner energy.

**AE 3: Analytical Techniques - I (PPECH201)**

**Prerequisite:** Nil

**Purpose:**

**Course Objectives:**

1. To follow the principles of various spectroscopic techniques and mass spectrometry.
2. To predict the spectral data for various organic and inorganic compounds based on these principles.
3. To predict the structure of organic and inorganic compounds based on various spectral data.

**Syllabus**

**Module I**

Introduction to spectroscopic techniques for structure elucidation. Electromagnetic radiation, absorption of energy by organic compounds, types of spectroscopic methods for structural elucidation of organic and inorganic molecules.

***IR – Spectroscopy*** – Basic principles, characteristic frequencies of common functional groups.

UV – Visible Spectroscopy: Basic principles. Born-Oppenheimer approximation, Frank Condon principle, laws of photochemical equivalence. Application of UV – Visible spectroscopy to organic structure elucidation, Woodward – Fisher rules.

**Module II**

***Nuclear Magnetic Resonance (NMR)Spectroscopy:*** JJ coupling, vicinal and germinal coupling and,Applications of 1H and 13C NMR spectroscopy in the structural determination of organic compounds. One-dimensional NMR of common heteroatoms present in organic compounds (N, F and P).

***Electron Spin Resonance (ESR) Spectroscopy:*** Analysis of ESR spectra of systems in liquid phase, radicals containing single set, multiple sets of protons, triplet ground states. Transition metal ions/complexes.

**Module III**

***Mass spectrometry:*** Basic principles of mass spectrometry, fragmentation and rearrangements (including McLafferty rearrangement) of organic molecules, basics of high resolution mass spectrometry, ionization potential and isotopic distribution, experimental setup, application of mass spectrometry to organic and inorganic compounds in structural determination.

Problem solving exercises involving UV, IR, NMR & MS data: Problems involving interpretation of spectral details of organic compounds.

**Essential Readings:**

1. Structural Methods in Inorganic Chemistry, E. A. O. Ebsworth, Blackwell Scientific Publications, 2nd Edn., 1991.
2. Physical Methods in Chemistry, R. S. Drago, Saunders Co., 2nd Edn., 1992.
3. Introduction to Magnetic Resonance, Carrington, A. & McLachlan, A. D. Chapman & Hall, 3rd Edn., 1983.
4. Magnetism and Transition Metal Complexes, F. E. Mabbs, & D. J. Machin, Chapman and Hall, 2nd Edn., 2008,.
5. Spectrometric Identification of Organic Compounds, R. M. Silverstein and F. X. Webster, John Wiley and Sons.Inc., 6th Edn., 1997.
6. Organic Spectroscopy, W. Kemp, MacMillon, 3rd Edn., 1994.
7. Introduction to Spectroscopy, Pavia, Lampman and Kriz, Brooks/Cole Pubs. Co., 3rd Edn., 2000.
8. Spectroscopic Methods in Organic Chemistry, D. H Williams and Ian Fleming, Tata McGraw Hill, 6th Edn., 2014.
9. Spectroscopy of Organic Compounds, P. S. Kalsi, New Age Intl., 6th edn., 2006.
10. Electron Paramagnetic Resonance: Elementary Theory and Practical Applications, J. A. Weil, J. R. Bolton and J. E. Wertz, Wiley Interscience, New York, 1994.
11. Basic One and Two Dimensional NMR Spectroscopy, H.Friebolin, Wiley VCH, 1991

**Course Outcomes**

* Knowledge on principles of various spectroscopic techniques and mass spectrometry.
* Envisage the spectral data for various organic and inorganic compounds based on these principles.
* Deduce the structure of organic and inorganic compounds based on various spectral data.

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| **PPECH201**:Analytical Techniques - I |
| 1 | Program Outcomes | a | b | c | d | e | f | g | h | i | j | k |
| 2 | Mapping of Course Outcomes with Program Outcomes | \* | \* |  | \* |  |  |  |  |  |  |  |
| 3 | Category | Core | Allied Elective | Free Elective |
|  |  | \* |  |

**FE 1: Chemical Biology (POECH201)**

**Prerequisite:** Nil

**Purpose:**

**Course Objectives:**

* 1. To introduce the structure and function of selected biomolecules.
	2. To learn the fundamentals on bioenergetics and metabolism of glucose.
	3. To study the introductory idea on ion-channel and transport phenomena on biosystem.
	4. To know the essential knowledge on enzymes, their functions and enzyme kinetics.

**Syllabus**

**Module I**

***Introduction to Biomolecules****:*

Structure and Function: Carbohydrates (Monosaccharide, oligosaccharides, polysaccharides (starch, Glycogen, Cellulose); Lipids: Saturated and unsaturated fatty acids, triacylglycerols, phosphoglycerides, sphingolipids, waxes and sterol; amino acids and peptides, proteins - hierarchy of protein architecture, Ramachandran plot; nucleic acids: DNA, RNA, double helix model of DNA, denaturation and renaturation of DNA; replication, transcription and translation of DNA; hormones and vitamins.

**Module II**

***Principle of Bioenergetics****:* Bioenergetics and Thermodynamics; Phosphoryl group transfer and energy currency-ATP; Biological Oxidation and reduction reactions

Metabolic processes: Introduction to metabolism of carbohydrates: Glycolysis, TCA Cycle, Gluconeogenesis.

**Module III**

***Transport Mechanism***

Introduction to ion-channel, Na+/K+ transport (Ion pump); O2 transport by hemoglobin, CO2 transport by carbonic anhydrase.

***Enzymes****:* Properties of enzyme, classification of enzymes, mechanism of enzyme action, kinetics of enzyme action, activation energy, enzyme inhibition, coenzyme, apozyme and holozyme.

**Essential Readings:**

1. Principle of Bio-Chemistry, Alberf L. Lehninger, David L. Nelson, and Michael M. Cox. Worth Publishers: 33 Irving Place, 2nd Edn., 1993.
2. Biochemistry, Jeremy M Berg, John L Tymoczko, and Lubert Stryer, New York: W H Freeman, 5th Edn., 2002.
3. Fundamentals of Biochemistry, D. Voet, J. G. Voet and C.W. Pratt, Wiley, 2nd Edn, 2011.
4. Biochemistry, C. B. Powar & G. R. Chatwal, Himalaya Publishing House, 5th Edn., 2017.
5. Biochemistry, S. C. Rastogi, Tata McGraw Hill, 3rd Edn, 2010.

**Course Outcomes**

* Understand the structure and function of selected biomolecules.
* Get the knowledge on working of bioenergetics and metabolism of glucose.
* Identify the ion-channel and transport phenomena on biosystem.
* Get comprehensive knowledge on the enzymes, their functions and kinetics.

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| **POECH201**:Chemical Biology |
| 1 | Program Outcomes | a | b | c | d | e | f | g | h | i | j | k |
| 2 | Mapping of Course Outcomes with Program Outcomes |  |  |  |  |  |  | \* |  |  |  |  |
| 3 | Category | Core | Allied Elective | Free Elective |
|  |  |  | \* |

**Lab 3: Advanced Inorganic Chemistry Laboratory (PLCCH201)**

**Prerequisite:** Nil

**Purpose:**

**Course Objectives:**

* 1. To carry out synthesis of simple complexes and pursue the quantitative analysis of metals or the ligands in those complexes.
	2. To carry out volumetric analysis of metals in a mixture of their salts.

**Syllabus**

1. Preparation and quantitative analysis of complexes
* Preparation of pentamminechloro cobalt(III)chloride.
* Chrome alum
* trans- bis-(ethylenediamene)dichlorocobalt(III) chloride
* sodium tris-(oxalate)iron(III)
* Tris(thiourea) copper(I) complex
* ammonium tetrathiocyanatocobaltate(II)
* Potassium tris-(oxalato)aluminate(III)
* Tetraaminecopper(II) sulphate.
1. Volumetric analysis
* Volumetric estimation of Fe & Cu in their mixture.
* Volumetric estimation of Zn & Cu in their mixture.
* Volumetric estimation of Ni and Zn in their mixture.

**Course Outcomes**

* Synthesize of simple complexes and analyze quantitatively the metal or ligand components in the complexes.
* Quantitatively analyze the metals in a mixture of their salts by volumetric methods.

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| **PLCCH201**: **Advanced Inorganic Chemistry Laboratory** |
| 1 | Program Outcomes | a | b | c | d | e | f | g | h | i | j | k |
| 2 | Mapping of Course Outcomes with Program Outcomes |  | \* |  | \* | \* | \* |  |  |  |  |  |
| 3 | Category | Core | Allied Elective | Free Elective |
|  | \* |  |  |

**Lab 4: Physical Chemistry Laboratory-I (PLCCH202)**

**Prerequisite:** Nil

**Purpose:**

**Course Objectives:**

* 1. To impart training on different basic physical laboratory experiments for quantitative analysis and titrimetric methods.

