CURRICULUM STRUCTURE

The total minimum credits required for completing the M.Sc. in Chemistry is 80.

SEMESTER 1					
Code	**Course of Study**	**L**	**T**	**P**	**C**
CHPC601	Organic Reaction Mechanisms and Aromaticity	3	-	-	3
CHPC603	Coordination Chemistry	3	-	-	3
CHPC605	Quantum Chemistry and Group Theory	3	-	-	3
CHPC607	Analytical Chemistry	3	-	-	3
CHPC609	Theory of Spectroscopy and Molecular Excitons	3	-	-	3
	Program Elective 1/*Online courses	3	-	-	3
CHLR601	Inorganic and Analytical Chemistry Lab	-	-	6	2
					20
SEMESTER II					
CHPC602	Stereochemistry, Photochemistry, Pericyclic and Rearrangement reactions	3	-	-	3
CHPC604	Organometallic Chemistry and Inorganic Spectroscopy	3	-	-	3
CHPC606	Rates and Energetics of Chemical Reactions	3	-	-	3
CHPC608	Spectroscopy-Applications in Organic Chemistry	3	-	-	3
	Program Elective 2/*Online courses	3	-	-	3
CHLR602	Organic Chemistry Lab	-	-	6	2
CHLR604	Physical Chemistry and Spectroscopy Lab	-	-	6	2
		-	-	-	**19**
***CHPC611**	Summer Internship (6- 8 weeks)	-	-	-	**2**
SEMESTER III					
CHPC613	Synthetic Organic Chemistry	3	-	-	3
CHPC615	Main Group, Bioinorganic and Nuclear Chemistry	3	-	-	3
CHPC617	Statistical Thermodynamics, Photochemistry, and Surfaces	3	-	-	3
CHPC619	**Project Work Phase I**	-	-	-	12
					21
SEMESTER IV					
CHPC610	**Project Work Phase II**	-	-	-	**12**
	Program Elective 3/*Online courses	3	-	-	3
	Program Elective 4/*Online courses	3	-	-	3
					18
	Total Credits	-	-	-	**80**
	*** Evaluation methodology as per senate decision**				

PROGRAM ELECTIVES

Code	Course of Study	L	T	P	C
CHPE601	Catalysis	3	-	-	3
CHPE603	Principles and Applications of Fluorescence Spectroscopy	3	-	-	3
CHPE605	Medicinal Chemistry	3	-	-	3
CHPE607	Nano Science and Technology	3	-	-	3
CHPE609	Electronic Structure Methods and Modelling	2	-	3	3
CHPE611	Natural Products Chemistry	3	-	-	3
CHPE613	Advanced Heterocyclic Chemistry	3	-	-	3
CHPE602	Polymer Chemistry	3	-	-	3
CHPE604	Computational Methods in Chemistry	2	-	3	3
CHPE606	Interfacial Chemistry and Sonochemistry	3	-	-	3
CHPE608	Lanthanide and Actinide Chemistry	3	-	-	3
CHPE610	Fuel cells for Stationary and Automotive Applications	3	-	-	3
CHPE612	Inorganic Rings, Cages and Clusters	3	-	-	3
CHPE614	Advanced Bioinorganic Chemistry	3	-	-	3
CHPE616	Organometallic Chemistry for Organic Synthesis	3	-	-	3
CHPE618	Environmental Chemistry	3	-	-	3
CHPE620	Biocatalytic processes in Chemical Industries	3	-	-	3
CHPE622	Photoredox and Electro-Catalysis	3	-	-	3
CHPE624	Multiscale Simulation Methods	2	-	3	3
CHPE626	Semiconductor process integration and skills development by Virtual Fabrication	2		1	3
	NPTEL, SWAYAM, Coursera, edX Online courses	-	-	-	3

CURRICULUM COMPONENTS

Category	Total	Total Credits
Program Core courses	12	36
Program Elective courses/Online courses	4	12
Essential Laboratory Requirements	3	6
Summer Internship	1	2
Project work	1 (2 Phases)	24
Total		**80**

PROGRAMME OUTCOMES (POs)

PO1	An ability to independently carry out research /investigation and development work to solve practical problems
PO2	An ability to write and present a substantial technical report/document
PO3	Students should be able to demonstrate a degree of mastery over the area as per the specialization of the program. The mastery should be at a level higher than the requirements in the appropriate bachelor program

COURSE OUTCOME AND PROGRAMME OUTCOME MAPPING

PROGRAMME CORE (PC)

Course Outcomes: On successful completion of the course, students will be able to:

Course Code	Course Title	CO	Course outcomes At the end of the course student will be able to	PO1	PO2	PO3
CHPC601	Organic Reaction Mechanisms and Aromaticity	CO1	the basics of reaction mechanism and the mechanistic concepts	3	2	
		CO2	the fundamentals of substitution reactions and reactive intermediates	2	3	
		CO3	the addition reactions of C=C and C=O bonds	3	2	1
		CO4	the mechanism of elimination reactions and important redox reagents	1	2	3
		CO5	the concept of aromaticity and reactions of aromatic compounds	2	3	
CHPC603	Coordination Chemistry	CO1	learn about the theories and bonding of coordination compounds	3	2	1
		CO2	learn about the reactions and structures of coordination compounds	3	1	2
		CO3	learn about the electronic spectra and magnetism of coordination compounds	2	3	
		CO4	learn about the basics of solid-state chemistry	1	2	3
CHPC605	Quantum Chemistry and Group Theory	CO1	apply principles of quantum mechanics to calculate observables on known wave functions	3	2	
		CO2	apply the concept of quantization of energy	3	3	1

			and relate to molecular systems or nanomaterials			
		CO3	apply the variational method, and the perturbation theory to solve important molecular problems	2	2	3
		CO4	apply group theory and character table to analyse the molecular properties	3	2	3
CHPC607	Analytical Chemistry	CO1	learn the basic principles, working, and applications of Advanced chromatographic techniques	3		1
		CO2	learn the working principles and applications of Ion selective electrodes		2	1
		CO3	learn the principles and application of electroanalytical techniques	3	2	3
		CO4	learn the principles and instrumentation of Atomic spectroscopic techniques and physical characterization methods.			3
CHPC609	Theory of Spectroscopy and Molecular Excitons	CO1	lean the fundamentals of interactions between electromagnetic radiation and matter	3	2	
		CO2	lean the theory of rotational, vibrational and Raman spectroscopic methods, and analysis of spectral data to examine physicochemical properties of matter	2	3	
		CO3	lean the different electronic spectroscopic methods and their utilization in understanding optoelectronic properties of molecules for practical applications	3	2	1

		CO4	lean the theory of molecular exciton models and their applications lies in the field of photovoltaics and photosynthetic systems.	2	1	3
CHPC602	Stereochemistry, Photochemistry, Pericyclic and Rearrangement reactions	CO1	understand the stereochemistry of organic molecules in detail.	3	2	
		CO2	solve various problems on photochemical transformations.	3	3	2
		CO3	plan synthetic routes to complex organic molecules through cycloaddition reactions.	3	3	
		CO4	understand the various types of rearrangement reactions and their mechanism.	3	3	2
CHPC604	Organometallic Chemistry and Inorganic Spectroscopy	CO1	learn about the organometallic bonding principles	3	2	
		CO2	learn about the industrially important homogenous catalytic cycles	3	2	1
		CO3	learn about the inorganic NMR & IR spectroscopy	2	3	
		CO4	learn about the EPR spectroscopy	2	3	
		CO5	learn about the Mössbauer spectroscopy	3	2	2
CHPC606	Rates and Energetics of Chemical Reactions	CO1	understand the equilibrium and non-equilibrium properties of the system.	3	2	
		CO2	understand the interrelationship between partial molar properties of phase equilibrium.	3	2	
		CO3	analyse and apply the principles of electrochemistry in real world problems.	2	3	

