Department of Chemistry
JRF Course

Monsoon Semester

Sl. No.	Course Code	Subject Name	L-T-P	Credit
1	HSI500	Research and Technical Communication	3-0-0	9
2	CYC 540	Research Methodology and Statistics	3-0-0	9
3	CYC 521	Advanced Spectroscopic Methods	3-0-0	9
4	CYC 522	Advanced Techniques in Materials Characterization	3-0-0	9
5	DE-1	Any one out of Table 2	3-0-0	9

Winter Semester

Sl. No.	Course Code	Subject Name	L-T-P	Credit
1	CYC 523	Numerical Analysis and Methods in Chemistry	3-0-0	9
2	DE-2	Any one out of Table 2	3-0-0	9
3	DE-3	Any one out of Table 2	3-0-0	9
4	DE-4	Any one out of Table 2	3-0-0	9

Table 1: List of Core Courses

List of Core Courses			
Sl. No.	**Course No.**	**Course Name**	**L-T-P**
1	CYC 522	Advanced Techniques in Materials Characterization	3-0-0
2	CYC 523	Numerical Analysis and Methods in Chemistry	3-0-0
3	CYC 524	Advanced Spectroscopic Methods	3-0-0
4	CYC 540	Research Methodology and Statistics	3-0-0

Table 2: List of Elective Courses

List of Open Electives			
Sl. No.	Course No.	Course Name	L-T-P
1	CYO 501	Instrumental Techniques for Material Characterization	3-0-0
2	CYO 502	Material Sciences and Technology	3-0-0
3	CYO 506	Electrochemical Strategies in Energy Systems	3-0-0
4	CYO 507	Nuclear & Radiation Chemistry	3-0-0
5	CYO 508	Surface Science & Catalysis	3-0-0
List of Departmental Electives			
Sl. No.	Course No.	Course Name	L-T-P
1	CYD 501	Medicinal Chemistry	3-0-0
2	CYD 502	Polymer Chemistry	3-0-0
3	CYD 503	Cluster Chemistry	3-0-0
4	CYD 504	Symmetry in Bonding	3-0-0
5	CYD 505	Asymmetric Synthesis	3-0-0
6	CYD 506	Computational Chemistry	3-0-0
7	CYD 507	Bio-inorganic Chemistry	3-0-0
8	CYD 508	Chemistry of *f*–Block Elements	3-0-0
9	CYD 509	Modern Terpyridine Chemistry	3-0-0
10	CYD 510	Chemistry of Nanostructured Materials	3-0-0
11	CYD 511	Advanced Methods in Organic Synthesis	3-0-0
12	CYD 512	Modern aspects of Catalysis and Surface science	3-0-0
13	CYD 513	Electroanalytical methods	3-0-0
14	CYD 514	Single crystal X-ray diffraction	3-0-0
15	CYD 515	Advances in Nonconventional Energy Systems	3-0-0
16	CYD 516	Advanced heterocyclic chemistry	3-0-0
17	CYD 517	Oligosaccharide synthesis	3-0-0
18	CYD 518	Metalloenzymes-Special Topics	3-0-0
19	CYD 519	Characterization Techniques for inorganic chemists	3-0-0
20	CYD 520	Advanced Fluorescence Spectroscopy	3-0-0
21	CYD 521	Nanomaterials for Advanced Applications	3-0-0
22	CYD 522	Advanced Biocatalysis	3-0-0
23	CYD 523	Supramolecular chemistry & Molecular recognition	3-0-0
24	CYD 532	Solid State Materials: Chemistry& Engineering	3-0-0
25	CYD 533	Advanced Electrochemistry	3-0-0
26	CYD 534	Heterocyclic Chemistry	3-0-0
27	CYD 535	Main Group Chemistry	3-0-0
28	CYD 536	Science of Corrosion & Corrosion Control	3-0-0

Course Content for Ph. D. PROGRAMME
CORE COURSES

CYC 540	**Research Methodology and statistics**	**(3-0-0)**

- **Course Philosophy:**
  The course is aimed to introduce the ethics of research, Literature survey, Designing a research scheme, execution, data handling, writing a research manuscript and patent filling.
- **Learning Outcomes:**
  At the end of the course, the learners should be able to:
  - ✓ identify the do's and don'ts of research work.
  - ✓ How to do literature survey and defining a research problem
  - ✓ Design a research scheme and data handling
  - ✓ Write research article and patent.

Unit I **[8L]**

Introduction to Research Methodology, Philosophy of Research, Ethics in Research, Conceptualizing, Literature Survey and defining the research problem. Evaluation of Research. Plagiarisms.

Unit II **[12L]**

Research Design, Sampling Design, Measurement and Scaling Techniques, Methods of Data Collection, processing and Analysis of Data, Sampling Fundamentals, Practical Aspects of Chemical Analysis.

Unit III **[12L]**

Tools and Techniques for scientific writing, writing a Research Paper, Preparing a Manuscript for Submission, Fundamental of patent filling.

Unit IV **[10L]**

Handling of air and moisture sensitive compounds, dry box, glove box, Schlenk line and vacuum line techniques and Fume Hood. General procedures for handling all chemicals in addition to specific procedures for chemical hazard groups (Toxins, Flammables, Carcinogenic, Corrossives, Compressed Gases, Peroxide Formers, Reactive chemicals).

Reference:

1. Research-Methodology: Methods-and-Techniques by C.R. Kothari, New age international (p) limited, 2004, ISBN-10: 8122436234.
2. Research Methods Knowledge Base by William Trochim, Atomic Dog; 3rd edition, 2015, ISBN-10: 1592602916.
3. From Research to Manuscript: A Guide to Scientific Writing by Michael Jay Katz, Springer, 2006, ISBN-10: 1402094663.

CYC 524	**Advanced Spectroscopic Methods**	**(3-0-0)**

- **Course Philosophy:**
  The subject offers the readers a fundamental understanding of the spectroscopic techniques and their application for structure elucidation of natural and synthetic molecules.
- **Learning Outcomes:** At the end of the course the student will be able to analyze the spectral data for elucidating chemicals structure and correlate with their properties.

Unit-I [**14 L**]

One-dimensional spectroscopy (1H, 13C, DEPT, steady-state NOE, saturation transfer), two-dimensional NMR (COSY, NOESY, and HSQC) and their use in structure elucidation.

Unit-II **[14L]**

Applications of Mass spectroscopic methods (EI, CI, SIMS, FAB, MALDI, and ESI) in organometallic and supramolecular chemistry. EPR spectra of transition metal ions and complexes, Zero-field splitting and Kramer's degeneracy, application of ESR spectroscopy.

Unit-III **[14L]**

Applications of UV, IR, and NMR spectral methods in structure determination of natural and synthetic compounds. Advancement of NMR spectroscopy for determination of absolute configuration of chiral molecules and it's application in structural revision of natural products. Principle and applications of Circular Dichroism (CD) and Optical rotatory dispersion (ORD). Chiroptical methods in the stereochemical analysis of natural products.

References:

1. Organic spectroscopy, William Kemp, 3rd edition, Macmillan, 2011.
2. Introduction to Spectroscopy – D. L. Pavia, G.M. Lampman, G. S. Kriz, 4th Edition, Cengage Learning, 2008.
3. Electron Paramagnetic Resonance: Elementary Theory and Practical Applications, John A. Weil, James R. Bolton, 2nd Edition, Wiley, 2007.

CYC 522	**Advanced Techniques in Materials Characterization**	**(3-0-0)**

- **Course Philosophy:**

  The course is aimed to introduce the applications of different advanced characterization methods related to electron microscopy, X-Ray techniques and thermal techniques.

- **Learning Outcomes:**

  At the end of the course, the learners should be able to:
  - ✓ Prepare samples for Electron microscopy, X-Ray and thermal analysis.
  - ✓ Analyze samples by Electron microscopy, X-Ray and thermal techniques.
  - ✓ Data interpretation and plotting.
  - ✓ Learn recent advancement in microscopic, X-Ray and thermal techniques.

Unit I **[18L]**

Applications of Electron Microscopic Techniques: SEM, TEM, EPMA and SPM. Specimen Preparation and Interpretation of data with specific examples. Recent advances in electron microscopic technique and their application.

Unit II **[15L]**

Applications of X-Ray techniques: PXRD, XPS and XRF. Sample Preparation and Interpretation of data with specific examples.

Unit III **[9L]**

Applications of Thermal Techniques: DTA, TGA, DSC. Sample Preparation and data interpretation with specific examples. Evolve gas analysis for various applications.

References:

1. Elements of X-Ray Diffraction, B.D. Cullity S.R. Stock, Third Edition, Pearson Education Limited 2014.
2. Materials Characterization Introduction to Microscopic and Spectroscopic Methods, Yang Leng, John Wiley & Sons (Asia), 2008.
3. Fundamentals of analytical chemistry, Douglas Skoog, Donald West, F. Holler, Stanley Crouch, 9th Edition, Cengage Learning, 2013.

CYC 523	**Numerical Analysis and Methods in Chemistry**	**(3-0-0)**

- **Course Philosophy:**

  The course is aimed to introduce the basics of theoretical and numerical methods for computer simulation of model systems. It also intends to develop elementary

programming skills in C++ to enable them write short programs for performing scientific calculations. Introduction of various simulation techniques using standard softwares.