**Syllabus**

* + - 1. pHmetry / conductometry / potentiometry and precipitation titrations.
			2. Determination of acid dissociation constant by spectrophotometric technique.
			3. Determination of inversion of sucrose using polarimeter.
			4. Determination of critical miceller concentration (CMC) of surfactants.
			5. Determination of polarizability from refractive index measurements.
			6. Determination of composition of a complex by Job’s method.
			7. Determination of polarity of solvent by dye absorption.

**Essential Readings:**

1. Experiments in Physical Chemistry, D. P. Shoemaker, C. W. Garland & J. W. Nibber, McGraw Hill, 5th Edn., 1989.
2. Text book of Practical Organic Chemistry, I. Vogel, ELBS, London, 5th Edn., 1989.
3. Laboratory Manual of Organic Chemistry, B. Dey and M. V. Sitharaman, Revised by T.R. Govindachari, Allied Publishers Ltd., New Delhi. 4th Edn., 1992.

**Course Outcomes**

* Expertise on different basic physical laboratory techniques for quantitative analysis and titrimetric experiments.

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| **PLCCH202: Physical Chemistry Laboratory-I** |
| 1 | Program Outcomes | a | b | c | d | e | f | g | h | i | j | k |
| 2 | Mapping of Course Outcomes with Program Outcomes |  | \* |  | \* | \* |  |  |  |  |  |  |
| 3 | Category | Core | Allied Elective | Free Elective |
|  | \* |  |  |

**Lab 5: Computational Chemistry Laboratory-I (PLCCA203)**

**Prerequisite:** Nil

**Purpose:**

**Course Objectives:**

1. To promote the students to learn on programming in C and to write the program on C also.

**Syllabus**

**Module – I**

Programming Lab-1

C program - header files, C pre-processor, standard library functions, etc., identifiers, basic data types and sizes, constants, variables, arithmetic, relational and logical operators, increment and decrement operators, conditional operator, bit-wise operators, assignment operators, expressions, type conversions, conditional expressions, Input-output statements, if and switch statements, loops: -while, do-while and for statements, break, continue, etc.

1. Write a C program to find the sum of individual digits of a positive integer.
2. Write a C program to find Fibonacci sequence.
3. Write a C program to generate all the prime numbers between 1 and n.
4. Write a C program to find the roots of a quadratic equation.
5. Write a C program to find both the largest and smallest number in a list of integers.

**Module – II**

Designing structured programs: - Functions, parameter passing, storage classes- extern, auto, register, static, scope rules, user defined functions, recursive functions. Arrays - concepts, declaration, definition, accessing elements, and functions, Pointers- concepts, initialization of pointer variables, pointers and function arguments, address arithmetic, Character pointers and functions, pointers to pointers, Dynamic memory management.

* 1. Write C programs that use both recursive and non-recursive functions
		1. To find the factorial of a given integer.
		2. To find the GCD (Greatest Common Divisor) of two given integers.
		3. To solve Towers of Hanoi problem.
	2. Write a C program that uses functions to perform the following:
		1. Addition of Two Matrices
		2. Multiplication of Two Matrices
	3. Write a C program that uses functions to perform the following operations:
	4. To insert a sub-string in to given main string from a given position.
	5. To delete n Characters from a given position in a given string.
	6. Write a C program to determine if the given string is a palindrome or not
	7. Write a C program to construct a pyramid of numbers.

**Module – III**

Derived types- structures- declaration, definition and initialization of structures, accessing structures, nested structures, arrays of structures, structures and functions, pointers to structures, union.

1. Write a program to display Name, Roll Number, Marks of different subjects etc. of n number of students.
2. Write a C program to count the lines, words and characters in a given text.
3. Write a C program that uses structure to perform the following operations:
4. Reading a complex number
5. Writing a complex number
6. Addition of two complex numbers
7. Multiplication of two complex numbers

(Note: represent complex number using a structure.)

**Course Outcomes**

* Acquire fundamental knowledge in C programming and able to write the structured programme in C.

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| **PLCCA203: Computational Chemistry Laboratory-I** |
| 1 | Program Outcomes | a | b | c | d | e | f | g | h | i | j | k |
| 2 | Mapping of Course Outcomes with Program Outcomes |  |  | \* | \* | \* |  | \* |  |  |  |  |
| 3 | Category | Core | Allied Elective | Free Elective |
|  |  |  | \* |

**Lab 6: Chemical Biology Laboratory (PLCCH204)**

**Prerequisite:** Nil

**Purpose:**

**Course Objectives:**

1. To get practical knowledge in estimating proteins, DNA and RNA by spectroscopic techniques.
2. To practice the separation of different biomolecules following standard procedures.
3. To study on enzyme activity and enzyme kinetics.

**Syllabus**

1. Spectroscopic/Colorimetric estimation of protein using Lowry’s and Bartford methods.
2. Spectroscopic estimation of DNA using DPA method
3. Spectroscopic estimation of RNA using Orcinol method
4. Estimation of Iodine number and saponification value of fatty acids
5. Separation of amino acids by paper chromatography
6. Separation of sugars by thin layer chromatography
7. Separation of proteins by SDS-PAGE.
8. Assay of Enzyme activity: Protease from bacteria.
9. Assay of enzyme activity: Amylase from plant tissue & saliva.
10. Determination of Km and Vmax of enzyme catalysed reaction.

**Essential Readings:**

1. Introduction to Practical Biochemistry, Plummer Mu, David T. Plummer, Tata McGraw-Hill Education, 3rd Edn., 2008.

**Course Outcomes**

* Estimate proteins, DNA and RNA by spectroscopic techniques.
* Learn separation techniques for separating different biomolecules.
* Understand the enzyme activity and enzyme kinetics.

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| **PLCCH204**: **Chemical Biology Laboratory** |
| 1 | Program Outcomes | a | b | c | d | e | f | g | h | i | j | k |
| 2 | Mapping of Course Outcomes with Program Outcomes |  | \* |  | \* | \* | \* | \* |  |  |  |  |
| 3 | Category | Core | Allied Elective | Free Elective |
|  |  |  | \* |

**Semester-3**

**Core 7: Solid State Chemistry (PPCCH301)**

**Prerequisite:** Nil

**Purpose:**

**Course Objectives:**

* 1. To provide an introductory idea on structure of solids, their classification and importance of lattice energy.
	2. To encompass the electronic properties of solids and to understand various types of defects in solids.
	3. To elucidate the structure of solids by different characterization techniques such as optical and electron microscopy and X-ray diffraction methods

**Syllabus**

**Module I**

Chemical crystallography: Introduction, Space lattice, Crystal point groups, space group (working knowledge), Packing in solids, Crystal structures of representative systems, Silicates and Zeolites, Cements, Glasses, Quasicrystals, Nanostructures.

***Bonding in solids and Crystal energetics:*** Crystal classifications, Madelung constant and Lattice energy.

**Module II**

***Electronic properties and Band theory of solids:*** Metals, insulators and semiconductors, electronic structure of solids- Band theory, band structure of metals, insulators and semiconductors. Intrinsic and extrinsic semiconductors, doping semiconductors, p-n junctions, super conductors (Low temperature superconductor, BCS theory, High temperature superconductor).

***Defects, Nonstoichiometry and Diffusion:*** Perfect and imperfect crystals, intrinsic and extrinsic defects–point defects- vacancies Schottky defects and Frenkel defects. Thermodynamics of Schottky and Frenkel defect formation, colour centres, non-stoichiometry defects, line defect- edge dislocation and Screw Dislocation and Plane defects- Grain boundaries, Tilt boundaries Diffusion mechanisms, Fick’s law, Kirkenall effect.

**Module III**

***Characterization techniques***

***Optical Microscopy:*** Optical microscope - Basic principles and components, Different examination modes (Bright field illumination, Oblique illumination, Dark field illumination, Phase contrast, Polarised light, Hot stage, Interference techniques), Stereomicroscopy, Photomicroscopy, Colour metallography, Specimen preparation, Applications.

***Electron Microscopy:*** Interaction of electrons with solids, Scanning electron microscopy Transmission electron microscopy and specimen preparation techniques, Scanning transmission electron microscopy, Energy dispersive spectroscopy, Wavelength dispersive spectroscopy.

**Module IV**

***X-ray Diffraction Methods:*** Generation of X-rays, Properties of X-rays: Continous spectrum, characteristic spectrum, Filters, Bragg condition, Miller indices, Structure factor and its relation to intensity, identification of unit cells from systematic absences in diffraction pattern. Structure factor calculation for NaCl and KCl. Description of the procedure for an X-ray structure analysis, Laue method, Bragg method, Debye-Scherrer method of X-ray structural analysis of crystals, indexing of crystals.