		CO4	familiarize with the theories of reaction rate and their utilization.	3	3	
		CO5	understand the equilibrium and non-equilibrium properties of the system.	3	2	2
CHPC608	Spectroscopy-Applications in Organic Chemistry	CO1	have a detailed understanding about the spin dynamics and magnetic resonance	3	2	
		CO2	learn about the different pulse sequences and applications of NMR spectroscopy to the structural characterization of molecules	3	2	3
		CO3	apply mass spectrometry for the structural characterization of molecules	3	3	2
		CO4	use combined spectroscopic approach for problem solving and structural analysis	3	2	
		CO5	have a detailed understanding about the spin dynamics and magnetic resonance	3	2	1
CHPC613	Synthetic Organic Chemistry	CO1	the concept of retrosynthesis and the terms involved	3	2	
		CO2	about one group and two group disconnections	1	2	3
		CO3	the various protection and deprotection of important functional groups	3	2	
		CO4	the use of important reagents in organic synthesis	3	2	2
		CO5	about selected name reactions in Organic synthesis	3	3	
CHPC615	Main Group, Bioinorganic and Nuclear Chemistry	CO1	learn about the different rules concerning the main group and TM clusters and isolobal analogy	3	2	1
		CO2	learn about the inorganic chains, rings, cages and polymers	3	3	

		CO3	learn the role of metal ions in biological process.	3	2	3
		CO4	learn bio-energetic processes and metals in medicine.	3	3	
		CO5	learn about the basics of nuclear chemistry and its applications	3	2	
CHPC617	Statistical Thermodynamics, Photochemistry, and Surfaces	CO1	apply the principles of statistical mechanics on ensembles of molecules	2	3	2
		CO2	understand the association between statistical mechanics and thermodynamics	3	2	
		CO3	apply the theories of light-matter interactions in various photophysical processes	1	2	3
		CO4	define and explain surface- and interfacial phenomena	2	3	

PROGRAMME ELECTIVE (PE)

Course Outcomes: On successful completion of the course, students will be able to:

Course Code	Course Title	CO	Course outcomes At the end of the course student will be able to	PO 1	PO2	PO3
CHPE601	Catalysis	CO1	Learn about the fundamentals of catalysis	3	2	
		CO2	Learn about the C-H and C-C activation reactions	3	2	2
		CO3	Learn about the asymmetric catalysis	3	1	
		CO4	Learn about the photocatalytic reactions	3	2	1
		CO5	Learn about the heterogeneous catalysis	3	3	
CHPE603	Principles and Applications of Fluorescence Spectroscopy	CO1	learn the basic principles of fluorescence spectroscopy and their applications to chemistry materials and biology	3	3	
		CO2	measure and understand the fluorescence properties of various small molecules and	3	2	1

			bio-macromolecule that important in sensing and other application			
		CO3	analyse time-resolved fluorescence data for detailed understanding of the excited state processes	3	2	
		CO4	have understanding of advanced fluorescence spectroscopic and microscopic techniques	2	3	
CHPE605	Medicinal Chemistry	CO1	know the history and fundamentals of medicinal chemistry	3	3	
		CO2	classify the drugs and relationship between structure and activity.	2	2	
		CO3	understand the bio-mechanism of the antibiotics along with their synthetic routes	3	2	
		CO4	know the structure of enzymes, their activity and different types of interactions in bio-molecules	1	2	3
CHPE607	Nano Science and Technology	CO1	describe important physical methods in the field of nanoscience	3	2	
		CO2	describe important of structures in the field of nanoscience	2	3	
		CO3	describe important experimental tools in the field of nanoscience	3	2	
		CO4	familiarize with the applications of nanotechnology in sensors	3	2	2
CHPE609	Electronic Structure Methods and Modelling	CO1	explain the most important concepts of electronic structure theory	3	3	
		CO2	understand the structure and reactivity of chemical and biological systems	3	2	2

		CO3	discuss the structural and physical properties of solids in different dimensions	3	2	
		CO4	design and optimize the efficient materials for specific potential applications	2	3	1
CHPE611	Natural Products Chemistry	CO1	Classify the natural products based on their structures.	3	2	
		CO2	Know various types of amino acids, their structures, and importance.	3	2	2
		CO3	Understand the bio-functions of steroids and their structures.	2	3	
		CO4	Get a comprehensive knowledge about carbohydrates and some heterocycles	3	2	2
CHPE613	Advanced Heterocyclic Chemistry	CO1	identify the commonly used synthetic routes to heterocycles and major advances in the field of heterocyclic chemistry.	3	3	
		CO2	plan synthetic routes to complex organic molecules containing heterocyclic motifs	3	2	3
		CO3	be familiar with general synthetic approaches used in drug discovery and synthetic routes to major drugs containing heterocyclic motifs	2	3	3
		CO4	critically evaluate heterocyclic chemical literature, present seminars and short reviews in heterocyclic chemistry	3	2	2
CHPE602	Polymer Chemistry	CO1	know the classification of polymers and its nomenclature.		2	3
		CO2	learn the different polymerization methods and kinetics	2		3
		CO3	learn the theories of polymer structures	3	2	3
		CO4	learn the uses of polymers for commercial purposes	3		2

CHPE604	Computational Methods in Chemistry	CO1	develop c program for any chemistry problem.	3	2	
		CO2	apply numerical methods to evaluate experimental data.	3	2	2
		CO3	conceive the suitable force field methods and parameterization for force field energy.	3	2	3
		CO4	carry out geometry optimization, energy calculation using software	3	2	
CHPE606	Interfacial Chemistry and Sonochemistry	CO1	describe important physical methods in the field of Advanced Oxidation Processes	3	2	
		CO2	describe importance of sonochemistry	3	2	
		CO3	describe importance of ozonation	2	3	
		CO4	familiarize with the applications of sonochemistry	3	2	1
CHPE608	Lanthanide and Actinide Chemistry	CO1	Learn about the lanthanides and their extraction	3	2	
		CO2	Understand the lanthanide Chemistry and spectroscopy	2	2	3
		CO3	Learn about the organometallic chemistry of lanthanides and actinides	2	3	
		CO4	Learn about the actinides and their extraction	2	3	
		CO5	Learn about the electronic and magnetic properties of actinides	2	3	
CHPE610	Fuel cells for Stationary and Automotive Applications	CO1	apply the fundamental laws governing conversion from chemical to electrical energy.	3	2	
		CO2	understand the need to switch from hydrocarbon economy to hydrogen economy, specifically in the transportation sector.	2	3	
		CO3	select the right type of fuel cell for specific application.	3	2	

		CO4	quantify performance related parameters, such as power density, operational life and cost.	2	3	
CHPE612	Inorganic Rings, Cages and Clusters	CO1	Study different rules concerning the main group element containing clusters	3	2	2
		CO2	Study different rules concerning the transition element containing clusters	3	2	
		CO3	Have a clear understanding of the structural paradigms in chemistry and isolobal analogy	3	2	
		CO4	Study the inorganic homo and heterocyclic systems of main group elements	2	2	3
		CO5	Study the inorganic polymers in detail	3	2	2
CHPE614	Advanced Bioinorganic Chemistry	CO1	Understand the metal ions in life	2	3	2
		CO2	Understand the metalloenzyme chemistry	3	2	
		CO3	Understand the electron transport phenomena in body	3	3	2
		CO4	Understand the bio-organometallic catalysis	3	3	3
CHPE616	Organometallic Chemistry for Organic Synthesis	CO1	Analyse various synthetic strategies	3	2	
		CO2	Understand the reaction mechanisms in advanced synthesis	2	2	3
		CO3	Evaluate the organometallic based organic synthesis	2	3	
		CO4	Identify the different named reactions	3	2	1
CHPE618	Environmental Chemistry	CO1	Familiarize the basics of Environmental chemistry and its numerous facets.	3	2	
		CO2	Find out the important causes of pollution.	3	2	3
		CO3	Will work out the analysis data for its control.	2	3	2