- **Learning Outcomes:**

  At the end of the course, the learners should be able to:

  ✓ Write short simple programs in C++ .

  ✓ The students should be perform basic molecular modeling for various chemical and physical problems using standard softwaress such as TeraChem, Gaussian, NAMD, AMBER, etc. The student should be also understand simulated results and correlate with corresponding experimental observations.

UNIT-I **[6 L]**

Errors in Chemical Analyses, Random Errors in Chemical Analysis, Statistical Data Treatment and Evaluation, Sampling. Standardization, and Calibration. Usage of packages (e.g. ORIGIN; EXCEL) for data analysis. Curve Fitting: Linear and Non-linear fitting of data.

UNIT -II **[15 L]**

Introduction to programming languages (C++) : data types, arrays, functions, classes and objects, constructors and destructors, function overloading, operator overloading; Basic numerical analysis: solution of linear and nonlinear equations.

UNIT – III **[21 L]**

Review of Basic Concepts: Length and Time Scales, Intermolecular Interactions and Potential Energy Surfaces, Classical Molecular Dynamics (MD): Langevin and Newtonian equations of motions, Various integration algorithms, and Force calculations. All atom and ab-initio molecular dynamics, Quantum mechanics/molecular mechanics (QM/MM) approaches. Use of various commercially available molecular modelling and simulation software (NAMD, AMBER, TeraChem, and GAUSSIAN).

References:

1. Elementary Numerical Analysis-An Algorithm Approach, by S.D. Conte and C. De Boor. McGraw Hill, 1980.
2. Programming: Principles and Practice Using C++ by Bjarne Stroustroup, Addison-Wesley, 2017.
3. Introduction to Computational Chemistry, F. Jensen, John Wiley & Sons, 2007.

ELECTIVES COURSES
OPEN ELECTIVES

CYO 501	Instrumental Techniques for Materials Characterization	(3-0-0)

❖ **Course Philosophy:**
- ✓ With this course students will learn Principle, instrumentation and applications of various X-Ray, Microscopic and Thermal techniques for materials characterizations.

❖ **Learning Outcome:**
- ✓ Characterize materials using advanced characterization techniques.
- ✓ Select and interpret analysis results.
- ✓ Design experiments with improved sample preparation, new measurement procedures and tools
- ✓ Utilize the concept of different materials characterization techniques for qualitative and quantitative analysis.

UNIT -I: **X-Ray Techniques** **[14L]**

Principle, Instrumentation and applications of XRD, XRF (EDS, WDS) and XPS. Crystal Structure determination by XRD. Qualitative and Quantitative elemental analysis by XRF. Surface chemical analysis by XPS. Neutron Diffraction for materials characterization.

UNIT -II: **Microscopic Techniques** **[20L]**

Resolution, magnification, depth of field, Imaging – theory and concepts. Principle, Instrumentation and applications of Scanning electron microscopy, Transmission electron microscopy, Scanning Tunnelling Microscopy, Atomic Force Microscopy. Sample Preparation Techniques for microscopic analysis. Elemental analysis by EPMA. Electron energy loss spectroscopy (EELS) and selected area electron diffraction (SAED) in TEM.

UNIT -III: **Thermal Techniques** **[8L]**

Principle, Instrumentation and applications of TGA, DSC and DTA. Factors affecting thermal analysis. Determination of degradation and cure kinetics by TGA and DSC.

Reference Books:

1. Elements of X-Ray Diffraction, B.D. Cullity, S.R. Stock, Third Edition, Pearson, 2014.
2. Materials Characterization: Introduction to Microscopic and Spectroscopic Methods, Y.Leng, Wiley, 2008.
3. Thermal Analysis, W. M. Wandlandt, Third Edition, Wiley, 1986.

CYO 502	Materials Science and Technology	(3-0-0)

❖ **Course Philosophy:**
- ✓ With this course students will be introduced to the concepts related to materials science and technologies, their classifications and relation between processing, structure, and physical properties

❖ **Learning Outcome:**
- ✓ Classify materials based on their properties and establish structure properties relationship.
- ✓ Correlate effect of crystal structure, defects and imperfections on materials properties.
- ✓ Identify the causes of failures and characterize materials with Thermal, spectroscopic and mechanical methods.
- ✓ Identify importance of composites, their processing, and characterization.

Unit -I **[14 L]**

Introduction to Materials Science, Classification of Materials, Modern Materials Needs, Processing/Structure/Properties/ Performance Correlations. Structure of Crystalline Solids, Geometry of crystals- the Bravais lattices, Crystal directions and Planes- Miller

indices, Structure determination-X-ray diffraction, Braggs Law, the power method. Imperfections in Solids: Point Imperfections, Line imperfections- edge and screw dislocations, Surface imperfections. Phase Diagrams.

Unit -II **[14L]**

Mechanical Properties, Failure: Fracture, Creep, Fatigue. Electrical, Magnetic, Thermal and optical properties of materials. Characterization of Materials: Mechanical, Thermal and Spectroscopic techniques. Properties of Selected Engineering Materials.

Unit -III **[14L]**

Polymer Structures. Characteristics, Applications, and Processing of Polymers, Composites: Significance and Classification. Processing, Characterization and Applications of Composites. Advanced Materials: Smart materials, Biomaterials, Nanomaterial and Nanocomposites.

Reference Books:

1. Materials Science and Engineering: An Introduction, William D. Callister, Jr. David G. Rethwisch, 2013, Wiley.
2. Solid State Chemistry and its Applications, Second Edition, Anthony R. West, 2014, Wiley.
3. Polymer Science & Technology – Plastics, Rubbers, Blends and Composites. Premamoy Ghosh. 3rd Edition, McGraw Hill Edu. (India) Private Limited, 2010.

CYO 506	**Electrochemical Strategies in energy systems**	**(3-0-0)**

- **Course Philosophy:** This course will impart
  - ✓ Fundamental understanding of the applications of electrochemistry
  - ✓ Electrochemical techniques related to conversion and storage energy.
- **Learning Outcome:** After studying this course, students should be able to:
  - ✓ Understand the basic electrochemical techniques used in energy systems.
  - ✓ Study the stability limits and the interpretation of E_H-P_H (Pourbaix) diagram.
  - ✓ Use concepts and models of mimicking systems in artificial photosynthesis.
  - ✓ Understand the basic principles and advances in Fuel-Cell and its technology.

UNIT -I **[18 L]**

Voltammetric, Amperometric, Potentiometric and Coulometric methods in energy systems. Stability limits of water,Pourbaix diagram and its features, Difference in Pourbaix diagram of $[Ru(tpy)(bpy)(OH_2)]^{2+}$ and $[Ru(tpy)(bpm)(OH_2)]^{2+}$. Understanding and case studies of Pourbaix diagram.

UNIT -II **[14 L]**

NAD^+/NADH as a model redox system: Reaction path and case studies. Electrochemical, chemical and photochemical oxidation of Water, reduction of CO_2, Proton Reduction. Case Studies of each system. Electrochemical analogues of Water-gas shift (WGS) reaction and WGS in homogeneous systems; Syn Gas, Fischer-Tropsch process.

UNIT -III **[10 L]**

Fuel Cells Technology: alkaline fuel cells, phosphoric acid fuel cell, molten carbonate fuel cells, solid oxide fuel cells, polymer electrolyte fuel cells; cell components, thermodynamics and kinetics, operation and performance, applications.

Reference Books:

1. Electrochemical Methods: Fundamentals and Applications 2nd Edition, Allen J. Bard and L. R. Faulkner, 2001.
2. Modern Analytical Chemistry, D. Harvey,1st Edition, 2000.
3. Hydrogen and Fuel Cells. Emerging Technologies and Applications. B. Sørensen. 2nd Edition, 2011.

CYO 507	Nuclear & Radiation Chemistry	(3-0-0)

❖ **Course Philosophy:**

- ✓ The course is meant to develop a better understanding of nuclear structure, various nuclear reactions and their implication in harvesting of nuclear energy. The course also introduces important information on nuclear reactor, theory involved and reactor design. It also enhance the knowledge of various applications of radiation chemistry and tracers in various fields.

❖ **Learning outcome:** At the end of the course the students should be able to:

- ✓ The develop an understanding of the nuclear structure, explain the origin of nuclear reactions
- ✓ Differentiate different nuclear energy harvesting technologies, and identify the conditions and parameters for optimum function of nuclear reactor
- ✓ Solve problems involving nuclear reactions, reactors, and those related application of nuclear radiations/tracers
- ✓ Develop understanding of various application of tracers and nuclear radiation in various fields

UNIT -I **[10L]**

Structure of Nucleus, Shell Model, liquid drop model, Collective model, optical model, merits and demerits. Radioactivity: Decay kinetics, α, β decay, γ emission, Parent – daughter decay –growth relationship, secular and transient equilibrium, Theory of α, β and γ decay, selection rules. Artificial radioactivity.

UNIT -II **[15L]**

Nuclear Reactions: Elastic, inelastic, Photonuclear, radiative capture, evaporation, spallation, Fragmentation, and Transfer reactions. Nuclear fission and fusion; Theory of Nuclear fission, fission energy and fission cross-section, Nuclear Reactors: Classification of reactors, reactor power, critical size, Breeder reactor.