***Surface Analysis:*** Atomic force microscopy, scanning tunneling microscopy, X-ray photoelectron spectroscopy.

**Essential Readings:**

1. Materials Characterization Techniques, Sam Zhang, Lin Li, Ashok Kumar, CRC Press, 2nd Edn. 2009.
2. Elements of X-Ray Diffraction, B.D. Cullity, and R.S. Stock, Prentice-Hall, 3rd Edn., 2001.
3. Solid State Chemistry and Its Applications, A. R. West, John Wiley & Sons, 2nd Edn., 2014.
4. Solid State Chemistry: An Introduction, L. Smart and E. Moore, Chapman and Hall, 4th Edn., 2012.
5. New Directions in Solid State Chemistry, C. N. R. Rao and J. Gopalkrishanan, Cambridge Univ. Press, 2nd Edn., 2010.
6. Basic Solid-State Chemistry, A.R. West, Wiley, 3rd Edn., 2012.

**Course Outcomes:**

* Distinguish the structure of solids, their classification and the significance of lattice energy.
* Define the electronic properties of solids and various types of defects in solids.
* Characterize the structure of solids by different characterization techniques such as optical and electron microscopy and X-ray diffraction methods.

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| **PPCCH301**: **Solid State Chemistry** |
| 1 | Program Outcomes | a | b | c | d | e | f | g | h | i | j | k |
| 2 | Mapping of Course Outcomes with Program Outcomes |  | \* |  | \* |  | \* |  |  |  | \* | \* |
| 3 | Category | Core | Allied Elective | Free Elective |
|  | \* |  |  |

**AE 4: Analytical Techniques – II (PPECH301)**

**Prerequisite:** Nil

**Purpose:**

**Course Objectives:**

* 1. To learn on data accuracy and their uses in various experiments; various standard methods for calculating the multifunctional parameters.
	2. To gain knowledge on basic principles of chromatography and separation techniques for purifying samples.
	3. To understand the basic principles on various thermal and electroanalytical techniques and their applications.
	4. To study the basic principles of fluorescence and optical activity techniques and their applications.

**Module I**

***Data Handling:*** Errors and Statistics: significant figures, rounding off, accuracy and precision, determinate and indeterminate errors, standard deviation, propagation of errors, non-linear least square fittings, confidence limit, test of significance, rejection of a result.

**Module II**

***Separation Techniques:*** Solvent Extraction: distribution coefficient, distribution ratio, solvent extraction of metals, multiple batch extraction, counter current distribution. Chromatographic Techniques: classification, theory of chromatographic separation, distribution coefficient, retention, sorption, efficiency and resolution. - Column, ion exchange, paper, TLC & HPTLC: techniques and application. - Gas

***Chromatography:*** retention time or volume, capacity ratio, partition coefficient, theoretical plate and number, separation efficiency and resolution, instrumentation and application.

**Module III**

***Thermal Analysis:*** TGA, DTA and DSC: Basic principles, instrumentation and their applications.

Electroanalytical Methods: Classification of electroanalytical methods, principles and applications of voltammetry, cyclic voltaammetry, anodic stripping voltammetry, polarography, amperometry, coulometry, conductometry and ion selective electrodes (Extensive instrumentations are to be excluded).

**Module IV**

Fluorescence Spectroscopy; Basic principles of fluorescence spectroscopy; quantum yield and lifetime; static & dynamic quenching; the Stern-Volmer equation, fluorescence anisotropy. Basic idea on green fluorescent protein.

Optical Activity and ECD Spectroscopy: Optical activity; absorption and dispersion; principles of circular dichroism; CD of small molecules.

**Essential Readings:**

1. Quantitative Chemical Analysis, D. C. Harris, W. H. Freeman, 8th Edn., 2010.
2. Instrumental Analysis, G. D.Christian & J. E. OReily, Allyn & Balon, 2nd Edn., 1986.
3. Instrumental Analysis, D. A. Skoog, F. J. Holler, S. R. Crouch, Cengage Learning, 11th Edn., 2012.
4. Principle and Applications of Thermal Analysis, P. Gabbott, Blackwell Publshing, 1st Edn., 2009.
5. Structure Determination of Organic Compounds, E. Pretsch, P. Bühlmann, M. Badertscher, Springer, 4th Edn., 2009.
6. Introduction to Modern Liquid Chromatography, Lloyd R. Snyder, Joseph J. Kirkland, Wiley, 3rd Edn., 2009.
7. Gas Chromatography, Ian A. Fowlis, John Wiley & Sons, 2nd Edn., 1995.
8. Validating Chromatographic Methods: A Practical Guide, D. Bliesner, John Wiley & Sons, 2nd Edn.,2006.
9. Principles of Fluorescence Spectroscopy J. R. Lakowicz, 3rd Edn., 2006.
10. NMR Spectroscopy, James Keeler, Wiely, 2nd Edn., 2011.
11. Introduction to Thermal Analysis: Techniques and Application, Brown, Michael Ewart, Kluwer Academic Publishers, 2nd Edn. 2001.
12. An Introduction to Error Analysis, J. R. Teller, University Science book, 2nd Edn. 1997.
13. Data reduction and Error Analysis for the Physical Sciences, P. Bavington and D.K. Robinson, McGraw-Hill, 3rd Edn., 2003.

**Course Outcomes:**

* Demonstrate on data accuracy principles and their uses in various experiments; various standard methods for calculating the multifunctional parameters.
* Understand the basic principles of chromatography and separation techniques for purifying samples.
* Acquire comprehensive knowledge on the basic principles of various thermal and electroanalytical techniques and their applications.
* Validate photochemical laws through fluorescence spectroscopic techniques and optical activity experiments.

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| **PPECH301**: **Analytical Techniques - II** |
| 1 | Program Outcomes | a | b | c | d | e | f | g | h | i | j | k |
| 2 | Mapping of Course Outcomes with Program Outcomes |  | \* |  | \* |  | \* | \* |  |  |  |  |
| 3 | Category | Core | Allied Elective | Free Elective |
|  | \* |  |  |

**FE 2: Pharmaceutical Chemistry – I (POECH301)**

**Prerequisite:** Nil

**Purpose:**

**Course Objectives:**

1. To demonstrate the basic principles of medicinal chemistry, QSAR and drug metabolism.
2. To describe the classification of drugs and their synthesis of drugs acting on autonomic, somatic and central nervous system.
3. To underline the synthesis of some selected antihistamine and analgesic drugs.

**Syllabus**

**Module -I**

1. ***Basic Principles of Medicinal Chemistry:*** Physico-chemical aspects (Optical, geometric and bioisosterism) of drug molecules and biological action
2. ***Brief concept on Quantitative Structure Activity Relationship (QSAR):* Hansch analysis –** its derivation and discussion on different parameters like electronic parameters, steric factor, and partition coefficient. Free Wilson model.

**Virtual drug screening techniques and their applications.**

**3-D QSAR Analysis:** Receptor independent 3-D QSAR Analysis, Receptor dependent

3-D QSAR Analysis

1. ***Basic concepts of:*** Drug metabolism, Prodrugs, Receptors and drug receptor interaction

**Module II**

Classification, mode of action, uses and structure activity relationship of the following classes of drugs. Synthesis of those compounds only exemplified against each class.

1. ***Drugs acting on autonomic nervous system:***
2. **Cholinergics and Anticholinesterase:** Acetylcholine, Carbachol, Bethanechol, methacholine and Neostigmine.
3. **Adrenergic drugs and adrenergic blocking agents:** Adrenaline, Salbutamol, Naphazoline ,Propranolol, Atenolol
4. **Antispasmodic and antiulcer drugs:** Homatropine, Cyclopentolate, Diclomine, Tropicamide.
5. ***Drugs acting on somatic nervous system:***
6. **Neuromuscular blocking agents:** Gallamine, succinylcholine
7. **Local Anaestahetics :** Benzocaine, Procaine, Lignocaine, Dibucaine.

**Module -III**

1. ***Drugs acting on the Central Nervous System:***
2. **General Anaesthetics:** Ananesthetic ether, Halothane, Thiopental sodium.
3. **Hypnotics and Sedatives:** Phenobarbitone, Cyclobarbitone, Glutethimide, Diazepam
4. **Opioid analgesics:** Pethidine, Methadone.
5. **Anticonvulsants:** Phenytoin, Ethosuximide, Primidone, Carbamazepine
6. **Antiparkinsonism drugs:** Levodopa, Amantidine
7. **CNS stimulants:** Nikethemide, Ethamivan, Amphetamine
8. **Psychopharmacological agents** (neuroleptics, antidepressants, anxiolytics): Chlorpromazine, Haloperidol, Impiramine, Phenelzine, Chlordiazepoxide, Alprazolam.

**Module -IV**

1. ***Autacoids:***
2. **Antithistamines:** Diphenhydramine, Mepyramine, Chlorpheniramine, Promethazine, Chlorcyclizine, Ranitidine.
3. **Eicosanoids:** Occurrences, Chemical nature, Medicinal applications
4. **Analgesic – antipyretics, anti-inflammatory (non-steroidal) agents:** Aspirin, Paracetamol, Ibuprofen, Naproxan, Diclofenac sodium.