		CO4	Know the health hazard in day-to-day life.	3	2	2
CHPE620	Biocatalytic processes in Chemical Industries	CO1	familiarize the basics industrial microbiology	3	2	3
		CO2	understand the application of microbial techniques in chemical synthesis	3	2	
		CO3	understand the biocatalysis	3	2	
		CO4	understand the applications of microbiology in chemistry	2	2	3
CHPE622	Photoredox- and Electro-Catalysis	CO1	familiarize with the modern strategies in organic synthesis.	3	2	
		CO2	understand the reactivities of organic molecules under light and electrochemical cell	3	2	
		CO3	plan synthetic routes to complex organic molecules following photo- /electro-catalysis	3	2	2
		CO4	know the major advances and the current state-of-the-art methods in organic chemistry	3	2	3
CHPE624	Multiscale Simulation Methods	CO1	understand the fundamentals of molecular dynamics techniques.	3	2	
		CO2	understand the mesoscale simulation methods.	3	2	
		CO3	understand the methodologies of enhanced sampling techniques.	3	2	2
		CO4	understand the application of big-data analysis in chemistry and biology.	3	3	
		CO5	understand the practical applications of computational chemistry and biology.	3	2	2
CHPE626	Semiconductor process integration and skills development by Virtual Fabrication	CO1	Understand the semiconductor manufacturing ecosystem	3	2	
		CO2	Understand the advantages of microfabrication and scaling	3	2	
		CO3	Seamlessly relate circuit abstraction with device cross-section and mask layout.	3	2	2

		CO4	Module-level understanding of advanced CMOS FinFET process	3	3	
		CO5	Use SEMulator3D® Software for semiconductor process development	3	2	2

LABORATORY (LR)

Course Outcomes: On successful completion of the course, students will be able to:

Course Code	Course Title	CO	Course Outcomes At the end of the course student will be able to	PO1	PO2	PO3
CHLR601	Inorganic and Analytical Chemistry Lab	CO1	learn about the semi-micro analysis of mixture of cations	3	3	
		CO2	learn about the volumetric estimation of mixture of cations	2	3	3
		CO3	learn about the gravimetric estimation of mixture of cations	3	3	2
		CO4	learn about the analysis of various samples in day-to-day life	3	3	1
CHLR602	Organic Chemistry Lab	CO1	separate the organic mixtures and identify the compounds	3	2	
		CO2	perform various reactions	2	3	
		CO3	perform natural product extraction	2	2	3
		CO4	learn about the estimation of organic compounds	2	2	
		CO5	learn about the analysis of oils	3	2	3
CHLR604	Physical Chemistry and Spectroscopy Lab	CO1	design and conduct experiments.	3	3	
		CO2	optimize the reaction conditions for the intended product.	3	2	
		CO3	use different instrumental methods of analysis and estimation	3	2	
		CO4	analyse and interpret the data.	3	2	

		CO5	do the analysis of samples using these techniques in day-to-day life	3	2	3
		CO6	develop the experimental skills required for analysis	2	3	

Course Code	**:**	CHPC601
Course Title	**:**	Organic Reaction Mechanisms and Aromaticity
Type of Course	**:**	PC
Prerequisites	**:**	B.Sc. Chemistry
Contact Hours	**:**	45
Course Assessment Methods	**:**	Continuous Assessment, End Assessment

COURSE LEARNING OBJECTIVES (CLO)

To introduce the students

CLO1	to the basics of reaction mechanism and the mechanistic concepts
CLO2	to the fundamentals of substitution reactions and reactive intermediates
CLO3	to the addition reactions of C=C and C=O bonds
CLO4	to the mechanism of elimination reactions and important redox reagents
CLO5	to the concept of aromaticity and reactions of aromatic compounds

COURSE CONTENT

Reaction mechanism: Definition of reaction mechanism, Experiments for studying mechanism, Trapping and competition/crossover, isotope scrambling experiments, Techniques to study Radical: Clock and trap. transition state theory, kinetics, qualitative picture. Substituent effects, linear free energy relationships, Hammett equation and related modifications. Basic mechanistic concepts like kinetic vs thermodynamic control, Hammond postulate, Curtin-Hammett principle, isotope effects, general and specific acid-base catalysis, and nucleophilic catalysis.

Aliphatic Nucleophilic Substitution: reactivity, structural and solvent effects, substitution in S_N1, S_N2, S_Ni. Neighbouring group participation -Norbornyl and bridgehead systems, substitution at allylic and vinylic carbons, substitution by ambident nucleophiles. Reactive intermediates-Carbenes, nitrenes, radicals, ylides-Formation, stability and their applications.

Addition to carbon-carbon multiple bonds: Electrophilic, nucleophilic and free radical addition. Stereochemistry and orientation of the addition. Hydrogenation, Halogenation, hydroxylation, hydroboration and Epoxidation. Addition to carbonyl compounds- 1,2 and 1,4-addition, benzoin, and Darzen glycidic ester reactions. Stereochemistry of Aldol and Michael addition reactions- Felkin- Ahn Model.

Elimination Reactions: E1, E2, E1CB- mechanism, stereochemistry, orientation of double bonds Hofmann, Zaitsev, Bredts rule-pyrolytic elimination, Chugaev reaction. Oxidation and reduction: Reduction using hydride reagents, $LiAlH_4$, $NABH_4$ and other organoboranes: chemo - and stereo selectivity, Catalytic hydrogenation (homogenous and heterogeneous catalysts) Swern and Dess-Martin oxidations, Corey-Kim oxidation, PCC, $KMnO_4$ oxidations.

Theories of Aromaticity: Aromaticity, Antiaromaticity and Pseudo aromaticity Huckel's rule, Molecular orbital description Polygon method. Annulenes and heteroannulenes, cyclopropenium, Cyclopentadienyl, tropylium, ions and fullerenes (C60). Aromatic electrophilic substitution: Orientation, reactivity, and mechanisms. Substitution in thiophene and pyridine. Aromatic nucleophilic substitution, S_N Ar, benzyne, S_N1. Aromatic Nucleophilic substitution of activated halides.

REFERENCES

1.	M. B. Smith, J. March, *March's Advanced Organic Chemistry,* John Wiley & Sons, 6th Edition, 2007.
2.	R. R. Carey and R. J. Sundburg, *Advanced Organic Chemistry, Part A and Part B,* Springer, 5th Edition, 2007.
3.	Peter Sykes, *A Guide Book to Mechanism in Organic chemistry,* Orient-Longman, 6th Edition, 1996.
4.	P. Y. Bruice, *Organic Chemistry,* Pearson Education, 7th Edition, 2013.
5.	E. V. Anslyn and D. A. Dougherty, *Modern Physical Organic Chemistry,* University Science Books, 1st Edition, 2005

COURSE OUTCOME

Upon completing the course, the student will be able to understand

CO1	the basics of reaction mechanism and the mechanistic concepts
CO2	the fundamentals of substitution reactions and reactive intermediates
CO3	the addition reactions of C=C and C=O bonds
CO4	the mechanism of elimination reactions and important redox reagents
CO5	the concept of aromaticity and reactions of aromatic compounds

Course Code	**:**	CHPC603
Course Title	**:**	Coordination Chemistry
Type of Course	**:**	PC
Prerequisites	**:**	B.Sc. Chemistry
Contact Hours	**:**	45
Course Assessment Methods	**:**	Continuous Assessment, End Assessment

COURSE LEARNING OBJECTIVES (CLO)

To introduce the students:

CLO1	to the theory and bonding of coordination compounds
CLO2	to the reactions and structures of coordination compounds
CLO3	to the electronic spectra and magnetism of coordination compounds
CLO4	to the solid-state chemistry and properties of lanthanides and actinides

COURSE CONTENT

Basics and theories: Basics of coordination chemistry - HSAB concept - stabilities of complexes - Irving-Williams series - chelate and macrocyclic effect - VB theory - CFT - splitting of d orbitals in ligand fields and different symmetries - CFSE - factors affecting the magnitude of Δ_o - evidence for crystal field stabilization - spectrochemical series - site selection in spinels - tetragonal distortion from octahedral symmetry - Jahn-Teller distortion - Nephelauxetic effect - MO theory - octahedral - tetrahedral and square planar complexes - bonding and molecular orbital theory - experimental evidence for - bonding.