UNIT -III **[17L]**

Application of radioactivity: Tracers in medicine, agriculture, chemical investigations; Analytical applications, Industry and in age determinations. Neutron Activation Analysis, advantages and applications. Radiation detectors, Radiolysis of water, Dosimeters

Reference Books:

1. Essentials of Nuclear Chemistry H. J. Arnikar, 4th edition, New Age Publishers, 1995.
2. Nuclear and Radiochemistry, G. Friedlander, J. W. Kennedy, E. S. Macias and J. M. Miller, John Wiley & Sons, 1985.
3. Nuclear and Radiochemistry: Fundamentals and Applications, Karl H. Lieser, 2nd edition, 2001, Wiley, NY.

CYO 508	Surface Science and Catalysis	(3-0-0)

❖ **Course Philosophy:**

- ✓ The course Surface Science and Catalysis has been designed for the students who willpursue their research in the area of heterogeneous catalysis which is related to oil industry, petrochemical industry, and fine chemical synthesis.
- ✓ Apart from catalysis thin film, several techniques for its preparation will be taught.

❖ **Learning Outcome:**

- ✓ Student will come out with a thorough understanding of catalyst preparation, characterization by different techniques, surface chemistry associated with

different reactions which will be useful for them to join in different R&D as well as industry.

- ✓ The thin film, molecular beam epitaxy as well as other topics can be useful for several interdisciplinary researches.

UNIT -I **[12 L]**

Elementary gas phase reaction, Kinetics of diffusion controlled reaction, spill-over effect, multiplet theory, Kinetics of Gas-solid reaction, LH and LR Mechanism Promotional and poisoning effect on catalyst surface, Physisorption and adsorption isotherm, Langmuir and BET isotherm, Hysteresis loop, Chemisorption of gas molecules to the solid surface, Determination of particle size from chemisorption measurement, TPR/TPD/TPO techniques,

UNIT -II **[12L]**

Brief overview of catalytic reactor, fixed bed and batch reactor, mass transfer and heat transfer on the catalyst surface**,** selective oxidation reaction, Hydrogenation reaction, Dehydrogenation reaction Dehydration reaction, Alkylation reaction

UNIT-III **[11L]**

Energy related Catalysis, Oil refining, Hydro treating, Hydrodesulfurization, Hydrodenitrogenation reactions, methane decomposition, steam reforming, cracking and isomerisation reaction Fischer-Troph synthesis, Bio-fuel

UNIT -IV **[7L]**

Mesoporous material, Organic-inorganic hybrid material, Thin film, PVD, CVD, Molecular beam epitaxy techniques, Langmuir-blodget thin film , self-assembled monolayers

Reference Books:

1. Chemical Kinetics, K. J. Laidler, 3rd Edition, Pearson Education India, 1987.
2. Handbook of Heterogeneous Catalysis Vol 1-8, Edited by Gerhard Ertl, HelmuthKnözinger, FerdiSchüth, Jens Weitkamp Wiley-VCH Verlag GmbH& Co. KGaA, Weinheim, Germany, ISBN: 978-3-527-31241-2, 2008
3. The Surface Science of Metal Oxides, Victor E. Henrich, P. A. Cox, Cambridge University Press; New Ed edition, 1996. 2. Current Trends of Surface Science and Catalysis, Jeong Young (Ed.) Park (Author), Jeong Young Park(editor), 1st Edition, Springer, 2013.

DEPARTMENTAL ELECTIVES

CYD 501	Medicinal Chemistry	(3-0-0)

- ❖ **Course Philosophy:**
  - ✓ With this course student will learn the basics of medicinal chemistry and fundamental of drug discovery
- ❖ **Learning Outcome:** By the end of this course, each student should be able to learn:
  - ✓ Knowledge on the fundamental principles of medicinal chemistry and, drug design.
  - ✓ Acquiring knowledge on the strategy of computer aided drug design and their application in modern drug discovery.
  - ✓ Apply the pharmacodynamics and pharmacokinetic principles that describe drug actions.
  - ✓ Basics of Intellectual property (IP) and Regulatory affairs.
  - ✓ Learning the art of synthesis of FDA approved drugs.

UNIT -I **[12L]**

Basics of Drug Action– Enzymes, proteins, antagonist, agonist, Drug-receptor interactions, Drug action through enzyme inhibition, Examples based on kinase inhibition, Drug likeness, Pharmacokinetics, ADME, bioavailability and bioequivalence.Drug metabolism and

elimination, Chirality and drug action.

UNIT -II **[12 L]**

Drug Design-Ligand based drug design,Structure Activity Relationships studies from Hit identification to lead optimization,De Novo drug design techniques: Receptor/enzyme cavity size prediction. Pharmacophore concept: Pharmacophore mapping. Molecular docking, quantitative structure and relationship (QSAR). Informatics methods in drug design, bioinformatics, chemoinformatics.

UNIT –III **[12 L]**

Classification of drugs- Based on structure or pharmacological basis with examples. Anti-bacterials, antivirals, antifungal, anticancer agents, statins, antidiabetic drugs, cardiovascular drugs

UNIT-IV **[6L]**

Synthesis of Marketed Drugs. Introduction to Clinical trials, Fundamentals of Intellectual Property (IP) and regulatory affairs.

Reference Books:

1. Medicinal Chemistry-An Introduction, Gareth Thomas, 2nd edition, 2007,Wiley, NY.
2. An introduction to medicinal Chemistry, Graham L. Patrick, 4th Edition,Oxford,2009.
3. The Organic Chemistry of Drug Design and Drug Action, R.B. Silverman, Academic Press.

CYD 502	Polymer Chemistry	(3-0-0)

- **Course Philosophy:**
  - ✓ With this course students will learn synthesis, structure, properties of polymers and mechanism of polymerizations along their processing and characterizations.
- **Learning Outcome:**
  - ✓ Classify different polymers based on their sources and properties.
  - ✓ Establish mechanism and kinetics of polymerizations along with molecular weight property relationship.
  - ✓ Identify the importance of polymers in field of Biomedical, electronics and advanced applications.
  - ✓ Utilize the concept of polymerization for copolymer and stereo regular polymers synthesis.

UNIT -I **[14L]**

Introduction and common applications of polymers. Classification of polymers. Kinetics and mechanism of chain growth and step growth polymerization. Polymerization processes (Bulk, Solution, Emulsion and Suspension). Molecular weight, molecular weight distribution and degree of polymerization. Significance of Molecular weight and distribution, Experimental methods for determination of molecular weight. Structure-property relationship of polymers. Commercial thermoplastic and thermosetting polymers- Synthesis, properties and applications.

UNIT -II **[14L]**

Copolymers: Classification, synthesis and application. Stereochemistry of Polymerization. Polymer synthesis procedures – FRP, ATRP, RAFT, ROMP, MP, ROP. Synthesis and applications of biodegradable, biomedical polymers. Conducting Polymers. Inorganic Polymers, Vulcanization of Rubbers.

UNIT -III **[14L]**

Polymer processing, Glass transition temperature: significance and determination. Analysis and Testing of Polymers. Advanced Polymers: Smart Polymers, Shape Memory Polymers, Self-Healing Polymers, LCP, Branched polymers (star, dendritic and hyper branched polymers).

Reference Books:

1. Principles of polymerization, George G. Odian, 4th Edition, A John Wiley &Sons, Inc., Publication, 2004.
2. Textbook of Polymer Science, W. F. Billmeyer, 3 rd Edition, A John Wiley & Sons, Inc., Publication, 2007.
3. Polymer Science & Technology–Plastics, Rubbers, Blends and Composites. Premamoy Ghosh. 3rd Edition, McGraw Hill Education (India) Private Limited, 2010.

CYD 503	Cluster Chemistry	(3-0-0)

- Course Philosophy:
  - ✓ The course is intended to provide students the chemistry behind formation of various types of cluster compounds, develop understanding about the bonding involved and predict their structures. It also intended to introduce the role of cluster compound as catalysts.
- **Learning outcome:**

  At the end of the course students should be able to-
  - ✓ Construct the valence bond scheme of boron clusters
  - ✓ Predict the structure of the clusters
  - ✓ Rationalise structure of clusters

UNIT -I **[10 L]**

Clusters: Definition, Clusters of Main Group elements, Clusters of Alkali and Alkaline earth metals, Preparation, structure and bonding, Reactivity of clusters.

UNIT -II **[15 L]**

Higher Boranes: Preparation structure, bonding and reactivity of Higher Boranes and carboranes, Naming of Boranes and carboranes, styx numbers, Wades rules. Clusters of early and late main group elements. Role of ligands in cluster formation, design methodology

UNIT -III **[17L]**

Transition Metal carbonyl clusters, early and late transition metal clusters, Mingo's Rules, Jemmi's '*mno'* rule. Metal-metal multiple bonded systems, structure, bonding and reactivity, Isopoly &h eteropoly acids & salts, PSEP Theory, violations, capping principle, Metal carbonyl hydride clusters, Electron precise molecules, Catalysis by clusters

Reference Books:

1. Basic Organometallic Chemistry: Concepts, Syntheses and Applications, B.D. Gupta, Anil J. Elias, 2nd Edition, University Press, 2013.
2. Inorganic and Organometallic Polymers, V. Chandrasekhar, Springer India, 2005.
3. Concepts and Models of Inorganic Chemistry, Bodie E. Douglas, Darl H. McDaniel and John J. Alexander, 3rd Edition, John Wiley and Sons, 1994.