**Essential Readings:**

1. Text Book of Organic Medicinal and Pharmaceutical Chemistry, J. M Beale, John Block, Lippincott Williams & Wilkins, 12th Edn., 2011.
2. Foye’s Principles of Medicinal Chemistry, Lippincott Williams & Wilkins, 7th Edn., 2012.
3. A Text Book of Medicinal Chemistry: Synthetic and Biochemical Approach, S. N. Pandeya, Vol.2, S. G. publisher, 1st Edn., 2009.
4. Medicinal Chemistry, Ashutosh Kar, New Age International Publishers, 5th revised and expanded Edn., 2010.
5. Bentley’s and Driver’s Text Book of Pharmaceutical Chemistry, Oxford Medical Publications, 8th illustrated Edn., 1969.
6. Introduction to Medicinal Chemistry, Graham L. Patrick, Oxford, 6th dn., 2017.

**Course Outcomes:**

* Develop an understanding on the basic principles of medicinal chemistry, QSAR and drug metabolism.
* Categorize the classification of drugs and elaborate the synthesis of some selected drugs acting on autonomic, somatic and central nervous system.
* Describe the synthesis of some selected antihistamine and analgesic drugs.

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| **POECH301**: **Pharmaceutical Chemistry – I** |
| 1 | Program Outcomes | a | b | c | d | e | f | g | h | i | j | k |
| 2 | Mapping of Course Outcomes with Program Outcomes |  |  |  |  |  |  | \* |  |  | \* | \* |
| 3 | Category | Core | Allied Elective | Free Elective |
|  |  |  | \* |

**FE 2: Chemical Rate Processes (POECH302)**

**Prerequisite:** Nil

**Purpose:**

**Course Objectives:**

1. To describe various techniques for measurement of fast reactions, types of chain reactions and effect of solvents on reactions.
2. To illustrate on oscillatory reactions and various models.
3. To emphasizes the dynamics of chemical reactions.
4. To provide an introductory idea on femtosecond kinetics.

**Syllabus**

**Module -I**

Kinetic Measurements: General features of fast reactions; study of fast reactions by relaxation methods (ultrasonic, pulse radiolysis, NMR); flash photolysis; solvent effects on reactions in solutions.

Chain Reactions: Features of chain reactions; thermal and photochemical reactions (hydrogen-bromine reaction, decomposition of aldehydes and ketones).

**Module-II**

Kinetics of oscillatory reactions: introduction to oscillatory reactions; Belousov- Zhabotinsky and Field-Koros-noyes models.

**Module-III**

Rate Theory: Concept of potential energy surfaces, transition state theory including its statistical mechanical treatment, phenomenological theories of unimolecular reactions (Lindemann, Hinshelwood), statistical mechanical theories of unimolecular reactions (RRKM).

Chemical Dynamics: Collision theory and Reaction Dynamics, Reaction Cross section and rate constant, Brief idea of Molecular Beam Scattering, Dynamics in condensed phase.

**Module-IV**

Femtochemistry: Concepts and perspectives; applications to studies of dynamics and control of chemical reactions.

**Essential Readings**

* 1. Physical Chemistry, I. Levine, Tata Mcgraw Hill, 5th Edn., 2007.
	2. Physical Chemistry: A Molecular Approach, D. A. McQuarrie and J. D. Simon, University Science Books, 1997.
	3. Chemical Kinetics and Dynamics, J. I. Steinfeld, J. S. Francisco and W. L. Hase, Prentice Hall, 1999.
	4. Chemical Dynamics in Condensed Phases: Relaxation, Transfer and Reactions in Condensed Molecular Systems, A. Nitzan, Oxford Univ. press, 2006.
	5. Basic Chemical Kinetics, H. Eyring, S. H. Lin and S. M. Lin, John Wiley & Sons, New York, 1980.
	6. The World of Physical Chemistry, K. J. Laidler, Oxford University press, 1993.

**Course outcomes**

* Understand the principles of fast reactions and various techniques to study these reactions.
* Acquire knowledge on oscillatory reactions and their concepts.
* Exhibit understanding on the chemical dynamics of reactions.
* Envisage femtosecond kinetics.

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| **POECH302**: **Chemical Rate Processes** |
| 1 | Program Outcomes | a | b | c | d | e | f | g | h | i | j | k |
| 2 | Mapping of Course Outcomes with Program Outcomes |  | \* |  | \* |  | \* |  |  |  | \* |  |
| 3 | Category | Core | Allied Elective | Free Elective |
|  |  |  | \* |

**FE 2: Chemistry of Natural Products (POECH303)**

**Prerequisite:** Nil

**Purpose:**

**Course Objectives:**

* 1. To provide a brief introduction to types of natural products
	2. To explore various synthetic routes for synthesis of some selected natural products.
	3. To enumerate the total synthetic approaches for synthesis of some selected drugs.

**Syllabus**

**Module-I**

Introduction to natural products: Isolation and structure elucidation of terpenes, alkaloids, flavonoids, xanthones. Structural elucidation of strychinine, tylophorine, morphine, abietic acid.

**Module-II**

Biosynthetic aspects and Synthesis of selected natural products of biological and structural importance: benzylisoquinoline alkaloids, colchicines, quinine, terpenes (mono, di and tri), isoflavones, anthraquinones.

**Module III**

Total Synthesis: Taxol, erythronolide B, penicillin V, Prostaglandins F2-alpha and E2.

**Essential Reading:**

1. Classics in Total Synthesis III: Further Targets, Strategies, Methods, K. C. Nicolaou, Jason S. Chen, Wiley-VCH, 1st Edn., 2011.
2. The Way Synthesis, T. Hudlicky and J. W. Reed, Wiley-VCH, 1st Edn., 2007.
3. The Logic of Chemical Synthesis, E. J. Corey and X-M. Cheng, John-Wiley & Sons, 1st Edn.,1989.
4. Comprehensive Natural Products Chemistry, D.H. R. Barton, K. Nakanishi, O. Meth-Cohn, Elsevier, Vols 1-9, 1999.
5. Chemistry of Natural Products, N. R. Krishnamurty, University Press, 2nd Edn., 2010.
6. Organic Chemistry of Natural Products. Vol.-I and II, G.R. Chatwal, Himalaya Publishing House

**Course outcomes:**

* Identify different types of natural products, their occurrence, structure, importance as medicines) and properties.
* Demonstrate various synthetic routes for synthesis of some selected natural products.
* Describe the total synthetic approaches for synthesis of some selected drugs.

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| **POECH303**: **Chemistry of Natural Product** |
| 1 | Program Outcomes | a | b | c | d | e | f | g | h | i | j | k |
| 2 | Mapping of Course Outcomes with Program Outcomes | \* |  |  |  |  |  | \* |  |  |  | \* |
| 3 | Category | Core | Allied Elective | Free Elective |
|  |  |  | \* |

**Lab 7: Environmental Chemistry Laboratory (PLCCH301)**

**Prerequisite:** Nil

**Purpose:**

**Course Objectives:**

* 1. To determine the physical properties of water.
	2. To estimate the dissolved impurities in water.
	3. To verify the quality of water for their applications.

**Syllabus**.

**Water Quality Analysis**

1. Determination of pH
2. Determination of turbidity.
3. Determination of alkalinity and acidity.
4. Determination of Optimum dose of coagulants by jar test.
5. Determination of Total Hardness.
6. Determination of Total solids and suspended solids.
7. Determination of Residual chlorine.
8. Determination of Chloride, phosphate and sulphate.
9. Chemical Oxygen Demand.
10. Determination of Biochemical Oxygen Demand.
11. Determination of Dissolved Oxygen.

**Essential readings:**

1. A Laboratory Manual for Environmental Chemistry, R. Gopalan, Amirtha Anand, R. Wilgred Sugumar, I. K. International Pvt Ltd, 1st Edn., 2008.
2. Principles of Environmental Chemistry, James E Girard, Jones & Bartlett, 2nd Edn., 2009.

**Course Outcomes:**

* Ascertain the physical properties of water.
* Determine quantitatively the amount of dissolved impurities in water.
* Establish the quality of water for their applications.

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| **PLCCH301**: **Environmental Chemistry Laboratory** |
| 1 | Program Outcomes | a | b | c | d | e | f | g | h | i | j | k |
| 2 | Mapping of Course Outcomes with Program Outcomes |  |  |  | \* | \* |  | \* |  |  | \* |  |
| 3 | Category | Core | Allied Elective | Free Elective |
|  | \* |  |  |

**Major Project: Project & Literature Search (PPRCH301)**

**Prerequisite:** Nil

**Purpose:**

**Course Objectives:**

* 1. To expose the students to handle the instruments to know their practical uses.
	2. To get knowledge on scientific advances in a particular field of research.
	3. To improve upon the technical writing skills on presenting the research outcomes.

A student has to carry out an original and innovative research work according to his/her area of interest in applied chemistry under the guidance of faculty member of CET and or in collaboration with expert(s) from other institutes. He/she has to submit a report of the findings and present the outcome of the research work.