Reactions: Substitution reactions in square planar complexes - the rate law for nucleophilic substitution in a square planar complex - the *trans* effect - theories of *trans* effect - mechanism of nucleophilic substitution in square planar complexes - kinetics of octahedral substitution - stereochemical outcome in octahedral substitution - mechanism of substitution in octahedral complexes - reaction rates influenced by acid and bases - racemization and isomerization - mechanisms of redox reactions - outer sphere mechanism - excited state outer sphere electron transfer reactions - inner sphere mechanism - mixed valence complexes.

Electronic spectra and magnetism: Microstates, terms and energy levels for d^1-d^9 ions in cubic and square fields - selection rules - band intensities and band widths - correlation diagrams - Orgel and Tanabe-Sugano diagrams - evaluation of Δ_o and β for octahedral complexes - charge transfer spectra - magnetic properties of coordination compounds - change in magnetic properties of complexes in terms of spin-orbit coupling - temperature dependent paramagnetism - spin cross-over phenomena - magnetic anisotropy and magnetism of dinuclear complexes - Van Vleck equation and its consequence to magnetic properties of transition metal complexes.

Structures: Structures of coordination compounds with reference to the existence of various coordination numbers (2, 3, 4, 5 & 6) - site preferences - isomerism - trigonal prism - absolute configuration of complexes - stereo selectivity and conformation of chelate rings - coordination number seven and eight - spectral and magnetic properties of lanthanide and actinide complexes.

Solid-state chemistry: Close packing of atoms and ions - bcc, fcc and hcp voids - structures of rock salt - cesium chloride - wurtzite - zinc blende - rutile - fluorite - antifluorite - diamond and graphite - perovskite - band theory of solids - dislocation in solids - Schottky and Frenkel defects - colour centres - electrical properties - insulators, semiconductors and conductors - Hall effect - super conductors - high Tc materials.

REFERENCES

1.	J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, *Inorganic Chemistry: Principles of Structure and Reactivity*, Pearson, 5th Edition, 2022.
2.	*F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, Advanced Inorganic Chemistry*, Wiley, 6th Edition, 2007.
3.	G. L. Miessler and D. A. Tarr, *Inorganic Chemistry*, 3rd Edition, Pearson, 2008.
4.	P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, *Inorganic Chemistry*, W. H. Freeman & Co, 4th Edition, 2006.
5.	L. V. Azaroff, *Introduction to Solids*, Mc.Graw Hill, New York, Indian Edition, 2017.

COURSE OUTCOMES (CO)

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

CO1	learn about the theories and bonding of coordination compounds
CO2	learn about the reactions and structures of coordination compounds
CO3	learn about the electronic spectra and magnetism of coordination compounds
CO4	learn about the basics of solid-state chemistry

Course Code	**:**	CHPC605
Course Title	**:**	Quantum Chemistry and Group Theory
Type of Course	**:**	PC
Prerequisites	**:**	B.Sc. Chemistry
Contact Hours	**:**	45
Course Assessment Methods	**:**	Continuous Assessment, End Assessment

COURSE LEARNING OBJECTIVES (CLO)

To introduce the students

CLO1	to solve elementary model problems in quantum mechanics and its applications
CLO2	to understand symmetry properties of molecules and application of group theory in understanding the electronic properties of systems

COURSE CONTENT

Foundation of Quantum Mechanics: Historical background, the wave function, Time-independent Schrodinger equation, the particle-in-a-box, tunnelling phenomenon, operators, principles/postulates of quantum mechanics, Hermitian operators, Solution of the Schrodinger equation for harmonic oscillator and rigid rotor, the particle-on-a-ring.

Angular Momentum and Hydrogen Atom: Angular momentum, representation of angular momentum operators and commutation relationships, the shape of wavefunctions, Coupling of angular momenta, the particle-on-a-sphere, Solution of the Schrodinger equation for hydrogen atom, radial and angular probability distributions, atomic orbitals, and electron spin, Pauli's exclusion principle.

Techniques of Approximation: Time-independent perturbation theory, First order correction to the energy and wavefunction, the closure approximation, the variation theory, the Raleigh-Ritz method, the Hellmann-Feynman theorem, Time-dependent perturbation theory, the Rabi formula, the Einstein transition probabilities. the Born-Oppenheimer approximation.

Fundamental of Group Theory: Symmetry elements and operations, Definition of a group, Group multiplication tables, point groups and assignment to molecules, Matrix representation, reducible and irreducible representations, construction of character tables, bases for irreducible representation, direct product, projection operators, Orthogonality theorem - its consequences.

Application of Group Theory: Molecular orbital theory - The LCAO ansatz, the symmetry adapted linear combination, the Hückel approximation for conjugated π-systems, MOs for σbonding in various ABn molecules, the selection rule for electronic transitions in formaldehyde and ethylene, the selection rules for fundamental vibrational transition, IR and Raman activity in CO_2, H_2O, N_2F_2, the exclusion rule and Fermi resonance.

REFERENCES

1.	N. Levine, *Quantum Chemistry,* Prentice Hall India, 4th Edition, 1994.
2.	Peter Atkins and Ronald Friedman, *Molecular Quantum Mechanics,* Oxford University Press, 4th Edition., 2005.
3.	F. A. Cotton, *Chemical Applications of Group Theory,* Wiley Eastern Ltd., 2nd Edition., 1990.
4.	A. K. Chandra, *Introductory Quantum Chemistry,* Tata McGraw Hill, 1994.
5.	M. S. Gopinathan and V. Ramakrishnan, *Group Theory in Chemistry,* Vishal Publishers, 1988.
6.	D. A. McQuarrie, *Quantum Chemistry,* University Science Books, 1983.
7.	R. K. Prasad, *Quantum Chemistry,* Tata McGraw Hill, 1995.

COURSE OUTCOMES (CO)

At the end of the course student will be able to

CO1	apply principles of quantum mechanics to calculate observables on known wave functions
CO2	apply the concept of quantization of energy and relate to molecular systems or nanomaterials
CO3	apply the variational method, and the perturbation theory to solve important molecular problems
CO4	apply group theory and character table to analyse the molecular properties

Course Code	**:**	CHPC607
Course Title	**:**	Analytical Chemistry
Type of Course	**:**	PC
Prerequisites	**:**	B.Sc. Chemistry
Contact Hours	**:**	45
Course Assessment Methods	**:**	Continuous Assessment, End Assessment

COURSE LEARNING OBJECTIVES (CLO)

To introduce the students:

CLO1	to the basic principles, working, and applications of Advanced chromatographic techniques
CLO2	to the working principles and applications of Ion selective electrodes
CLO3	to the principles and application of electroanalytical techniques
CLO4	to the principles and instrumentation of Atomic spectroscopic techniques and physical characterization methods.

COURSE CONTENT

Advanced chromatographic techniques: Theory of separation methods: HPLC, GC, GC/MS, LC/MS, GPC, Supercritical fluid chromatography, Detectors in Chromatography, Applications of Chromatography. Mathematical data analysis: Confidence intervals, statistical aids to hypothesis testing- analysis of variance and Regression analysis.

Ion selective electrodes: Working principles and applications– theoretical considerations - types of ion-selective electrodes – properties of ion-selective electrodes – sources of errors – construction and working of cation-specific electrodes for analysis of cadmium, lead, arsenic and anion-specific electrodes for fluoride, chloride and sulphide ions.

Electroanalytical techniques: Polarography - Introduction, Dropping mercury electrode (DME), Instrumentation, Ilkovic equation, and its verification, Determination of half wave potential, applications. Voltammetry –A three-electrode system concept – diffusion-controlled and adsorption-controlled electron-transfer reactions; Single sweep voltammetry, cyclic voltammetry – Randles-Sevcik equation, Criteria for reversible and irreversible processes - applications. Electrochemical sensors, ISFETs, CHEMFETs.