CYD 504	Symmetry in Bonding	(3-0-0)

- **Course Philosophy:**

  This course will communicate the fundamental understanding of the applications of group theory related to:
  - ✓ The hybrid orbitals,
  - ✓ Molecular orbitals and
  - ✓ Chemical bonding.
- **Learning Outcome:**

  After studying this course, students should be able to:
  - ✓ Bring into fore the molecular orbital theory
  - ✓ The techniques in group theory to interpret bonding in organic molecules as well as transition metal complexes.

- ✓ Use of symmetry in vibrational spectra and structural interpretation.

UNIT -I **[12 L]**

Hybrid orbitals and their symmetries, Hybrid orbitals for σ and π-bonding, Hybrid orbitals as linear combination of atomic orbitals, descending symmetry in Jahn-Teller distortion. The Projection operator, Application of Projection operator method in multi-dimensional representations.

UNIT -II **[20 L]**

Molecular orbitals and hybrid orbitals: Criteria of LCAO Approximation, Construction of SALCs for different geometry of molecules. Designation and symmetry of molecular orbitals. Molecular orbitals of sandwich complexes. Hückel π-orbital method and applications, 1,3 butadiene, Carbocyclic systems. Three centre bonding.

UNIT -III **[10 L]**

Application of normal mode analysis: Geometrical isomer prediction, Structure determination and Linkage isomer prediction, Denticity of anionic ligands, Coordinate bond vibrations, and bonding mode in metal carbonyls.

Reference Books:

1. Chemical Applications of Group Theory, F. A. Cotton, 3rd Edition, John Wiley & Sons, 2008.
2. Group Theory and Chemistry, D. M. Bishop, 1st edition, Dover Publications; Una Rev Edition, 1993.
3. Introduction to Ligand Fields, B. N. Figgis**,** John Wiley & Sons Ltd., London and New York 1966.

CYD 505	**Asymmetric Synthesis**	**(3-0-0)**

- ❖ **Course Philosophy:**
  - ✓ Why asymmetric synthesis is required?
  - ✓ History and progress of asymmetric synthesis.
  - ✓ Understanding the major strategies, techniques and tools for asymmetric synthesis.
- ❖ **Learning Outcome:**
  - ✓ Grasp of the fundamentals of asymmetric synthesis.
  - ✓ Understanding the current tools of asymmetric synthesis.
  - ✓ Designing an asymmetric synthesis

UNIT I **[10L]**

Introduction –Introduction to and recapitulation of terminologies associated to stereochemistry and asymmetric synthesis. Concepts and necessity for asymmetric synthesis.

Chiral induction – Concepts of substrate and reagent controlled asymmetric induction; Concepts of diastereoselective synthesis and double diastereoselective synthesis; Concepts of catalytic asymmetric synthesis, Chiral Pool approach: Advantages and Limitations

"Chirons"– terpenes and carbohydrates as chiral source material – Steven"s steroid intermediate synthesis, Syntheses of biologically relevant compounds, Chiral auxiliary based asymmetric synthesis: Introduction, advantages and disadvantages.

Basic requirements of a chiral auxiliary popular and generally adaptable chiral auxiliaries (Oppolzer, Evans, Enders, Davies, 8-phenyl-menthol, BINOL, etc.)

UNIT II **[14L]**

Chiral diasteroselective and catalytic reactions involving - Asymmetric alkylations of enolates and azaenolates based on organolithiums. Asymmetric 1,2 and 1,4 addition to C=X; Asymmetric aldol and related reactions.

UNIT III **[18L]**

Chiral diasteroselective and catalytic reactions involving - Asymmetric Pericyclic reactions, Asymmetric hydroborations and other reductions. Asymmetric oxidations. Asymmetric

organocatalysis: Chiral amine catalysis.

Reference Books:

1. Principles of Asymmetric Synthesis – R. E. Gawley and J. Aube, Pergamon, 2nd Edition, Elsevier, 2012.
2. Catalytic Asymmetric Synthesis, I. Ojima (ed.), 3rd Edition, Wiley, 2010.
3. Principles and Applications of asymmetric synthesis - Guo-Qiang Lin, Yue-Ming Li, Albert S.C. Chan, John Wiley & Sons, 2001.

CYD 506	Computational Chemistry	(3-0-0)

- **Course Philosophy:**
  - The course is aimed at developing elementary programming skills in C++ to enable them write short programs for performing scientific calculations. Introducing the basics of theoretical and numerical methods for computer simulation of model systems. Introducing various simulation techniques using standard softwares based on time and length scales of various phenomena.
- **Learning Outcome:**
  - ✓ At the end of the course, the learners should be able to:
  - ✓ Write short simple programs in C++ and be able to compile and execute them in a host of machines. Using TeraChem software the students should be able to do basic electronic structure calculations. Use standard software tools such as NAMD, AMBER to perform molecular dynamics simulation of various phenomena. The student should be also able to interpret the simulated data (with its limitations) and correlate with experimental observations.

UNIT –I **[10 L]**

Programming languages (C++) : C++ basics, loop and decision making, functions, classes and objects, pointer and references, overloading and type conversions; inheritance and polymorphism;

UNIT -II: **[8 L]**

Review of postulates of quantum chemistry, The Born-Oppenheimer approximation, variational method and principle, Hartree-Fock method, restricted and unrestricted references, selfconsistent- field (SCF) procedure, Geometry optimization, basis set, semiempirical methods, geometry optimization, vibrational frequency analysis, Density-functional theory.

UNIT -III **[12 L]**

Molecular Mechanics / Force Field Methods: Introduction to molecular mechanics; review of basic Concepts; comparison of popular force fields; performance of molecular mechanics, Lagrangian, Hamiltonian, and Newtonian equations of motions, integration algorithms, Periodic boundary conditions, force calculations, methods for long range interactions calculation.

UNIT -IV **[12 L]**

Modelling of macromolecules: all atom and ab-initio molecular dynamics, Coarse-Graining and Multiscale Simulations for Nanoscale Systems, Quantum mechanics/molecular mechanics (QM/MM) approaches, study of self-organized assemblies, biomolecules like peptides, proteins, membranes and ion channels. Dynamical and structural studies of molecules using molecular dynamics simulations.

Reference Books:

1. Programming: Principles and Practice Using C++, B. Stroustroup, Addison Wesley, 2014.
2. Introduction to Computational Chemistry, F. Jensen, Wiley Publishers, 2007.Let Us C++, Y. P. Kanetkar, BPB Publications, 2003.
3. Understanding Molecular Simulations: From Algorithms to Applications, D. Frenkel

and B. Smit, Academic Press, 2002.

CYD 507	**Bio-inorganic Chemistry**	**(3-0-0)**

- **Course Philosophy:**
  - ✓ The course in intended to impart knowledge and understanding about the role of various metal ions in biology, either as part of enzymes or as a participant various biological processes. The provide information about the structure and mechanistic aspect of various metallo-enzymes.
- **Learning outcome:** At the end of the course students should be able to-
  - ✓ Develop understanding about how metal ions are transported and stored in biological systems
  - ✓ Explain how the active site structure of the enzyme and protein folding influence the activity of the enzymes
  - ✓ Develop understanding about the interaction of metal with proteins/nucleic acids and their implication in biological processes.

UNIT -I **[18L]**

Essential and trace elements in biological processes, Metal Storage and Transport: Ferritin, transferrin, and siderophores, ionophores. Biological role of alkali and alkaline earth metal ions, transport and regulation, molecular aspects of intramolecular processes,.Metalloenzymes, Iron enzymes, Mn, Ni, Zn and Cu containing Enzymes, SODs, Molybdenum/Tungsten containing enzymes, Coenzyme vitamin B_{12}, Zinc in transcription and regulation.

UNIT -II **[12 L]**

Photosynthesis, Oxygen Evolution Complex (OEC), Oxygen Binding and transport: Biological Dioxygen carriers: Hemoglobin, hemerythrin, hemocyanin, allosteric regulation, artificial dioxygen carriers, metallo-porphyrins, Electron-transfer proteins, long distance electron transfer.

UNIT -III **[11 L]**

Metal-Nucleic Acid Interactions: Metals in Medicine, Metal deficiency and disease, toxic effects of metals, metals used for diagnosis and chemotherapy with particular reference to anticancer drugs

Reference Books:

1. Bioinorganic Chemistry: A Survey, Ei-Ichiro Ochiai, academic press, 2008.
2. Bio-inorganic Chemistry: A short course, Rossette M. Roat –Malone, 2nd edition, Wiley, NY, 2007.
3. Bioinorganic Chemistry, Ivano Bertini, Harry B. Gray, Stephen J. Lippard, Joan Silverstone Valentine, University Science Books, 1994.

CYD 508	**Chemistry of f-block elements**	**(3-0-0)**

- **Course Philosophy:**
  - ✓ This course contains the chemistry of f-block elements, extraction, fundamental properties and their application. Electronic, magnetic properties, organometallic chemistry f-block elements are explored. Applicability of these elements in organic synthesis, material chemistry are also included.
- **Learning Outcome:**
  - ✓ General synthetic procedures and characterization of f-block elements.
  - ✓ Structure, binding and reactivity
  - ✓ Application in multidisciplinary areas.