**Course Outcomes:**

* Create interest on R&D activities.
* Get experience in handling of instruments for their practical applications.
* Garner knowledge on scientific advances in a particular field of research.
* Improve upon the technical writing skills on presenting the research outcomes

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| **PPRCH301**: **Project & Literature Search** |
| 1 | Program Outcomes | a | b | c | d | e | f | g | h | i | j | k |
| 2 | Mapping of Course Outcomes with Program Outcomes |  | \* |  | \* |  | \* | \* | \* | \* | \* | \* |
| 3 | Category | Core | Allied Elective | Free Elective |
|  | \* |  |  |

**Semester-4**

**Core 8: Organic Chemistry-III (PPCCH401)**

**Prerequisite:** Nil

**Purpose:**

**Course Objectives:**

* 1. To describe the orbital concepts explaining the pericylic reactions and their classifications.
	2. To discuss on various facets of sigmatropic rearrangements.
	3. To explore the synthetic strategies through asymmetric synthetic approaches.
	4. To enumerate heterocyclic compounds, their structures and classifications.
	5. To encompass on principles of green chemistry and its applications including synthesis of organic compounds using green chemistry routes.

**Syllabus**

**Module I**

***Pericyclic Reactions and Photochemistry***

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 and PMO approach. Electrocyclic reactions: Conrotatory and disrotatory motion, 4n, 4n+2 and allyl systems.

Cycloadditions: Antarafacial and suprafcial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3 dipolar cycloadditions and cheleotropic reactions.

Sigmatropic rearrangements: Suprafacial and antarafacial shifts of H, Sigmatroic shifts involving carbon carbon moieties, [3,3] and [5,5] Sigmatropic rearrangements, Claisen, Cope and aza-Cope rearrangements, fluxional tautomerism, ene reaction. Norrish Type-I and Type-II reactions. Paternobuichi reaction

**Module II**

***Synthetic Strategies:***

Umpolung reactivity – formyl and acyl anion equivalents. Selectivity in organic synthesis – chemo-, regio- and stereoselectivity. Concepts of asymmetric synthesis – resolution (including enzymatic), desymmetrization and use of chiral auxiliaries. Carbon-carbon bond forming reactions through enolates (including boron enolates), enamines and silyl enol ethers. Michael addition reaction. Stereoselective addition to C=O groups (Cram and Felkin-Anh models).

**Module III**

***Heterocyclic Compounds:***

Introduction to heterocycles, nomenclature, structure, preparation, properties and reactions of furan, pyrrole, thiophene, pyridine, indole, quinoline and isoquinoline.

***Green Chemistry:*** Principles, green solvents, concepts of atom economy, Domino and multi component reactions. Principle and applications to green synthesis of pharmaceuticals and industrial chemicals.

**Essential Readings:**

1. Advanced Organic Chemistry: Part A & B, F. A. Carey and R.J. Sundberg, Springer International, 5th Edn., 2007
2. Principles of Organic Synthesis, R. O. C. Norman and J.M. Coxon, Blackie Academic and Professional, 3rd Edn., 1993.
3. Organic Chemistry, Jonathan Clayden, Nick Greeves, and Stuart Warren, Oxford press, 2nd Edition, 2012.
4. Heterocyclic Chemistry, Thomas. L. Gilchrist, Prentice Hall PTR, 3rd Edn., 1997
5. Heterocyclic Chemistry, J. A. Joules., K. Mills, G.F. Smith, Springer, 3rd Edn., 1995.
6. Green Chemistry and Catalysis, R.A. Sheldon, I. Arends, Ulf Hanefeld, Wiley-VCH. 2007
7. Green Chemistry: Theory and Practice, P.T. [Anastas](http://www.amazon.com/Paul-T.-Anastas/e/B001JSE6SY/ref%3Dntt_athr_dp_pel_1), J.C. [Warner](http://www.amazon.com/John-C.-Warner/e/B00H4B8SYS/ref%3Dntt_athr_dp_pel_2), Oxford University press, 2005.
8. New Trends in Green Chemistry, [V.K. Ahluwalia](https://www.amazon.in/-/e/B001JP25EO/ref%3Ddp_byline_sr_ebooks_1?ie=UTF8&text=V.K.+Ahluwalia&search-alias=digital-text&field-author=V.K.+Ahluwalia&sort=relevancerank), M. ,[Kidwai](https://www.amazon.in/s/ref%3Ddp_byline_sr_ebooks_2?ie=UTF8&text=M.+Kidwai&search-alias=digital-text&field-author=M.+Kidwai&sort=relevancerank), Sringer, 2004.
9. Photochemistry and Pericyclic Reactions, Jagadamba Singh, New age international, Revised 3rd Edn, 2012
10. Pericyclic Reactions A Mechanistic and Problem-Solving Approach, Sunil Kumar, Vinod Kumar, S.P. Singh, Academic Press, 1st Edn., 2016

**Course Outcomes:**

* Comprehensive knowledge on the orbital concepts explaining the pericylic reactions and their classifications.
* Understand various facets of sigmatropic rearrangements.
* Predict the synthetic strategies through asymmetric synthetic approaches.
* Describe heterocyclic compounds, their structures and classifications.
* Illustrate the principles of green chemistry and its applications.
* Elucidate synthetic strategies for synthesis of organic compounds using green chemistry routes.

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| **PPCCH401**: **Organic Chemistry-III** |
| 1 | Program Outcomes | a | b | c | d | e | f | g | h | i | j | k |
| 2 | Mapping of Course Outcomes with Program Outcomes | \* |  |  |  |  |  |  |  |  |  |  |
| 3 | Category | Core | Allied Elective | Free Elective |
|  | \* |  |  |

**Core 9: Polymer Chemistry (PPCCH402)**

**Prerequisite:** Nil

**Purpose:**

**Course Objectives:**

1. To demonstrate the principles of polymerisation and techniques used for polymerisation reactions.
2. To estimate the degree of polymerization and determination of their properties.
3. To illustrate on plastics and to describe the applications of polymers.

**Syllabus**

**Module I**

Fundamental concepts - functionality - principle of polymerisation - addition, condensation polymerisation - ring opening polymerisation - classification - production from coal tar and petrochemicals - Techniques of polymerisation - gas polymerisation, - bulk, solution, suspension and emulsion - melt condensation. Mechanism of polymerisation and general characteristics - free radical - cationic, anionic and coordination polymerisation (Ziegler-Natta catalyst) auto acceleration - Kinetic chain length - degree of polymerisation kinetics of polymerisation (Detailed study) - copolymerisation.

**Module II**

Polymer characterisation - molecular weight, MWD - Mn, Mw, Mv and Mz - end group analysis - viscometry - osmometry - Light scattering - spectral analysis-Thermal properties – Electrical properties, Mechanical and dynamic properties - polymer degradation. Phase transitions of polymers, crystallization and glass transition, mechanism of glass transition, methods of determining Tg.

**Module III**

Studies on individual polymers - plastics, polyurethanes, FIR plastics, GR plastics. Alkyd resins, epoxy resins - phenolics - Melamine resins - compounding of plastics. Rubber - elastomer - vulcanisation, compression mouldings - injection mouldings – lamination, Medicinal applications of polymers, high temperature and fire-resistant polymers. Polymer impregnated concrete, conducting polymers.

**Essential Readings**

1. Test Book of Polymer Science, Jr. Billmeyer, Fred, W. John Wiley & Sons, New York, 3rd Edn., 1984.
2. Polymer Characterization: Physical Techniques, Dan Campbell, Richard A. Pethrick, Jim R. White, CRC Press, 2nd Edn. 2012.
3. Principles of Polymer Systems’, F. Rodrigues, M. Elpaw Hill Book Company, 2nd Edn., l982.
4. Handbook of Biopolymer-Based Materials: From Blends and Composites to Gels and Complex Networks, [S.Thomas](http://www.amazon.com/s/ref%3Ddp_byline_sr_book_1?ie=UTF8&field-author=Sabu+Thomas&search-alias=books&text=Sabu+Thomas&sort=relevancerank) & [D. Durand](http://www.amazon.com/s/ref%3Ddp_byline_sr_book_2?ie=UTF8&field-author=Dominique+Durand&search-alias=books&text=Dominique+Durand&sort=relevancerank), Wiley – VCH, 1st Edn. 2013.

**Course Outcomes:**

* Reveal the principles of polymerisation and techniques used for polymerisation reactions.
* Determine the degree of polymerization, physical properties and describe their properties.
* Distinguish between polymers and plastics; depict the applications of polymers.