Atomic Absorption, Flame Emission, and Inductively Coupled Plasma Analysis: Atomic Absorption Spectroscopy and Flame Emission Spectroscopy - Basic principles–

Instrumentation – analytical applications. ICP-MS/OES - Basic principles- sources of radiation – instrumentation – analytical applications.

Physical methods of characterization: Surface Techniques: Principles and applications of electron spectroscopy for chemical analysis (ESCA) and Scanning Probe Microscopy.

REFERENCES

1.	Gary D. Christian, Purnendu (Sandy) Dasgupta, Kevin Schug, *Analytical Chemistry,* Wiley & sons, 7th Edition, 2013.
2.	Douglas A Skoog, Donald M West, F James Holler, Stanley R. Crouch, *Fundamentals of Analytical Chemistry,* Wadsworth Publishing Co Inc., 9th Edition, 2014.
3.	H.A. Willard, L.L.Merrit, J.A. Dean, Von Nostrand, *Instrumental Methods of Analysis,* 7th Edition, CBS Publishers, 1986.
4.	S.M. Khopkar, *Analytical Chemistry: Problems and Solutions,* New Age International Pvt. Ltd., 2nd Edition, 2010.
5.	J. Basset, R.C. Denny, C.H. Jaffery and J. Mendhan, *Vogel's Text Book of Quantitative Chemical Analysis,* ELBS, Longman Group Publishers, 6th Edition, 2009.

COURSE OUTCOMES (CO)

At the end of the course student will be able to

CO1	learn the basic principles, working, and applications of Advanced chromatographic techniques
CO2	learn the working principles and applications of Ion selective electrodes
CO3	learn the principles and application of electroanalytical techniques
CO4	learn the principles and instrumentation of Atomic spectroscopic techniques and physical characterization methods.

Course Code	**:**	CHPC609
Course Title	**:**	Theory of Spectroscopy and Molecular Excitons
Type of Course	**:**	PC
Prerequisites	**:**	B.Sc. Chemistry
Contact Hours	**:**	45
Course Assessment Methods	**:**	Continuous Assessment, End Assessment

COURSE LEARNING OBJECTIVES (CLO)

The learning objectives are to enable students

CLO1	to acquire knowledge on light-matter interactions
CLO2	to have specialized understanding of different spectroscopic methods
CLO3	to use quantum mechanical and group theoretical approach to understand molecular spectra
CLO4	to utilize different spectroscopic methods to examine chemical and physical properties of materials

COURSE CONTENTS

Rotational spectroscopy: Interaction of radiation with matter, Einstein coefficients - transition probability- Population of States – Boltzman Distribution-Molecular Hamiltonian, Born-Oppenheimer approximation- width of spectral lines- Principal moments of Inertia - Diatomic and polyatomic molecules- selection rules – Diatomic Rigid Rotor – Non Rigid Rotor – Nonlinear poly atomic molecules- Effect of Nuclear spin –Inversion Phenomenon – The Stark Effect

Vibrational Spectroscopy: Polyatomic molecules -harmonic and anharmonic oscillators-Morse potential-selection rules– Fermi Resonance-Group Frequencies - normal modes of vibrations of polyatomic molecules-selection rules- Group theoretical approach to spectral activity - FTIR spectrometer –Instrumentation and sampling. Raman Spectroscopy-Fundamentals- quantum mechanical description- Selection rules -rotational Raman - vibrational Raman spectra— Resonance Raman – Surface Enhanced Raman –Non-linear effects – Instrumentation and sampling

Atomic & Electronic spectroscopy: Atoms and molecules-term symbols- Russel – Saunders coupling — Zeeman Effect - Frank Condon principle- Vibronic transitions- selection rules-polarization of transitions- Transition dipole moment and Fermi's Golden Rule-Instrumentation and sampling - Fluorescence Spectroscopy – Jablonski Diagram- Kashas rules-Quenching

Molecular Exciton: Exciton states-binding energy, Frenkel-type exciton Hamiltonians, theories of exciton dynamics, coherent dynamics, local field and environment effects, exciton dynamics in molecular aggregates and conjugated polymer system, applications in organic photovoltaic materials and natural light-harvesting systems.

Photoelectron spectroscopy: Basic principles of electron spectroscopy, classification - electron energy analysis-photon sources - UV, X-ray, synchrotron, theory, angular dependence-cross section and its determination-valence and core photoemission - Koopmans' theorem.

REFERENCE BOOKS

1.	D. N. Sathyanarayana, *Handbook of Molecular Spectroscopy, From Radio waves to gamma rays*, I.K International Publishing house Pvt. Ltd, 2015
2.	C. N. Banwell, *Fundamentals of Molecular Spectroscopy*, 4th Edition, Tata McGraw Hill, 1996.
3.	J. M. Hollas, *Modern Spectroscopy*, 4th Edition, John Wiley& Sons, 1992.
4.	P. F. Bernath, *Spectra of Atoms and Molecules*, 2nd Edition, Oxford University Press, 2005.
5.	D. C. Harris and M. D. Bertolucci, *Symmetry and Spectroscopy*, Dover, 1989.
6.	P. K. Ghosh, *Introduction to Photoelectron Spectroscopy*, Wiley Interscience, 1983.
7.	A. B. P. Lever, *Inorganic Electronic Spectroscopy*, 2nd Edition, Elsevier, 1984
8.	Vladimir L. Broude, Emmanuel I. Rashba, Elena F. Sheka, *Spectroscopy of Molecular Excitons,* Springer-Verlag Berlin and Heidelberg GmbH & Co. K; Softcover reprint of the original 1st Edition, 1985.

COURSE OUTCOME

At the end of the course student will be able to

CO1	lean the fundamentals of interactions between electromagnetic radiation and matter
CO2	lean the theory of rotational, vibrational and Raman spectroscopic methods, and analysis of spectral data to examine physicochemical properties of matter
CO3	lean the different electronic spectroscopic methods and their utilization in understanding optoelectronic properties of molecules for practical applications
CO4	lean the theory of molecular exciton models and their applications lies in the field of photovoltaics and photosynthetic systems.

Course Code	**:**	CHLR601
Course Title	**:**	Inorganic and Analytical Chemistry Lab
Type of Course	**:**	PC
Prerequisites	**:**	B.Sc. Chemistry
Contact Hours	**:**	6 hours per week
Course Assessment Methods	**:**	Continuous Assessment, End Assessment

COURSE LEARNING OBJECTIVES (CLO)

To introduce the students

CLO1	to the semi-micro analysis of mixture of cations
CLO2	to the volumetric estimation of mixture of cations
CLO3	to the gravimetric estimation of mixture of cations
CLO4	to the analysis of various samples in day-to-day life

COURSE CONTENT

Semi-micro qualitative analysis (minimum 4 mixtures): Analysis of a mixture containing two common cations (Mg, Ca, Sr, Ba, Cr, Mn, Fe, Co, Ni, Zn, Cd, Al, Pb, Bi, NH_4^+) and two less common cations (Tl, W, Se, Te, Mo, Ce, Th, Ti, Zr, V, Be, U and Li).

Inorganic quantitative analysis: Analysis involving volumetric and gravimetric estimations of mixtures of cations Cu & Ni, Zn & Cu and Fe & Ni.