UNIT -I **[22 L]**

Introduction of Lanthanides, abundance, ores, extraction, electron configuration, f-orbitals, periodic properties, redox properties, energetics, coordination chemistry, electronic and

magnetic properties, lanthanide meta-organic frameworks, organometallic chemistry of lanthanides, lanthanide in organic synthesis.

UNIT -II **[20 L]**

Introduction of actinides, occurrence, extraction, characteristics, redox behaviour, binary compounds, coordination chemistry, electronic and magnetic properties, organometallic chemistry, Transactinides.

Reference Books:

1. The Rare Earth Elements: Fundamentals and Application, David A. Atwood, Wiley-Blackwell, 2012.
2. Lanthanide and Actinide Chemistry, Simon Cotton, Wiley & Sons Ltd, 2006.
3. Principles in Organolanthanide Chemistry, Reiner Anwander, Springer, 2001.

CYD 509	**Modern Terpyridine Chemistry**	**(3-0-0)**

- **Course Philosophy:** This course will impart
  - ✓ Fundamental understanding of the synthesis and applications of Terpyridine and corresponding metal complexes
- **Learning Outcome:** After studying this course, students should be able to:
  - ✓ Understand the basic techniques used in synthesis of Terpyridine and its derivatives along with corresponding metal complexes.
  - ✓ Study the models of supramolecular and photophysical properties of Terpyridine complexes.
    Study the homogeneous and surface anchored catalysis by Terpyridine complexes.

UNIT I: **[14L]**

Basic synthetic strategies, Ring assembly, Cross coupling methods, synthesis of 2,2':6',2''-Terpyridine derivatives, Unsymmetrically terminally substituted 2,2':6',2''-Terpyridines, Multi-functional 2,2':6',2''-Terpyridine with variable substituents.

UNIT II: **[14 L]**

Synthetic strategies for mono- and bis-chelate Terpyridine based transition metal complexes, Ruthenium Terpyridine complexes, luminescent and chiral properties of the complexes. Dyads, Triads, Helicates Rotaxanes and Catenanes in supramolecular Terpyridine architectures. Fullerene Terpyridine complexes.

UNIT III: **[14L]**

Homogeneous and Surface anchored catalysis by Terpyridine complexes: Oxidation and Reduction reactions by chemical, photochemical and electrochemical methods.

Reference Books:

1. Modern Terpyridine Chemistry, G. R. Newkome, H. Hofmeier, and U. S. Schubert WILEY -VCH Verlag GmbH & Co. KGaA, Weinheim, 2003, ISBN-3-527-30630-7.
2. Terpyridine-based Materials: For Catalytic, Optoelectronic and Life Science Applications, A. Winter, G. R. Newkome, and U. S. Schubert WILEY -VCH Verlag GmbH & Co. KGaA, Weinheim, 2012, ISBN- 978-3-527-63963-2.
3. Ruthenium Complexes: Photochemical and Biomedical Applications, Edited by A. A. Holder, L. Lilge, W. R. Browne, M. A.W. Lawrence, J. L. Bullock Jr., WILEY -VCH Verlag GmbH & Co. KGaA, Weinheim, 2018, ISBN: 978-3-527-33957-0.

CYD 510	**Chemistry of Nanostructured Materials**	**(3-0-0)**

- **Course Philosophy:**
  - ✓ With this course student will learn various strategy for control synthesis of nanomaterials, their characterization and applications in various fields.
- **Learning Outcome:**

At the end of this course the student will able to:

- ✓ Identify special properties of nanomaterials.
- ✓ Conceptualize various synthetic routes for nanomaterial synthesis.
- ✓ Characterize nanomaterials by various analytic tools and identify their potential area of application.

UNIT –I **[21L]**

Introduction; fundamentals of nanomaterials science, surface science for nanomaterials, colloidal chemistry; Classical methods of Synthesis, preparation and fabrication of nanomaterials;

UNIT –II **[21L]**

Shape and size control synthesis of nanomaterials. Recent advancement in Sonochemistry and Other Novel Methods for Nanoparticle synthesis. Characterization of Nanomaterials. Potential applications of nanomaterials in various fields.

Reference Books:

1. Solid State Chemistry – An Introduction, L. Smart and E. Moore, Taylor & Francis Group, 4th Edition, 2012.
2. Principles of the Solid State, H. V. Keer, 1st Edition, New Age International Publishers, 2005.
3. The Chemistry of Nanomaterials: Synthesis, Properties and Applications, C. N. R. Rao, Achim Muller, Anthony K. Cheetham, Wiley, 2004.

CYD 511	**Advanced Methods in Organic Synthesis**	**(3-0-0)**

- ❖ **Course Philosophy:**
  - ✓ Knowledge on various organic reactions in organic synthesis.
  - ✓ Acquire advanced synthetic tools applied in organic synthesis.
  - ✓ Chasing the synthesis of complex molecular architecture by means of developing new synthetic methods.
- ❖ **Learning Outcome:**
  - ✓ Gather the information about various modern synthetic methods.
  - ✓ Conceptualize various synthetic methods for organic synthesis.
  - ✓ Update to current trends of organic research

UNIT –I **[21L]**

Olefin Metathesis Reaction; Photoredox Catalysis; Metal-Free Iodinane Catalysis; C-H activation; Cross-Dehydrogenative Coupling (CDC); Counter ion Directed Catalysis;

UNIT- II **[21L]**

Remote Functionalization; Electrochemical Reaction; "On water" Reaction; Chiral Amine Catalysis; Memory of chirality; Relay Catalysis; Concept of Dual Catalysis; Ball-Milling Reaction; Frustrated Lewis pair (FLP) chemistry.

Reference Books:

1. Visible Light Photocatalysis in Organic Chemistry, Edited by Corey R. J. Stephenson, Tehshik P. Yoon, and David W. C. MacMillan, 1st Edition, © 2018 Wiley-VCH Verlag GmbH & Co. ISBN: 978-3-527-33560-2.
2. Hypervalent Iodine Chemistry: Preparation, Structure and Synthetic Applications of Polyvalent Iodine Compounds; Viktor V. Zhdankin; © 2014 John Wiley & Sons, ISBN:9781118341032.
3. From C-H to C-C Bonds: Cross-Dehydrogenative-Coupling, Chao-Jun Li; © 2015 The Royal Society of Chemistry; ISBN: 978-1-84973-797-5.
4. Chiral Amine Synthesis: Methods, Developments and Applications; edited by Thomas C. Nugent; © 2010 Wiley-VCH Verlag GmbH & Co. ISBN: 978-3-527-32509-2.

CYD 512	**Modern aspects of Catalysis and Surface science**	**(3-0-0)**

- ❖ **Course Philosophy:**
  - ✓ Catalysis is an interdisciplinary area which covers materials science, green chemistry and development of sustainable energy.

- ✓ The course is aimed to encourage student for understanding the correlation between different segment of chemistry along with chemical engineering as well as modern nanostructured materials.

❖ **Learning Outcome:**

- ✓ At the end of the course students will be comfortable to do research in fine chemicals synthesis in gas phase as well as liquid phase
- ✓ Students will also be able to do research in hydrocarbon sector as well as in sustainable energy

UNIT –I **[14L]**

Kinetics of Gas-solid reaction; LH and LR Mechanism, Adsorption and adsorption isotherm; Physisorption and Chemisorption of gas molecules to the solid surface; determination of particle size from chemisorptions measurement, TPR/TPD/TPO techniques;

UNIT –II **[18L]**

Elementary gas phase reaction, spillover effect, multiplet theory brief overview of catalytic reactor, fixed bed and batch reactor, mass transfer and heat transfer on the catalyst surface; promotional and poisoning effect on catalyst surface; selected organic reaction e,g selective oxidation, hydrogenation, dehydrogenation, dehydration, alkylation, aromatization etc. and their mechanism in gas phase,

UNIT –III **[10L]**

Energy related catalysis, petroleum refining, hydrotreating, methane decomposition, steam reforming, cracking and isomerization reaction; Fischer-Tropsch synthesis; bio-fuel.

Reference Books:

1. Current Trends of Surface Science and Catalysis, Jeong Young (Ed.) Park (Author), Jeong Young Park(editor), 1st Edition, Springer, 2013.
2. Handbook of Heterogenous Catalysis, G. Ertl, H. Knozinger, F. Schuth, J. Weitkamp, WILEY-VCH Verlag GmbH & Co. KGaA, ISBN 978-3-527-31241-2
3. Nanotechnology in Catalysis, Spinger,; ISBN-0387-34687-2; Edited by G A Somorjai Vol-1-3

CYD 513	**Electroanalytical methods**	**(3-0-0)**

❖ **Course Philosophy:**

- ✓ Electroanalytical techniques offer a unique access to information on chemical, biochemical, and physical systems.
- ✓ The purpose of this course is to provide both the instrumental basis and the theoretical fundamentals of electrochemical techniques, commonly used in recent time, so that an interest can be develop among the students to easily apply these techniques for real-time applications.

❖ **Learning Outcome:**

This course is rigorous examination of theory and applications of electro-analytical methods. Students completing this course will be:

- ✓ Knowledgeable of the current electroanalytical techniques,
- ✓ Comprehend the factors that must be controlled to obtain reliable and reproducible data during their electroanalytical experiments,
- ✓ Capable of selecting the most appropriate electroanalytical technique for a specific analysis,
- ✓ Adept at evaluating the electrode reaction mechanism from data obtained from various electroanalytical techniques.