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| **PPCCH402**: **Polymer Chemistry** |
| 1 | Program Outcomes | a | b | c | d | e | f | g | h | i | j | k |
| 2 | Mapping of Course Outcomes with Program Outcomes | \* |  |  |  |  |  |  |  |  |  |  |
| 3 | Category | Core | Allied Elective | Free Elective |
|  | \* |  |  |

**AE 5: Materials Chemistry (PPECH401)**

**Prerequisite:** Nil

**Purpose:**

**Course Objectives:**

* 1. To provide knowledge in understanding various common materials of industrial importance and their basic properties.
	2. To describe the basic principles for which the materials could exhibit dielectric and magnetic behaviour.
	3. To demonstrate the electronic and magnetic properties of materials.

**Syllabus**

**Module I**

Materials and their classification: Matter, materials science, broad classification of materials, -metal and alloys, polymers and elastomers, ceramics and refractories, semiconducting and electronic materials, super metal and super conductors, materials for nuclear technology and for aero-space technology, magnetic materials, dielectric materials, optical and opto-electronic materials, bio- medical materials, thermo- electrical materials, structural and construction engineering materials, special and nanomaterials, SMART materials.

General Strategies for preparation and production of materials: Wet chemical processes, the sol-gel route, precursor synthesis, carbo-thermic and thermo- chemical treatments, hydrothermal, pyrochemical, metallurgical and chemical routes, heat treatment methods, surface deposition and film formation methods, special fabrication and processing techniques.

Elementary ideas on basic properties of important materials (overview only): Mechanical properties and impact properties, brittle, malleable and ductile properties, crystalline, poly crystalline materials. Phase rule and phase diagram its applications.

**Module II**

***Dielectric and Magnetic Materials-I:*** Dielectric materials:Electrical dipole moment, dielectrics, dielectric constants and polarization, microscopic displacement, temperature and frequency dependence of dielectric constant, dielectric break down. Synthetic strategies for preparation of dielectric materials. Ferro electrics. Piezoelectric. Pyroelectrics. Application of dielectric materics. Magnetic materials: Concept/ origin of magnetism, dimagnetism, paramagnetism, ferromagnetism, hysteresis- soft and hard magnets. Synthetic strategies. Ferrites, ortho-ferrites and plumba ferrites. Applications of magnetic material, magnetic bubbles.

**Module III**

***Dielectric and Magnetic Materials-II:*** Semiconductor and electronic materials: Band concept for insulator, conductor and semi - conductor(elementary), intrinsic and extrinsic semi-conductor, conductivity, n- and p- type semiconductor, carrier and hole mobility and concentration Fermi level, density of electrons in the conduction band and density of holes in valence band, concentration of electrons in the CB of n- type and holes in VB of p-type semiconductor. Hall effect- hall voltage and Hall coefficient and application. Fabrication and processing of semiconductors. Film formation and surface coating techniques. Application of semiconductors. Film formation and surface coating techniques. Applications of semiconductors. Preparation of single crystals.

**Essential Readings:**

1. Calister’s Material Science and Engineering, R. Balasubramaniam, Wiley-India, 2nd Edn., 2014.
2. Magnetic and Dielectric Properties of Materials: Basics, Theories and Experiments, M. M. Rahman, LAP LAMBERT Academic Publishing, 1st Edn., 2012
3. Chemical Processing of Advanced Materials: L. L. Hench and J. K. West, John Wiley, 1st Edn., 1992.
4. Preparative Methods in Solid State Chemistry, P. Hagnmuller (ed), Academic Press, 1st Edn., 1972.
5. Sol-Gel Science, C. J. Brinker & G. W. Scherer, Academic Press, 1st Edn., 1980.
6. Semiconductor Material and Device Characterization, Dieter K. Schroder, Springer, 3rd Edn., 2006.
7. Introduction to Semiconductor Materials and Devices, M.S.Tyagi , John Wiley & Sons, 3rd Edn., 2008.
8. The Materials Science of Semiconductors, Angus Rockett, Springer, 1st Edn., 2008.

**Course Outcomes:**

* Identify various common materials of industrial importance and know their basic properties.
* Understand the basic principles of the dielectric and magnetic materials.
* Reveal the electronic and magnetic properties of materials for their applications.

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| **PPECH401**: **Materials Chemistry** |
| 1 | Program Outcomes | a | b | c | d | e | f | g | h | i | j | k |
| 2 | Mapping of Course Outcomes with Program Outcomes | \* | \* |  | \* |  |  |  |  |  | \* |  |
| 3 | Category | Core | Allied Elective | Free Elective |
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**AE 6: Bioinorganic & Supramolecular Chemistry (PPECH402)**

**Prerequisite:** Nil

**Purpose:**

**Course Objectives:**

1. To explain the importance of metal ions in living system and describe their storage and transport mechanisms.
2. To discuss various types of metalloenzymes and their roles in biological systems.
3. To explain the pathways of biological systems like nitrogen fixation and photosynthesis and to delineate the mechanism of oxygen transport and its storage.
4. To define the supramolecular chemistry, molecular recognition and some selected building blocks referred in supramolecular chemistry.

**Syllabus**

**Module I**

***Metal ions in biological systems and its storage transport and biomineralization:*** Essential and trace elements, Ferritin, transferrin, and siderophores.

***Calcium in Biology:*** Transported regulation, Intracellular Ca2+ transport, Ca2+ATpase, Na+/Ca2+ exchange, mitochondrial influx and efflux. Inositol triphosphate, Ca2+ regulated intracellular processes: Calmodulin, Troponin C.

***Metalloenzymes:*** Zinc enzymes: Carboxypeptidase and carbonic anhydrase; Iron enzymes: catalase peroxidase and cytochromes, Cyt-P450; Copper enzymes: Superoxide dismutase; Molybdenum oxatransferase enzymes: xanthine oxidase. Coenzyme vitamin B12. sulphur proteins

**Module II**

***Nitrogen fixation:*** Biological nitrogen fixation, molybdenum nitrogenase, spectroscopic and other evidence, other nitrogenases model systems.

***Photosynthesis****:* Chlorophylls, photo system I and photo system II in cleavage of water.

***Transport and storage of dioxygen****:* Heme proteins and oxygen uptake, structure and function of hemocyanin and hemerythrin, model synthetic complexes of iron, cobalt and copper.

**Module III**

***Supramolecular Chemistry****.*

Introduction-the meaning of supramolecular chemistry, phenomenon of molecular recognition and their quantification

Building blocks of supramolecular chemistry- acyclic receptors for neutral and charged guests, macrocycles and crown ethers, macrobicycles and cryptands, macropolycycles, cucurbiturils and cyclodextrins

**Essential Readings:**

1. Principles of Bioinorganic Chemistry, S.J. Lippard and J. M. Berg., University Science Books. 1994
2. Bioinorganic Chemistry, I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valenting, University Science Books.
3. Progress in Inorganic Chemistry, Vols 18 and 38 ed, by J. J. Lippard, Wiley.
4. Bioinorganic Chemistry, Asim K. Das, Books and Allied, 2nd Edn., 2007.
5. Supramolecular Chemistry, J. W. Steed and J. L. Atwood, Willey, 2nd Ed., 2009.
6. Bioinorganic and Supramolecular Chemistry, P. S. Kalsi, J. P. Kalsi, New Age International, 2nd Edn., 2012.
7. An Introduction of Supramolecular Chemistry, Asim K. Das, Books and Allied, 1st Edn., 2017.
8. Supramolecular Chemistry: Concepts and Perspectives, J.M. Lehn, VCH, Weinheim, 1995
9. Principles and Methods in Supramolecular Chemistry, H. J. Schneider and A. Yatsimirsky, Wiley, New York, 2000.
10. Supramolecular Chemistry - Fundamentals and Applications, Ariga, Katsuhiko & Kunitake, Toyoki, Iwanami Shoten Publishers, Tokyo, 2006,

**Course Outcomes:**

* Understand the role of metal ions in living system and depict their storage and transport mechanisms.
* Describe various types of metalloenzymes and their roles in biological systems.
* Demonstrate pathways of biological systems like nitrogen fixation and photosynthesis and explain the mechanism of oxygen transport and its storage.
* Illustrate supramolecular chemistry, molecular recognition and enumerate some selected building blocks referred in supramolecular chemistry.

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| **PPECH402 Bioinorganic & Supramolecular Chemistry** |
| 1 | Program Outcomes | a | b | c | d | e | f | g | h | i | j | k |
| 2 | Mapping of Course Outcomes with Program Outcomes | \* |  |  |  |  |  |  |  |  |  | \* |
| 3 | Category | Core | Allied Elective | Free Elective |
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**FE 3: Pharmaceutical Chemistry – II (POECH401)**

**Prerequisite:** Nil

**Purpose:**

**Course Objectives:**

1. To describe the classification, structure, mode of action, uses and synthesis of some selected drugs like steroid, thyroid, anti-thyroid, insulins.
2. To delineate the mechanism of action of some drugs like diuretics, cardiovascular and some anticoagulants.
3. To define the chemistry and chemotherapy of some common drugs.

**Syllabus**

**Module–I**

Classification, mode of action, uses and structure activity relationship of the following classes of drugs. Synthesis of those compounds only exemplified against each class.