Analytical experiments:

1) Milk analysis:
   a) Determination of specific gravity of milk
   b) Determination of acidity of milk
   c) Estimation of total solid content in milk
   d) Estimation of ash content in milk
2) Cement analysis
3) Analysis of antacid tablet

REFERENCES

1.	In-house laboratory manual and relevant literature.
2.	V. V. Ramanujam, *Inorganic Semi–micro Qualitative Analysis,* 3rd Edition, National Publishing Company, l990.
3.	A. I. Vogel, *Text Book of Quantitative Inorganic Analysis,* 5th Edition, Longman, 1989

COURSE OUTCOMES (CO)

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

CO1	learn about the semi-micro analysis of mixture of cations
CO2	learn about the volumetric estimation of mixture of cations
CO3	learn about the gravimetric estimation of mixture of cations
CO4	learn about the analysis of various samples in day-to-day life

Course Code	**:**	CHPC602
Course Title	**:**	Stereochemistry, Photochemistry, Pericyclic and Rearrangement reactions
Type of Course	**:**	PC
Prerequisites	**:**	CHPC601
Contact Hours	**:**	45
Course Assessment Methods	**:**	Continuous Assessment, End Assessment

COURSE LEARNING OBJECTIVES (CLO)

To introduce the students

CLO1	to provide a comprehensive information about the stereochemistry of organic molecules.
CLO2	to the fundamentals of photochemistry and various photochemical reactions in detail.
CLO3	to plan synthetic routes to complex organic molecules through cycloaddition reactions.
CLO4	to be familiar with various types of rearrangement reactions.

COURSE CONTENT

Optical activity and chirality: absolute and relative configuration-R-S Notation system, Molecules with more than one asymmetric center. Enantiotopic and diastereotopic atoms, groups and faces. Stereo specific and stereo selective synthesis Fundamental to asymmetric synthesis: discussion on resolution, chiral auxiliaries, chiral ligands, chiral catalysts and organocatalysts with suitable examples. Optical isomerism of biphenyls, allenes and spiranes. Compounds containing chiral nitrogen and sulfur Geometrical isomerism, E, Z- nomenclature of olefins, cumulenes and oximes.

Conformational analysis: Inter-conversion of Sawhorse, Newman and Fischer projections Conformational analysis of ethane and disubstituted ethane derivatives, cycloalkanes and substituted cyclohexane. Conformation and stereochemistry of cis and trans decalin and 9-methyldecalin. Anomeric effect in cyclic compounds.

Photochemistry: Qualitative introduction about different transitions, Cis-Trans isomerization, Paterno-Buchi reaction, Norrish type I and II reactions, photo reduction of ketones, photochemistry of arenes di-pi-methane and Hoffmann-Loeffler-Freytag rearrangements, Barton reaction, Photoredox catalysis, Photodynamic therapy

Pericyclic reactions: Classification, electrocyclic, sigmatropic, cycloaddition and ene reactions, Woodward-Hoffmann rules, and FMO theory, Claisen, Cope, Sommelet-Hauser, and Diels-Alder reactions in synthesis, stereochemical aspects.

Rearrangement Reactions: reactions involving electron deficient, carbon, nitrogen, oxygen centers, emphasis on synthetic utility of these rearrangements. [1,2]-Meisenheimer, [2,3]-Meisenheimer, Wagner-Meerwein, Favorskii, Pummerer, Wolff, Meyer–Schuster, Rupe, Schmidt, Neber, Smiles, Truce-Smiles rearrangement.

REFERENCES

1.	*Photochemistry and Pericyclic Reactions* by Jagdamba Singh, 3rd Edition, ISBN-13: 978-1906574161 ISBN-10: 1906574162, New Age Science publisher
2.	*Stereochemistry of Organic Compounds: Principles and Applications,* 4^{th} Revised Edition, by D. Nasipuri, Publisher: New Academic Science Ltd.
3.	House, *Modern Synthetic Reactions,* 1973.
4.	R.O.C. Norman and J. M. Coxon, *Principles of organic synthesis,* ELBS, 1994.
5.	J. J. Li, *Name Reactions,* Springer, 3rd Edition, 2006.
6.	B. P. Mundy, M. G. Ellerd, F. G., Jr. Favaloro *Name Reactions and Reagents in Organic Synthesis,* Wiley-Interscience, 2005.
7.	E. L. Eliel, S. H. Wilen. *Stereochemistry of carbon compound,* Tata McGraw Hill, 2006

COURSE OUTCOMES (CO)

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

CO1	understand the stereochemistry of organic molecules in detail.
CO2	solve various problems on photochemical transformations.
CO3	plan synthetic routes to complex organic molecules through cycloaddition reactions.
CO4	understand the various types of rearrangement reactions and their mechanism.

Course Code	**:**	CHPC604
Course Title	**:**	Organometallic Chemistry and Inorganic Spectroscopy
Type of Course	**:**	PC
Prerequisites	**:**	B.Sc. Chemistry
Contact Hours	**:**	45
Course Assessment Methods	**:**	Continuous Assessment, End Assessment

COURSE LEARNING OBJECTIVES (CLO)

To introduce the students

CLO1	to the organometallic bonding principles
CLO2	to the industrially important homogenous catalytic cycles
CLO3	to the inorganic NMR IR and Raman spectroscopy
CLO4	to the EPR spectroscopy
CLO5	to the Mössbauer spectroscopy

COURSE CONTENT

Bonding and Reaction mechanisms in organometallics: 18/16 electron rule – Chatt-Dewar-Duncanson Model - dihydrogen complexes - agostic bonds - metal–metal bonds - Fischer and Schrock carbenes - structure, bonding & reactivity – metallocenes - electronic structure and bonding in ferrocene - Reaction mechanism - Substitution, oxidative addition, reductive elimination, insertion and de-insertion.

Catalysis: Hydroformylation, Monsanto process, Hydrogenation, Wilkinson's catalyst – Ziegler-Natta polymerization, C-C Heck & Suzuki coupling reactions, Olefin Metathesis – ADMET- metathesis polymerization – Hartwig-Buchwald amination

Inorganic spectroscopy: NMR Chemical shifts and coupling constants involving different nuclei (^{1}H, ^{19}F, ^{31}P, ^{13}C) - Effect of quadrupolar nuclei (^{2}H, ^{10}B, ^{11}B) on the ^{1}H NMR spectra - – fluxional molecules –isotropic shifts contact and pseudo-contact interactions – lanthanide shift reagents – Applications of IR and Raman Spectroscopy in Inorganic/ Organometallic systems – Electronic Spectra of Lanthanides

EPR spectroscopy: Resonance condition**-** Isotropic and anisotropic systems- g values ($g_{\perp}$ and $g_{\parallel}$)- Hyperfine splitting – EPR of organic radicals - spin densities and McConnell relationship – factors affecting the magnitude of g and A tensors in metal complexes– Zero-field splitting and Kramers degeneracy– Model system for pulse EPR experiments- ENDOR spectroscopy–Applications of EPR

Mössbauer spectroscopy: Gamma ray emission – recoil – recoilless resonance absorption – Debye model – Instrumentation and techniques- hyperfine interaction - **I**somer shift – quadrupolar splitting - magnetic interactions –impact of Zeeman effect - applications to iron and tin compounds – Fe-S proteins -

REFERENCES

1.	J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, *Inorganic Chemistry: Principles of Structure and Reactivity*, Pearson, 5th Edition, 2023.
2.	G. L. Miessler, P. J. Fischer and D. A. Tarr, *Inorganic Chemistry*, 5th Ed., Pearson Prentice Hall, New York, 2014.
3.	R. H. Crabtree, *The Organometallic Chemistry Of The Transition Metals*, 7th Ed., Wiley- VCH, 2019.
4.	B. D. Gupta and A. J. Elias, *Basic Organometallic Chemistry: Concepts, Syntheses and Applications*, 2nd Ed., Universities Press (India) Pvt Ltd., 2022.
5.	Ajay Kumar, *Organometallic & Bioinorganic Chemistry*, 5th Ed., Aaryush Education.
6.	R. S. Drago, *Physical Methods in Inorganic Chemistry*, Litton Educational Publishing, Inc. 2023.
7.	R. C. Maurya and J. M. Mir, *Molecular Symmetry and Group Theory: Approaches in Spectroscopy and Chemical Reactions*, Walter de Gruyter GmbH, Berlin/Boston, 2019.
8.	K. Nakamoto, *Infrared and Raman Spectra of Inorganic and Coordination Compounds*, Part A & Part B, 2nd Edition, Wiley, 2009.
9.	D. N. Sathyanarayana, *Handbook of Molecular Spectroscopy, From Radio waves to gamma rays*, I.K international Publishing house Pvt. Ltd, 2015
10.	J. A. Weil, J. R. Bolton, *Electron Paramagnetic Resonance, Elementary Theory and Practical Applications*, Wiely-Interscience, 2007.
11.	A. K. Das, M. Das, A. Das, *Fundamental Concepts of Inorganic Chemistry*, Vol. 7., CBS Publishers & Distributers Pvt Ltd., 2022.