UNIT –I **[21L]**

Polarographic methods, Dropping Mercury Electrode, Current-voltage relationship, Voltammetry: Cyclic voltammetry, linear sweep voltammetry, pulse voltammetry, stripping voltammetry.

UNIT-II **[21L]**

Potentiometric techniques. Theory of electro-gravimetric analysis, electrode reactions, overpotential, completeness of deposition, and electrolytic separation of metals by controlled potential electrolysis/electrodeposition. Rotating disc and ring disc electrodes, concepts and applications of AC impedance techniques. Spectro-electrochemistry

Reference Books:

1. Fundamentals of analytical chemistry, Douglas Skoog, Donald West, F. Holler, Stanley Crouch, 9th Edition, Cengage Learning, 2013.

2. Electroanalytical Methods, F. Scholz, 2nd Edition, Springer, 2010.

CYD 514	Single crystal X-ray diffraction	(3-0-0)

❖ **Course Philosophy:**

✓ This course contains the theory and application of single crystal X-ray diffraction technique.

✓ With this course students will learn the concepts behind the technique and how to solve the structures of small molecules.

❖ **Learning Outcome:**

At the end of the course students will be able to-

✓ Gain knowledge about X-ray diffraction technique

✓ Solve structure of small molecules from diffraction data

UNIT-I **[21L]**

Unit cell, Bravais lattice, symmetry elements and space groups, examples, Hermann-Mauguin Symbolism, Reciprocal lattice concept, determination of space groups, Laue pattern, Ehwald's sphere, convolution, phase problem,

UNIT –II **[21L]**

Structure factor and its significance, Patterson Fourier synthesis, Direct methods, Isomorphous replacement, Harkar-Kasper inequalities, refinement of crystal structures. R factor, Difference fourier maps. Treatment of disorder.

Reference Books:

1. Crystal Structure Determination, Werner Massa, Robert O. Gould, 2nd Edition, Springer; 2004. Corr. 5th printing 2010 edition, 2010.
2. Introduction to macromolecular crystallography, Alexander McPhearson, Wiley-Liss, 2003.
3. Crystal structure analysis- A primer, 3rd edn. J. P. Glusker, K. N. Trueblood, Oxford Science Publications, 2010

CYD 515	Advances in Non-conventional Energy Systems	(3-0-0)

❖ **Course Philosophy:** This course will impart

✓ Electrochemical techniques related to conversion and storage energy.

✓ Fundamental understanding of the Chemical, Electrochemical and Photochemical processes in Energy generation, storage and Utilization.

❖ **Learning Outcome:** After studying this course, students should be able to:

✓ Understand the basic electrochemical techniques used in energy conversion and storage systems.

✓ Advantage and disadvantages in the Industrial methods for generation of Fuels.

✓ Use concepts towards the mimicking systems in artificial photosynthesis.

UNIT-I **[14L]**

Electrochemical Techniques and their application to Real Systems, Electrochemical Cells: Batteries, Supercapacitors.

UNIT –II **[14L]**

Fuels through industrial reforming, Fischer-Tropsch process, and Water-gas shift reactions, Multi electronic reservoirs for Electrochemical energy storage.

UNIT –II **[14L]**

Recent advances in Fuel Cells, Synthesis, Characterization and Application Energy Materials: Electrochemical, photochemical and chemical methods for HER and OER catalysis,

Reference Books:

1. Energy Production and Storage: Inorganic Chemical Strategies for a Warming World (Inorganic Chemical Strategies for a Warming World), edited by Robert H. Crabtree

ISBN: 978-0-470-74986-9, Wiley Publications.
2. Molecular Water Oxidation Catalysis, edited by Antoni Llobet ISBN: 978-1-118-41337-1, Wiley Publications.
3. Electrochemical and Electrocatalytic Reactions of Carbon Dioxide; Edited by: B.P. Sullivan, K. Krist and H.E. Guard; ISBN: 978-0-444-88316-2.

CYD 516	Advanced Heterocyclic Chemistry	(3-0-0)

❖ **Course Philosophy:**

✓ The subject offers the readers a fundamental understanding of the basics of heterocyclic chemistry and their occurrence in bioactive molecules in advanced level.

❖ **Learning Outcome:**

✓ Acquire knowledge about importance of heterocyclic molecules relevant to pharmaceutical chemistry.

UNIT –I **[10L]**

Different types of strains, interactions and conformational aspects of non-aromatic 3-and 4-membered heterocycles: Synthesis, reactivity, and importance of the following ring systems. Azirines, Oxaranes, Thiiranes, Diazirenes, Diaziridines, Azetidines and Oxetanes.

UNIT-II **[12L]**

5- and 6-Membered heterocyles containing two hetero atoms: Synthesis, reactivity, aromatic character and importance of the following heterocycles: Pyrazole, Imidazole, Oxazole, Thiazole, Isoxazole, Isothiazole, Pyridazine, Pyrimidine, Pyrazine, Oxazine, thiazine, benzimidazole, benzoxazole and benzthiazole.

UNIT –III **[10L]**

Heterocyles with Nitrogen-ring-junction: Synthesis and reactivity of Quinolizines, Indolizines and Imidazopyridines. Heterocycles with Dipolar structures: synthesis and reactivity of pyridine-*N*-oxides and pyridinium imides.

UNIT–IV **[10L]**

Synthesis of Drugs: Ranitidine, Lansoprazole and/or recently discovered molecules containing multiple hetero atoms and rings. Synthesis of few heterocyclic novel natural products.

Reference Books:

1. Heterocyclic Chemistry J. A. Joule and K. Mills, 5th Edition, Wiley-Blackwell publishing, 2010.
2. Heterocyclic Chemistry T. Gilchrist 3rd edition, Prentice Hall, 1997.
3. Modern Heterocyclic Chemistry, Julio Alvarez-Builla, Juan Jose Vaquero, José Barluenga, Wiley-VCH, 2011.

CYD 517	Oligosaccharide synthesis	(3-0-0)

❖ **Course Philosophy:**

✓ Introduction to important carbohydrate polymers in natural systems.

✓ Introduction to some of the most important methods in carbohydrate synthesis

❖ **Learning Outcome:**

✓ Biologically important carbohydrate polymers - their structural and repeating units.

✓ Synthetic tools and methodologies in carbohydrate synthesis.

✓ Knowledge of the synthetic routes to repeating units of some biologically interesting carbohydrates.

UNIT –I **[21L]**

Monosaccharides; Protecting group strategies – one-pot orthogonal protection; Glycosyl donors and glycosylation - glycosylation methods, photochemical glycosylation, substituent effects on glycosylation.

UNIT –II **[21L]**

Oligosaccharide synthesis – one pot glycosylation, iterative glycosylation, solid phase and automated synthesis. Structure, relevance and synthesis of some important oligosaccharides such as glycosaminoglycans, capsular polysaccharides of pathogens, etc.

References:

1. Carbohydrates- the sweet molecules of life R. V Stick, Academic press, 2001.
2. Essentials of Carbohydrate Chemistry and Biochemistry, T. K. Lindhorst, Wiley VCH, 2000.
3. Recent Primary literature

CYD 518	Metalloenzymes- Special Topics	(3-0-0)

❖ **Course Philosophy:**

✓ The course is intended to impart basic understanding about the structure and function of metal containing enzymes and its model

❖ **Learning Outcome:** At the end of the course the student is able to-

✓ Know the difference in the structure and function of various metalloenzymes
✓ Develop understanding about the role of metal ions and the mechanism of action
✓ Understand the design aspects of metalloenzyme model compounds

UNIT-I **[12L]**

Introduction to metalloenzymes: Coordination chemistry and basic characterization techniques, suggested mechanism of selected enzymes and synthetic analogues

UNIT –II **[16L]**

Vanadium: haloperoxidases; Cobalt: cobalamine based enzymes; Zinc: hydrolases, peptidases, ligases, transferases, lyases, oxido-reductases; Iron: heme and non-heme enzymes- Phosphatases, Mono oxygenases, dioxygenases, peroxidase, catalase, super-oxide dismutase, reductases;

UNIT –III **[14L]**

Manganese: Oxygen Evolving Complex in PS-II, super-oxide dismutase, catalase; Copper: Mono oxygenases, dioxygenases, super-oxide dismutase, catecholase and tyrosinase; Nickel: urease, hydrogenase, super-oxide dismutase; Molybdenum: Oxido-reductases.

References:

1. Bio-inorganic chemistry- A survey by Ei-ichiro Ochiai, 2006, Associated Press, Elsevier
2. Chemical Reviews 1996, Vol. 96 and other recent litterature.
3. Biological Inorganic Chemistry: Structure and reactivity by I. Bertini, H. B. Gray, E. I. Stiefel, J. S. Valentine, 2007, Abe Books
4. Physical Methods in Bio-inorganic Chemistry by Lawrence Que, 2000, University Science Books

CYD 519	Characterization Techniques for Inorganic Chemists	(3-0-0)

❖ **Course Philosophy:**

The course intended to provide

✓ Basic understanding about various techniques such as, infrared spectroscopy, electronic spectroscopy, EPR spectroscopy, voltammetric techniques, CD, ORD and Mossbauer Spectroscopy

❖ **Learning Outcome:**

At the end of the course the student will be able to-

✓ Develop understand the principle involved in various techniques used by inorganic chemists
✓ Interpret data such as IR, UV-visible, EPR, Cyclic voltammogram, CD, ORD and Mossbauer Spectra

UNIT –I **[10L]**

Interpretation of UV-visible and IR spectra of inorganic and organometallic compounds, case studies. Characterization methods for paramagnetic compounds:

UNIT –II **[10L]**

EPR: Fundamental principles of continuous wave EPR (CW-EPR), X, Q and W band modes, case

studies- interpretation, ENDOR. HYSCORE, methods for simulation, specific examples.