***Steroids and Related Drugs:*** General study on Steroidal nomenclature and stereochemistry, Androgens and anabolic agents, Estrogens and progestational agents. Synthesis of Progesterone from diosgenin, Diethyl satilboestrol, Synthesis of Testosterone from Cholesterol, General study of structural formula and therapeutic uses of steroidal ant-inflammatory agents.

***Thyroid and Anti thyroid drugs****:* Thyroxine, Liothyronine, Propythiouracil, Carbimazole

***Insulin, Insulin preparations and oral hypoglycaemic agents:*** Chloropropamide, Tolbutamide, Glibenclamide, Phenformin.

**Module-II**

***Diuretics:*** Acetazolamide, Chlorthiazide, Furosemide.

***Cardiovascular drugs:*** Antihypertensives, Anti-anginal agents, Anti-arrhythmics and Antilipidemics**:** Clonidine, Methyldopa, Procainamide, Nifedipine, Prazosin, clofibrate.

Anticoagulants: Heparin, Coumarins, Phenindione derivatives.

**Module III**

***Chemistry of Chemotherapy:***

***Sulphonamides****:* Sulphadiazine, Sulphamethoxazole, Sulphacetamide sodium.

General study of Qunolones and Fluoroqunolones.

***Antibiotics****:* General study of β-Lactum antibiotics (Penicillins and Cephalosporins), Aminoglycosides, Tetracyclines, Macrolides, Lincomycins, Polypeptides, Anticancer antibiotics: synthesis of Methecillin, Ampicillin.

***Anti-TB and anti-leprosy Drugs****:* Isoniazid, Ethambutrol, Pyrazinamide. Antifungal agents: Griseofulvin, Nystatin, Ketoconazole, Amphotericin B.

**Module–IV**

***Anti-Malarial Drugs****:* Chloroquine, Pamaquine, Mepacrine, Proguanil, Pyrimethamine

***Anti-amoebic agents****:* Metronidazole, Diloxamide furoate

***Anti-viral including anti-HIV agents****;* Acyclovir, Zidovudine

**Essential books**

1. Wilson and Grisvold’s Text Book of Organic Medicinal and Pharmaceutical Chemistry, J.M. Beale, Jr. J.H. Block, Lippincott Williams & Wilkins, 12th Edn, 2011.
2. Foye’s Principles of Medicinal Chemistry, Lippincott Williams & Wilkins, 7th Edn, 2012.
3. A Text Book of Medicinal Chemistry: Synthetic and Biochemical Approach, S.N. Pandeya, Vol.2, S. G. publisher, 1st Edn, 2009.
4. Medicinal Chemistry, Ashutosh Kar, New Age International Publishers, 5th revised and expanded Edn, 2010.
5. Text Book of Pharmaceutical Chemistry, A.O. Bentley, and J.E. Driver, Oxford Medical Publications, 8th illustrated Edn., 1969.
6. Introduction to Medicinal Chemistry, Graham L. Patrick, Oxford, 6th Edn., 2017.

**Course Outcomes:**

* Demonstrate the classification, structure, mode of action, uses and synthesis of some therapeutic drugs like steroid, thyroid, anti-thyroid, insulins.
* Understand the mechanism of action of some drugs like diuretics, cardiovascular and some anticoagulants.
* Describe the chemistry and chemotherapy of some common drugs.

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| **POECH401 Pharmaceutical Chemistry – II** |
| 1 | Program Outcomes | a | b | c | d | e | f | g | h | i | j | k |
| 2 | Mapping of Course Outcomes with Program Outcomes |  |  |  |  |  |  | \* |  |  | \* | \* |
| 3 | Category | Core | Allied Elective | Free Elective |
|  |  |  | \* |

**FE 3: Functional Materials (POECH402)**

**Prerequisite:** Nil

**Purpose:**

**Course Objectives:**

1. To discuss the salient features of combinatorial chemistry and its applications for synthesis of combinatorial libraries.
2. To describe the composites, their functions and uses.
3. To delineate the synthetic strategies for synthesis of some selected artificial important organic compounds.

**Syllabus**

**Module I**

Combinatorial chemistry: Resins, protecting groups, solid-phase synthetic strategies, synthesis of peptides, synthesis of some novel biologically important N-heterocyclic building blocks using amino acids, techniques for preparation of combinatorial libraries.

**Module II**

Composites: Micro and macro composites, fibre -reinforced composites (FRPs), matrix based composites. Polymer- matrix composites (PMCs), metal- matrix composite (MMCs), ceramic- matrix composites (CMCs) as in construction materials, carbon- carbon composites (CCCs), hybrid composites. Uses of composites.

**Module III**

[Cardiovascular drugs](http://en.wikipedia.org/w/index.php?title=Cardiovascular_drugs&action=edit&redlink=1), such as [Alapril](http://en.wikipedia.org/w/index.php?title=Alapril&action=edit&redlink=1) (lisinopril), [Captoril](http://en.wikipedia.org/wiki/Captoril%22%20%5Co%20%22Captoril) (captopril),  .antiulcerants (cimetidine. artificial sweetener [Aspartame](http://en.wikipedia.org/wiki/Aspartame) (N-L-α-Aspartyl-L-phenylalanine 1-methyl ester) , [riboflavin](http://en.wikipedia.org/wiki/Riboflavin) (B2), and [thiamine](http://en.wikipedia.org/wiki/Thiamine) (B1)

**References**

1. Eco-friendly Synthesis of Fine Chemicals, Edited by Roberto Ballini, James H. Clark and George A. Kraus, from RSC Green Chemistry Series, Royal Society of Chemistry, 1st Edn., 2009.
2. Aqueous Microwave Assisted Chemistry: Synthesis and catalysis, Ed. V. Polshettiwar and R. S. Verma, from RSC Green Chemistry Series, Royal Society of Chemistry, 1st Edn., 2010.
3. Fundamentals of Asymmetric Synthesis, G. L. David Krupadanam, Universities Press, 1st Edn. 2013.
4. W. Bannwarth, B. Hinzen, Combinatorial Chemistry - From Theory to Application

Wiley-VCH, 2nd edition, 2006.

1. Michael Pirrung, Molecular Diversity and Combinatorial Chemistry, Elsevier, 2004.

**Course Outcomes:**

* Understand the salient features of combinatorial chemistry and its applications for synthesis of combinatorial libraries for drug discovery.
* Illustrate the facets of composites, their functions and uses.
* Demonstrate the synthetic strategies for synthesis of some selected artificial important organic compounds.

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| **POECH402 Functional Materials** |
| 1 | Program Outcomes | a | b | c | d | e | f | g | h | i | j | k |
| 2 | Mapping of Course Outcomes with Program Outcomes | \* | \* |  | \* |  |  |  |  |  | \* |  |
| 3 | Category | Core | Allied Elective | Free Elective |
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**FE 3: Nuclear Chemistry (POECH403)**

**Prerequisite:** Nil

**Purpose:**

**Course Objectives:**

1. To describe various types of radioactive decay and detectors.
2. To explain the theories of nucleus and different types of nuclear reactions.
3. To demonstrate the principles of functioning of nuclear reactors and knowhow for nuclear waste management.
4. To discuss on radiation chemistry and the wide-spread applications of radioisotopes.

**Syllabus**

**Module I**

General Aspects of Nuclear Chemistry: Discovery- Types of decay-Decay kinetics: Decay constant, half-life period, mean life Parent daughter decay-growth relationships-Secular and transient equilibrium-Units of radioactivity- Alpha, beta and gamma decay: Theory of decay, energies and properties-Artificial radioactivity- Detectors: Ionization chamber, electron pulse counters, scintillation detectors, semiconductor, detectors, thermo luminescence detectors and neutron detectors. Bethe notation-Types of nuclear reactions: The compound nucleus theory-Reaction cross section- Transmutation reactions, elastic and inelastic scattering, spallation, fragmentation, stripping and pick-up, fission, fusion, photonuclear reactions, Thermonuclear reactions.

**Module II**

Nuclear Disintegration and Reactors: The fission energy – Reproduction factor - Classification of reactors- Based on Moderators, Coolant, Phase of Fuel and Generation -Principle of Thermal nuclear Reactors: The four factor formula - Reactor power – Critical size of a thermal reactor – Excess reactivity and control - Breeder reactor - Reprocessing of spent fuels - Nuclear waste management – Safety culture – Active and passive safety, containment building, nuclear criticality safety, ionizing radiation protection – enforcement agencies.

**Module III**

Radiation chemistry – Passage of radiation through matter – Units for measuring radiation absorption – Radiation dosimetry – Radiolysis of water – Free radicals in Water Radiolysis –Chemical dosimetry: Radiolysis of Fricke Dosimeter Solution.