COURSE OUTCOMES (CO)

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

CO1	learn about the organometallic bonding principles

CO2	learn about the industrially important homogenous catalytic cycles
CO3	learn about the inorganic NMR. IR and Raman spectroscopy
CO4	learn about the EPR spectroscopy
CO5	learn about the Mössbauer spectroscopy

Course Code	:	CHPC606
Course Title	:	Rates and Energetics of Chemical Reactions
Type of Course	:	PC
Prerequisites	:	B.Sc. Chemistry
Contact Hours	:	45
Course Assessment Methods	:	Continuous Assessment, End Assessment

COURSE LEARNING OBJECTIVES (CLO)

To introduce the students

CLO1	to learn the thermodynamic principles of systems in equilibrium and non-equilibrium systems and their associated properties.
CLO2	to understand the phases of coexistence in any reaction or equilibrium.
CLO3	to understand the basic principles of electrochemistry, interphases and their applications, the kinetics of reactions.

COURSE CONTENT

Advanced Thermodynamics: Equilibrium: Third law of thermodynamics and Nernst heat theorem. An apparent exception to the third law: Kauzmann paradox. Concept of chemical potential: Gibbs Duham equation. Relationship between partial molar quantities. Concept of standard states, fugacity, and activity coefficient. Experimental determination of activity coefficient of electrolytes.

Non-equilibrium Thermodynamics: Definition of non-equilibrium state and irreversible processes with examples. Concept of quasi-equilibrium stationary states, cross phenomenon, and microscopic reversibility. Concept of Correlation time. Minimum entropy production. Entropy production in open systems (matter flow, heat flow, mixing, chemical reactions, electrochemical reactions). Entropy flow and Entropy balance. Forces and fluxes. Phenomenological equations. Onsager reciprocal relations. Application in biological systems.

Electrochemistry-I: Ion transport in solution - migration, convention and diffusion -Fick's laws of diffusion conduction - influence of ionic atmosphere on the conductivity of electrolytes-The Debye-Hückel-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. The electrode-electrolyte interface-electrical double layer-electro capillary phenomena-

Lippmann equation - the Helmholtz- Perrin - Guoy-Chapmann and Stern models, electrokinetic phenomena. Tiselius method of separation of protons of proteins - membrane potential.

Electrochemistry-II: Electrodics - mechanism of electrode reactions-polarization and overpotential- the Butler Volmer equation for one step and multistep electron transfer reaction - the significance of equilibrium exchange current density and symmetry factor-significance of transfer coefficient-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 - electrodeposition. Electrochemical Impedance spectroscopy (EIS) basics, electrical elements, differential impedance, time domain results, graphical representation of impedance data in Bode and Complex plane plots.

Chemical kinetics: The steady-state approximation. Unimolecular theories of reaction rates (Lindeman-Hinshelwood). Transition state theory (derivation and comparison with collision theories). Enthalpy, Entropy, and Free Energy of Activation. Experimental methods for probing transition states (molecular-beam technique, femtosecond spectroscopy). Potential Energy Surfaces. Reaction Coordinates. Kinetic Isotope Effects. Factors determining reaction rates in solution. Solvent dielectric constant and ionic strength. Chain reactions - linear reactions, branching chains - explosion limits. Rice–Herzfeld scheme. Kinetics of free radical polymerization reactions. Enzyme catalysis - rates of enzyme-catalyzed reactions - effect of substrate concentration, pH, and temperature - determination of Michael's parameters.

REFERENCES

1.	S. Glasstone, *Thermodynamics for chemists*, Affiliated East West Press, 1965.
2.	P.W. Atkins, *Physical Chemistry*, Oxford University Press, 6th Edn., 1998.
3.	K. J. Laidler, *Chemical Kinetics*, Harper and Row Publishers, 3rd Edn., 1987.
4.	J. O. M. Bockris and A. K. N. Reddy, *Modern Electrochemistry*, Plenum Press, 1970.
5.	J. Rajaram and J. C. Kuriakose, *Thermodynamics for Students of Chemistry*, Shobanlal Nagin Chand Co, 1986.
6.	C. Kalidas, M. V. Sangaranarayanan, "*Non-equilibrium Thermodynamics*", Macmillan India 2012.

COURSE OUTCOMES (CO)

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

CO1	understand the equilibrium and non-equilibrium properties of the system.
CO2	understand the interrelationship between partial molar properties of phase equilibrium.
CO3	analyse and apply the principles of electrochemistry in real world problems.
CO4	familiarize with the theories of reaction rate and their utilization.
CO5	understand the equilibrium and non-equilibrium properties of the system.

Course Code	**:**	CHPC608
Course Title	**:**	Spectroscopy- Applications in Organic Chemistry
Type of Course	**:**	PC
Prerequisites	**:**	B.Sc. Chemistry
Contact Hours	**:**	45
Course Assessment Methods	**:**	Continuous Assessment, End Assessment

COURSE LEARNING OBJECTIVES (CLO)

To introduce the students

CLO1	to the spin dynamics and magnetic resonance
CLO2	to the different pulse sequences and applications of NMR spectroscopy to the structural characterization of molecules
CLO3	to apply mass spectrometry for the structural characterization of molecules
CLO4	to use combined spectroscopic approach for problem solving and structural analysis

COURSE CONTENT

Nuclear magnetic resonance I: Introduction to one dimensional NMR, magnetization, Larmor frequency, rotating and laboratory frame, free induction decay (FID), FT-generation of NMR peaks, relaxation phenomena, effect of pulses, FT-NMR instrumentation, NMR sample preparation, ^{1}H-NMR - chemical shift, diamagnetic anisotropy, spin-spin coupling- mechanism and sign of J coupling, analysis of first order multiplets, magnetic equivalence, second order coupling effects, Pople nomenclature - AX, AB, ABC, AMX, AABB, AA′BB′ systems, Karplus relationship, chemical shift reagents

Nuclear magnetic resonance II: ^{13}C-NMR – chemical shifts and line intensities, saturation and spin decoupling, homonuclear and heteronuclear spin decoupling experiments, nuclear Overhouser effect (NOE), NOE difference experiment, conformational analysis from NOE, multiple pulse sequences, J-modulated spin echo, polarization transfer – APT and DEPT experiments and analysis, dynamic processes by NMR- restricted rotation (DMF, DMA, biphenyls, annulenes), cyclohexane ring inversion, degenerate rearrangements, One dimensional NMR spectra of other-nuclei (^{13}C, ^{15}N, ^{31}P and ^{19}F)

Nuclear magnetic resonance III: Introduction to two dimensional NMR, 2D NMR techniques: Homo- and hetero-nuclear correlation (COSY, HETCOR, TOCSY, HSQC, HMBC), analysis of 2D NMR spectra, NOESY and ROESY experiments, INADEQUATE, introduction to solid state NMR, diffusion-NMR and magnetic resonance imaging (MRI) techniques

Mass spectroscopy: Methods of desorption and ionization (EI, CI, ESI, MALDI, FAB, TOF), instrumentation, magnetic sector analysis, quadrupole analyser, ion cyclotron resonance (FT), meta stable ions, study of fragmentation pattern, bond cleavage, McLafferty rearrangement, retro Alder fragmentation, applications in organic chemistry, isotope distribution analysis.

Structural Analysis of Molecules: Application of ^{1}H NMR, ^{13}C-NMR and Mass spectroscopy in structural analysis of molecules, case studies on 1D and 2D NMR, problem solving using combined UV-vis absorption, IR, NMR, and Mass analysis.