UNIT –III **[12L]**

Solution studies: Cyclic voltammetry, basic principles and applications, interpretation of redox peaks, case studies. Circular Dichorism (CD) and optical rotatory dispersion (ORD): Principles and application in inorganic and organometallic compounds.

UNIT –IV **[10L]**

Mossbauer Spectroscopy: Introduction and basic principles, selected examples, interpretation of data.

Reference Books:

1. Infrared and Raman spectra of Inorganic and coordination compounds: Part A & B, Kazuo Nakamoto, Wiley, 2009
2. Applications of Physical Methods to Inorganic and Bioinorganic Chemistry by Robert A. Scott, Charles M. Lukehart, 2007, Wiley –Blackwell.
3. Electron Paramagnetic Resonance: Elementary Theory and Practical Applications, John A. Weil, James R. Bolton, 2nd Edition, Wiley, 2007.
4. Physical Methods for Chemists, R. S. Drago, 2nd Edition, Saunders (W.B.) Co Ltd, 1992.

CYD 520	**Advanced Fluorescence Spectroscopy**	**(3-0-0)**

- **Course Philosophy:**
  This course will give an introduction to modern spectroscopic techniques including time-resolved laser methods and dynamic properties of materials.
- **Learning Outcome:**
  Understanding the fundamentals as well to have an insight of the many photo-physical processes and every possible deactivation pathways of the excited systems including organic, inorganic and nanoscales materials.

UNIT –I **[21L]**

Jablonski diagram, Fluorescence quantum yields and lifetimes, radiative and non-radiative rates, steady state and time-resolved fluorescence, quenching of fluorescence, Fluorescence anisotropy, Resonance energy transfer, Solvatochromism, TRES.

UNIT –II **[21L]**

Light sources, LASER, monochromator, optical filters, PMT, polarizers, corrected emission spectra, TCSPC, Fluorescence upconversion, transient recording, data analysis. Different examples correlating data recording and data analysis and information found.

Reference Books:

1. Principles of fluorescence spectroscopy by J.R.Lakowicz, *3rd ed., Springer, 2006*
2. Fundamentals of Photochemistry, K. K. Rohatgi-Mukherjee, John Wiley & Sons, 1978.
3. Molecular spectroscopy by Jeanne L. McHale, CRC Press, 2017.

CYD 521	**Nanomaterials for Advanced Applications**	**(3-0-0)**

- **Course Philosophy:**
  With this course student will learn various strategy for control synthesis of nanomaterials and their applications in biotechnology.
- **Learning Outcome:**

✓ Students will learn shape and size control synthesis of metallic, inorganic and magnetic nanomaterials.

✓ Applications of these nanomaterials in the field of biotechnology, photonics, imaging and sensors will be introduced to the students.

UNIT –I **[21L]**

The interface of bioscience, nanotechnology and photonics, Quantum dots for bioimaging, Metallic nanoparticles and nanorods for biosensing, Upconverting nanophores and Inorganic nanoparticles for nanosensors for In vitro bioanalysis and optical diagnostics.

UNIT –II **[21L]**

Magnetic targeting, magnetic separation and detection, Magnetic tweezers, Chemo therapy, MRI, Magnetic contrast agents, Hyperthermia, Application of various nanomagnetic materials in

biotechnology, core-shell structures and their applications. Nanoelectronics, Micro and nano electromechanical systems. Nanophotonics.

Reference Books:

1. Introduction to Nanophotonics, Sergey V. Gaponenko, Cambridge University Press, New York, (2010)
2. Nanofabrication towards Biomedical Applications, Techniques, Tools, Applications, and Impact. C. S. S. R. Kumar, J. Hormes, C. Leuschner, 2005, WILEY -VCH Verlag GmbH & Co. KGaA, Weinheim, ISBN-13 978-3-527-31115-6.
3. Nanoscale Technology in Biological Systems, Edited by Ralph S. Greco, Fritz B. Prinz, R. Lane Smith, CRC PRESS, Boca Raton London New York Washington,

CYD 522	Advanced Biocatalysis	(3-0-0)

❖ **Course Philosophy:**

- ✓ Biochemical studies for the metalloenzyme provide a useful starting point for the development of academically as well as industrially important synthetic analogues of bio-enzymes.

❖ **Learning Outcome:**

- ✓ Students will be familiar with some of the important enzymatic action.
- ✓ Students will be able to model the active site of the bio-enzyme of their interest.
- ✓ Students will understand the advantage of synthetic model over active enzymes.
- ✓ They will be able to develop a non-toxic, green, economic and energy-efficient synthetic method for the preparation of synthetically/industrially important chemicals.

UNIT –I **[21L]**

Introduction: potential of enzyme-catalysed processes in biology; Introduction to model complexes: Impact in catalysis; Structure and probable enzymatic action of galactose oxidase, catechol oxidase, tyrosinase, vanadium haloperoxidase, etc.;

UNIT –II **[21L]**

Immobilization on solid supports: Novel concepts, use of nano-, meso- and magnetic materials and characterization, limitations of catalysts, Plots and parameters for Michaelis-Menten kinetics, effect of local environment in catalysis, Supported catalysts, Effect and application in fine Chemicals Industry.

References:

1. Recent review articles/ Journals
2. Enzyme Kinetics and Mechanism; Paul F. Cook, W. W. Cleland. ISBN-13: 978-0815341406
3. Enzyme Kinetics and Mechanisms; Taylor, Kenneth B. ISBN 978-0-306-48025-6

CYD 523	Supramolecular Chemistry & Molecular recognition	(3-0-0)

❖ **Course Philosophy:**

The course aims to:-

- ✓ Demonstrate the importance of supramolecular forces for the assembly of complex nanomaterials
- ✓ Give an understanding of how the properties of ligands can be tuned in order to optimise the performance of metal complexes in their various applications.
- ✓ Examine the relevance of such Supramolecular systems to catalytic, biological, chemi-architectural, industrial processes and applications

❖ **Learning Outcome:**

By the end of the course the student will be able to:-

- ✓ Develop an understanding of the importance of intermolecular forces to define the "chemistry beyond the molecules"
- ✓ Use the basic understanding of such forces to rationalise the formation of complex nanomaterials
- ✓ Understand the importance of the bottom-up approach to prepare complex systems.

- ✓ Recognize the main types of supramolecular assemblies and suggest synthetic strategies for their preparation.

UNIT –I **[14L]**

Supramolecules: Supramolecular Chemistry and Molecular Recognition. Concepts, Definitions, Language, Receptor Design Principles. Supramolecular Interactions. Ion-ion interactions; Ion-dipole interactions; dipole-dipole -interactions; van der Wall interactions, π-π-interactions; cation-π interactions; hydrogen bonding; hydrophobic effect; metal-coordination bonds. Self-assembly processes in organic systems. Catenanes, rotaxanes, pseudorotaxanes. Synthetic strategies for their preparation. Examples of each type.

UNIT –II **[20L]**

Self-assembly processes in metal-containing compounds. Using the coordination bond to prepare large supramolecular assemblies. Cages, macrocycles and catenanes. Polymeric materials and grids. Nano-capsules and containers. Synthetic strategies for their preparation. Examples of each type. Potential uses of such assemblies as nano-reactors and for transport. Host-Guest Chemistry. Hosts for Cation Binding; Host for Anion Binding; Hosts for the Binding of Neutral Guests; Synthetic consideration; Templation; Kinetic and Thermodynamic Aspects of Binding Selectivity. Kinetic and Thermodynamic Considerations; Helicates. Supramolecular Chirality. Supramolecular Reactivity and Catalysis. Supramolecular Catalysts; Enzyme Models. Self-Replicating Systems. Kinetic Models; Self-replication in nature; Artifical Self Replicating Systems.

UNIT –III **[8L]**

Molecular switches and machines. Use of supramolecular forces to assemble components that respond (on-off) to external stimuli. Molecular shuttles, abacus and muscles. Assembling such components into surfaces for molecular electronics. Supramolecular Aggregates and Assemblies.

Reference Books:

1. Supramolecular Chemistry, J. W. Steed and J. L. Atwood, J. Wiley and Sons; 1st Ed. 2000.
2. Principles and Methods in Supramolecular Chemistry, Hans-Joerg Schneider & A. Yatsimirsky, J. Wiley & Sons, 1st Ed. 2000.
3. Control of Reactivity in Aggregates of Amphiphilic Molecules. P. Scrimin, in "Supramolecular control of Structure and Reactivity," John Wiley and Sons, 1996, Vol. 3, pp. 101-153.

CYD 532	**Solid State Materials: Chemistry and Engineering**	**(3-0-0)**

❖ **Course Philosophy:**

- ✓ With this course students will learn the concepts involved in the syntheses, structure and physical properties of crystalline solids along with their characterizations and applications.