Application of radioisotopes: probing by isotopes, reactions involved in the preparation of radioisotopes, The Szilard-Chalmer’s Reaction – Radiochemical principles in the use of Tracers – Applications of radioisotopes as tracers- Chemical investigations, analytical applications, agricultural and industrial applications -Neutron Activation Analysis – Carbon and Rock Dating – Use of nuclear reactions- Radioisotopes as source of electricity – Nuclear medicines.

**Essential Readings**

1. Essentials of Nuclear Chemistry, Arnikar, H. J., New Age International Publishers Ltd., New Delhi, 4th Edn., 1995.
2. Nuclear and Radiochemistry, K. H. Lieser, Wiley-VCH, 2nd revised Edn, 2001.
3. Radiochemistry and Nuclear Chemistry, G. Choppin, J. O Liljenzin and J. Rydberg. Butterworth-Heinemann, Oxford, 3rd Edn., 2002.
4. Modern Nuclear Chemistry, [Walter D. Loveland](http://www.amazon.com/Walter-D.-Loveland/e/B001HD1KZI/ref%3Ddp_byline_cont_book_1), [David J. Morrissey](http://www.amazon.com/s/ref%3Ddp_byline_sr_book_2?ie=UTF8&field-author=David+J.+Morrissey&search-alias=books&text=David+J.+Morrissey&sort=relevancerank), Wiley, 2nd Edn. 2006.

**Course Outcomes:**

* Encompass various types of radioactive decay and detectors.
* Illustrate the fundamental theories of nucleus and different types of nuclear reactions.
* Explain the principles of functioning of nuclear reactors and processes followed for nuclear waste management.
* Understand radiation chemistry and describe the wide-spread applications of radioisotopes.

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| **POECH403 Nuclear Chemistry** |
| 1 | Program Outcomes | a | b | c | d | e | f | g | h | i | j | k |
| 2 | Mapping of Course Outcomes with Program Outcomes | \* |  |  |  |  |  | \* |  |  |  | \* |
| 3 | Category | Core | Allied Elective | Free Elective |
|  |  |  | \* |

**Lab 8: Advanced Organic Chemistry Laboratory (PLCCH401)**

**Prerequisite:** Nil

**Purpose:**

**Course Objectives:**

* 1. To identify the functional groups in organic compound through qualitative analysis.
	2. To know the procedure of distillation and separation techniques and apply these to organic compounds.
	3. To characterize the functional groups of organic compounds through IR spectra.
	4. To practice standard synthesis procedure for synthesis of some organic compounds.
	5. To estimate organic compounds using standard methods.
	6. To use the ChemDraw software to draw the structure of compounds.

**Syllabus**

1. Separation, purification and identification of compounds of binary mixture using TLC and column chromatography.
2. Application of steam distillation in isolation of essential oil (clove) and perfume (rose).
3. Interpretation of IR spectra for functional group identification.
4. Preparation of paracetamol, aspirin, and some dyes and indicators.
5. Preparation of (i) o-iodobenzoic acid from anthranilic acid, furoic acid from furfural, (ii) Thiamine catalysed benzoin condensation and (iii) benzil from benzoin.

**Essential Readings:**

1. Experiments and Techniques in Organic Chemistry, D. J. Pasto, C. R. Johnson & M. J. Miller, Printice Hall, 6th Edn.,1992.
2. Systematic Qualitative Organic Analysis, H. Middleton, Rupa Publishing House, 2nd Edn., 1982.
3. Hand Book of Organic Analysis, Qualitative & Quantitative, M. T. Clarke, E. Arnold (publisher)
4. Text book of Practical Organic Chemistry, A. I. Vogel, ELBS (London), 5th Edn., 1989.
5. Macro-scale and Micro-scale Organic Experiments, K. L. Williamson, D. C. Heath & Co., 2nd Edn., 1994.

**Course Outcomes**

* Identify the functional groups in organic compound through qualitative analysis.
* Separate the organic compounds by distillation and separation techniques.
* Characterize the functional groups of organic compounds by IR spectra.
* Synthesis of some organic compounds following standard procedures.
* Estimate organic compounds using standard methods.
* Draw the structure of organic compounds using Chem-Draw software.
* Prediction of the molecular properties based on different quantum mechanical theories using Gaussian9 softwares.

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| **PLCCH401**: **Advanced Organic Chemistry Laboratory** |
| 1 | Program Outcomes | a | b | c | d | e | f | g | h | i | j | k |
| 2 | Mapping of Course Outcomes with Program Outcomes |  | \* | \* | \* | \* | \* |  |  |  |  |  |
| 3 | Category | Core | Allied Elective | Free Elective |
|  | \* |  |  |

**Lab 9: Physical Chemistry Laboratory – II (PLCCH402)**

**Prerequisite:** Nil

**Purpose:**

**Course Objectives:**

* 1. To perform some experiments for determination of physical properties/parameters of surfactants, solvents, acids etc.
	2. To apply the analytical and experimental techniques for validating photochemical laws and studying thermogravimetric analysis and fast reactions.

**Syllabus**

1. Determination of CMC of surfactants by different methods.
2. Adsorption isotherm studies.
3. pKa determination of tribasic acid by pH titration method
4. Iodination of acetone by spectrophotometric method
5. Fluorometry studies of naphthalene/anthracene.
6. Study of fast reactions by Stopped flow Spectrophotometry (reaction of Fe(III)thiocyanate and ascorbic acid).
7. Thermogravimetric analysis of calcium oxalate and copper sulphate.
8. Determination of surface tension by tensiometer.
9. Cyclicvoltametric study of Ferri-Ferrocyanide system

**Essential Readings:**

1. Experiments in Physical Chemistry, D. P. Shoemaker, C. W. Garland & J. W. Nibber, McGraw Hill, 5th Edn., 1989.
2. Text book of Practical Organic Chemistry, I. Vogel, ELBS, London, 5th Edn., 1989.
3. Laboratory Manual of Organic Chemistry, B. Dey and M. V. Sitharaman, Revised by T.R. Govindachari, Allied Publishers Ltd., New Delhi. 4th Edn., 1992.

**Course outcomes:**

* Develop expertise for performing experiments to determine the physical properties/parameters of surfactants, solvents, acids etc.
* Learn experimental techniques to validate photochemical laws.
* Study thermogravimetric analysis and fast reactions.

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| **PLCCH402 Physical Chemistry Laboratory – II** |
| 1 | Program Outcomes | a | b | c | d | e | f | g | h | i | j | k |
| 2 | Mapping of Course Outcomes with Program Outcomes | \* | \* |  | \* |  | \* |  |  |  |  |  |
| 3 | Category | Core | Allied Elective | Free Elective |
|  | \* |  |  |

**Lab 10: Computational Chemistry Laboratory - II (PLCCH403)**

**Prerequisite:** Nil

**Purpose:**

**Course Objectives:**

* + 1. To get conversant with drawing the structures uniformly using Chemdraw softwares.
		2. To predict the molecular properties based on different quantum mechanical theories using Gaussian9 softwares.
		3. To apply Gaussian softwares for molecular modelling studies.

**Syllabus**

1. Practicing Chem-Draw software to draw the structures.
2. Use of Gaussian9 software to predict the energies, bond angle, bond length, spectral properties of some small molecules using different methods and basis sets.

**Essential Readings:**

1. Introduction to Computational Chemistry, F. Jensen, John Wiley & Sons Ltd, 2nd edn, 2007.
2. Essentials of Computational Chemistry, C. J. Cramer, Wiley & Sons ltd., 2nd edn, 2004.
3. Computational Chemistry, D. C. Young, Wiley-Interscience, 1st edn, 2001.

**Course Outcomes:**

* Develop expertise on drawing the structures uniformly using Chemdraw softwares.
* Project molecular properties based on different quantum mechanical theories using Gaussian9 softwares.
* Perform molecular modelling studies using Gaussian9 softwares.

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| **PLCCH403 Computational Chemistry Laboratory - II** |
| 1 | Program Outcomes | a | b | c | d | e | f | g | h | i | j | k |
| 2 | Mapping of Course Outcomes with Program Outcomes |  |  | \* | \* | \* |  | \* |  |  |  | \* |
| 3 | Category | Core | Allied Elective | Free Elective |
|  | \* |  |  |

**Seminar: Seminar & Scientific Writing (PSECH401)**

**Prerequisite:** Nil

**Purpose:**

**Course Objectives:**

* 1. To develop the attitude and to build confidence for presenting scientific facts and or theories etc.
	2. To get the opportunities to explore own potentials on creative thinking through learning and writing skill.

**Course Outcomes:**

* Attain proper attitude and confidence for presenting scientific facts and or theories etc.
* Determine own potentials on creative thinking through learning and writing skill.

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| **PSECH401 Seminar & Scientific Writing** |
| 1 | Program Outcomes | a | b | c | d | e | f | g | h | i | j | k |
| 2 | Mapping of Course Outcomes with Program Outcomes |  |  |  |  |  |  |  | \* | \* |  | \* |
| 3 | Category | Core | Allied Elective | Free Elective |
|  | \* |  |  |