❖ **Learning Outcome:**

- ✓ Identify and apply suitable strategies for synthesizing crystalline solids in polycrystalline and single crystal forms.
- ✓ Correlate and Predict structure composition-properties (magnetic, electrical and optical) in crystalline solids.
- ✓ Characterize solids with X-Ray, microscopic and thermal techniques.

Unit -I **[14L]**

Crystal Structures and Crystal Chemistry, Bonding in Solids, Defect Chemistry and its applications in various fields. Electrical, Magnetic and Optical Properties of solids, Structure Property Relationship, Superconductors.

Unit -II **[14L]**

Synthesis, Processing and Fabrication Methods of solids, Nucleation and Growth in Solution, Solid State Reaction, ChimieDouce Methods, Gas-Phase Methods, Crystal Growth, Recent advances in solid state materials.

Unit -III **[14L]**

Characterization of Solids: Crystallography and Diffraction Techniques, Optical and Electron Microscopy Techniques, Spectroscopic Techniques, Thermal Techniques.

Reference Books:

1. Solid State Chemistry and its Applications, Second Edition, Anthony R. West, 2014, Wiley.
2. Metallic Nanostructures: From Controlled Synthesis to Applications, YujieXiong, Xianmao Lu, 2015, Springer.
3. Materials Science and Engineering: An Introduction, William D. Callister, Jr. David G. Rethwisch, 2013, Wiley.

CYD 533	**Advanced Electrochemistry**	**(3-0-0)**

- **Course Philosophy:**
  - ✓ The learners should be able to apply theories in electrochemistry to analyze electrode kinetics.
- **Learning Outcome**: At the end of the course, the learners should be able to:
  - ✓ **Write** equations representing electrochemical cell, **explain** various overpotential involved during the operation of the cell.
  - ✓ **Calculate** electrochemical cell parameters, electrochemical active surface area, current and overpotential under given condition, **Plot** potential vs current, surface coverage vs. potential, potential vs. pH, concentration profile vs. distance from the electrode.
  - ✓ **Understand** the basics of electrocatalysis and industrial applications of electrochemistry

UNIT -I **[10 L]**

Ionics: Electrochemistry of solutions, Ion-solvent interactions, ion-ion interactions, ionic migration and diffusion. Phenomenological description of transport processes. Electrodics: Equilibrium electrode potentials, Thermodynamics of electrochemical cells and applications.Theories of Double-Layer structure, diffuse-double-layer theory of Gouy and Chapman, the Stern Model, Adsorption of ions and neutral compounds

UNIT -II **[16L]**

Electrode kinetics: Current-potential relationship (derivation of Butler-Volmer and Tafel equations). Adsorption isotherms for intermediates formed by charge transfer (Langmuir adsorption and its limitations, relating bulk concentration to surface coverage), Electrocaplillary and differential capacitance measurements; Influence of double layer on charge transfer processes.potential of zero charge, pzc of solid electrodes, polarization: types of polarization, the charge transfer resistance Types of overpotentials: origin and minimization

UNIT-III **[14L]**

Electro-catalysis, Bio-electrochemistry, Electron transfer in homogeneous system and in heterogeneous system. Electrosynthesis: electroorganic and electroinorganic syntheses, mechanism of electro-organic reactions; hydrogen evolution and oxygen reduction reactions, Industrial processes: electroplating, anodization, Al production, electrosynthesis of selected industrial chemicals.

Reference Books:

1. Atkins' physical chemistry, P. Atkins and J. de Paula, 8th Edition, Oxford University Press, New Delhi, 2008.
2. E. Gileadi, Physical Electrochemistry, Fundamental, Techniques and Applications, Wiley-VCH, 2011
3. A. J. Bard and L. R Faulkner Electrochemical Methods: Fundamentals and Applications, 2nd Edition, Wiley, 2001

CYD 534	Heterocyclic chemistry	3-0-0

❖ **Course Philosophy:**
- ✓ The subject offers the readers a fundamental understanding of the basics of heterocyclic chemistry and their occurrence in bioactive molecules in advanced level.

❖ **Learning Outcome:**
- ✓ Acquire knowledge about importance of heterocyclic molecules relevant to pharmaceutical chemistry

Unit-I **[12 L]**

Synthesis and reactions of heteroaromatics containing one hetero atom. General approaches to heterocycle synthesis – cyclisation and cycloaddition routes.

Unit -II **[18 L]**

Synthesis, reactions and their mechanisms of aziridine, azetidine; pyrazines and their analogues; Synthesis of oxazole, thiazole, imidazole, iso-oxazole, isothiazole and corresponding fused systems; imidazopyridine, pteridines, folic acid. Synthesis of drugs like Nevirapine.

Unit III **[12 L]**

Nomenclature of bicyclic and tricyclic fused system. Synthesis of uracil, thymine and cytosine. Synthesis of adenine and guanine. Synthesis of uric acid, caffeine, pyrazine, synthesis of Triazole and tetrazole.

References Books:

1. I .L. Finar, Organic Chemistry, Vol.II, 5th Edition, ELBS, 1975.
2. Heterocyclic Chemistry J. A. Joule and K. Mills, 5th Edition, Wiley-Blackwell publishing, 2010.
3. Heterocyclic Chemistry T. Gilchrist 3rd edition, Prentice Hall, 1997.
4. Modern Heterocyclic Chemistry, Julio Alvarez-Builla, Juan Jose Vaquero, José Barluenga, Wiley-VCH, 2011.

CYD 535	Main Group Chemistry	(3-0-0)

❖ **Course Philosophy:**
- ✓ This course contains the chemistry of s- and p-block elements, synthesis, structure and bonding and their chemical reactivity. Organometallic chemistry of main group elements is included with a special focus on their applications in organic synthesis. Various applications of main group elements in catalysis and material chemistry will be explored.
- ✓ With this course students will learn the concepts involved in the syntheses, structure, physical and chemical properties of main group elements along with their application in various field

❖ **Learning Outcome:**
- ✓ General synthetic procedures and characterization for inorganic and organometallic compounds
- ✓ Structure, binding and reactivity
- ✓ Application in multidisciplinary areas.

UNIT -I **[12 L]**

s-block elements: Organometallic compounds of alkali and alkaline earth metals, synthetic methods, structure, bonding and reactivity, application catalysis, organometallic compounds of zinc, cadmium and mercury, application

UNIT -II **[12 L]**

p-block elements: General properties, synthesis, structure, bonding of organoelements

compounds, spectroscopic characterization and application. Multiple bonding in main group elements, Hypervalency in p-block elements, heavier carbene analogues, small molecule activation, and unusual oxidation states of main group elements.

UNIT-III **[18L]**

Inorganic rings, cages and polymers: boron, carbon, silicon, germanium, tin, nitrogen, phosphorus and arsenic, sulfur and selenium compounds, synthesis, structures, bonding, nomenclature, application in catalysis and material chemistry.

Reference Books:

1. Inorganic Rings and Polymers of the p-Block Elements: From Fundamentals to Applications, Tristram Chivers and Ian Manners, RSC, 2009.
2. Organometallics, A concise introduction, C. Elschenbroich, A. Salzer 3rdedition, 2006, Wiley-VCH Verlag GmbH& Co, KGaA,Weinheim, Germany.
3. Inorganic and Organometallic Polymers, V. Chandrasekhar, Springer India, 2005.

CYD 536	**Science of Corrosion & corrosion control**	**(3-0-0)**

❖ **Course Philosophy:**

- ✓ Most of the industries such as chemical, mining and petroleum industries are facing the corrosion problems. In a recent survey made in India it was estimated that the annual loss due to corrosion is approximately 3 – 4% loss of the GDP. We teach corrosion to paper to B. Tech students of Petroleum Engineering, Mechanical Engineering and Chemical Engineering students. Therefore we have floated this course as open elective.
- ✓ The course is offered to impart: Knowledge about the problem faced by industries
- ✓ Develop understanding about the mechanism and process of corrosion
- ✓ Knowledge about various methods for protection against corrosion

❖ **Learning Outcome:**

- ✓ Knowledge of corrosion and corrosion control to engineering students will help in their working in industries.

UNIT -I **[14L]**

Definition of corrosion, consequences of corrosion and economic aspects of corrosion. Types of corrosion: Chemical and electrochemical corrosion, Pilling Bedworth rule, Forms of corrosion, Theories of corrosion. Factors affecting corrosion. Kinetics of corrosion: Evan's diagram. Thermodynamics of corrosion- Pourbaix diagram.

UNIT-II **[16L]**

Measurement of corrosion: Weight loss, potentiodynamic polarization and electrochemical impedance spectroscopy methods. Corrosion prevention: modification of materials, modification of environment, modification in design, corrosion inhibitors, protective coatings, cathodic and anodic protection.

UNIT-III **[12L]**

Application of FTIR, SEM-EDX, XPS and AFM in corrosion inhibition studies. Corrosion problems in Chemical, Mining and petroleum industries.

Reference Books:

1. Corrosion Engineering, Mars. G. Fontana, 3rd Edition, McGraw-Hill, Inc. 1987.
2. Principles and prevention of corrosion, Denny A. Jones, 2nd Edition, Prentice Hall, 1995.
3. An Introduction to Science of Corrosion and Its Inhibition, S. N. Banerjee, Oxonian Press, 1985.