REFERENCES

1.	D. L. Pavia, G. M. Lampman, G. S. Kriz, J. A. Vyvyan, *Introduction to Spectroscopy,* 5th Edn., Brooks Cole, 2010.
2.	R. S. Macomber, *A Complete Introduction to Modern NMR Spectroscopy,* John Wiley & Sons Ltd, 1998.
3.	L. D. Field, S. Sternhell, J. R. Kalman, *Organic Structures from Spectra,* John Wiley & Sons, Ltd, 4th and 5th Edn. 2007 & 2013.
4.	M. Balci, *Basic ^{1}H- and ^{13}C-NMR Spectroscopy,* Elsevier, 2005.
5.	J. H. Simpson, *Organic Structure Determination using 2D-NMR Spectroscopy,* Academic Press, 2008.
6.	M. H. Levitt, *Spin Dynamics- Basics of Nuclear Magnetic Resonance,* 2nd Edn, John Wiley and sons, 2008.
7.	E. Breitmaier, *Structure Elucidation by NMR in Organic Chemistry - A Practical Guide,* 3rd Edn, John Wiley and Sons, 2002.

COURSE OUTCOMES (CO)

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

CO1	have a detailed understanding about the spin dynamics and magnetic resonance
CO2	learn about the different pulse sequences and applications of NMR spectroscopy to the structural characterization of molecules
CO3	apply mass spectrometry for the structural characterization of molecules
CO4	use combined spectroscopic approach for problem solving and structural analysis
CO5	have a detailed understanding about the spin dynamics and magnetic resonance

Course Code	**:**	CHLR602
Course Title	**:**	Organic Chemistry Lab
Type of Course	**:**	PC
Prerequisites	**:**	B.Sc. Chemistry
Contact Hours	**:**	6 hours per week
Course Assessment Methods	**:**	Continuous Assessment, End Assessment

COURSE LEARNING OBJECTIVES (CLO)

The learning objectives are to enable students

CLO1	to separate the organic mixtures and identify the compounds
CLO2	to perform various reactions
CLO3	to perform natural product extraction
CLO4	to estimate the organic compounds
CLO5	to the analysis of oils

COURSE CONTENT

1. **Separation, Purification and Identification of organic compounds**
    i. Preparation of TLC plates and analysis of mixtures (TLC plates, glass rods, TLC grade silica, Distilled water)
    ii. Separation using column chromatography and crystallization
    iii. Identification using IR and NMR Spectroscopy
2. **Preparation, Purification and Identification of products using spectroscopy**
    i. Claisen Schmidt reaction – Dibenzalacetone synthesis
    ii. Fischer Indole synthesis
    iii. Benzil reduction
    iv. Synthesis of dinitrobenzene
    v. Glucosazone
    vi. Diels-Alder reaction of Anthracene and maliec anhydride
    vii. preparation of diazoamino benzene
    viii. Preparation of 2-Iodoxybenzoic Acid (IBX)
    ix. Alkylation of Isatin
3. **Soxhlet extraction of natural product**
    i. Curcumin, Tea leaves, Neem leaves etc.

4. **Organic quantitative analysis:**

a. Estimations:

i. Estimation of phenol, aniline, ascorbic acid

ii. Estimation of ketone by volumetric method & gravimetric method

iii. Estimation of lactose in milk

iv. Estimation of glucose by Fehling's method

v. Estimation of glucose by Bertrand's method.

b. Analysis of Oils:

i. Determination of saponification value of an oil

ii. Determination of acetyl value of an oil

iii. Determination of iodine value of an oil

iv. Determination of acid value of an oil.

REFERENCES

1.	I. Vogel, *Text Book of Practical Organic Chemistry,* 5th Edn., ELBS, London, 1989.
2.	B. B. Dey and M. V. Sitharaman, *Laboratory Manual of Organic Chemistry,* Revised by T.R. Govindachari, Allied Publishers Ltd., New Delhi, 4th Revised Edn., 1992.
3.	A. I. Vogel, *Text Book of Practical Organic Chemistry*, 5th Edition, ELBS, 1989.

COURSE OUTCOME (CO)

Upon completing the course, the student will be able to

CO1	separate the organic mixtures and identify the compounds
CO2	perform various reactions
CO3	perform natural product extraction
CO4	learn about the estimation of organic compounds
CO5	learn about the analysis of oils

Course Code	:	CHLR604
Course Title	:	Physical Chemistry and Spectroscopy Lab
Type of Course	:	PC
Prerequisites	:	B.Sc. Chemistry
Contact Hours	:	6 hours per week
Course Assessment Methods	:	Continuous Assessment, End Assessment

COURSE LEARNING OBJECTIVES (CLO)

The learning objectives are to enable students

CLO1	to perform various laboratory experiments for analysis of sample
CLO2	to acquire hands-on experience in studying thermodynamics and kinetics of chemical systems
CLO3	to interpret experimental data for physical and chemical characterizations of systems
CLO4	to record and analyse spectral data of molecular systems

COURSE CONTENT

Physical Chemistry

1. Kinetic study of hydrolysis of ester. Determination of order, I^- and $S_2O_8^{2-}$.
2. Kinetics of iodination of acetone by spectrophotometer.
3. Partition coefficient of NH_3 between water and chloroform.
4. Determination of partition coefficient and equilibrium constant for $KI + I_2 \rightarrow KI_3$.
5. Adsorption of oxalic acid on activated charcoal.
6. Determination of heat of solution and heat of fusion.
7. Study of three component system.
8. Determination of solubility product.
9. Study of chain linkages in PVA and its molecular weight determination by viscometry.
10. Partial molar volume of NaCl.
11. Buffer preparation and pH-metric titration.
12. Conductometric titration of mixture of acids and precipitation titration (KCl Vs $AgNO_3$) using conductivity bridge.
13. Potentiometric titrations.

14. Determination of the capacitance of electrochemical interfaces, formal potential and diffusion coefficient of $[Fe(CN)_6]^{3-}$ by cyclic voltammetry.
15. Estimation of Pb^{2+} ion by amperometric titration.

Spectroscopy

1. Michelson's interferometer- Wavelength of light and refractive index determination
2. Calculation of molar extinction coefficient
3. Absorption spectroscopy- Beers law –Deviations-Titrations
4. Photoelectric effect- Planks constant- Work function of material determination
5. Fluorescence spectroscopy- Excitation and emission, Kashas rule
6. Relative quantum yield determination of unknown fluorophores
7. Fluorescence quenching experiment and Stern-Volmer coefficient determination
8. Study of twisted intramolecular charge transfer of molecules (such as, DMABN) in different solvents
9. Polarization of light- Malus Law Verification
10. Synthesis of quantum dots (such as, perovskite quantum dots) and their spectral properties
11. Demonstration of Raman Spectroscopy

REFERENCES

1.	C. Garland, J. Nibler and D. Shoemaker, *Experiments in Physical Chemistry***,** McGraw-Hill Education; 8th Edn., 2008.
2.	A. I. Vogel, *Text Book of Quantitative Inorganic Analysis*, 5th Edn, Longman, 1989.
3.	Manual provided by the Department.

COURSE OUTCOME (CO)

Upon completing the course, the student will be able to

CO1	design and conduct experiments.
CO2	optimize the reaction conditions for the intended product.
CO3	use different instrumental methods of analysis and estimation
CO4	analyse and interpret the data.
CO5	do the analysis of samples using these techniques in day-to-day life
CO6	develop the experimental skills required for analysis

Course Code	**:**	CHPC613
Course Title	**:**	Synthetic Organic Chemistry
Type of Course	**:**	PC
Prerequisites	**:**	CHPC601 and CHPC602
Contact Hours	**:**	45
Course Assessment Methods	**:**	Continuous Assessment, End Assessment

COURSE LEARNING OBJECTIVES (CLO)

CLO1	The concept of retrosynthesis and the terms involved
CLO2	About one group and two group disconnections
CLO3	The various protection and deprotection of important functional groups
CLO4	The use of important reagents in organic synthesis
CLO5	About selected name reactions in Organic synthesis

COURSE CONTENT

Introduction to retrosynthesis: synthon, synthetic equivalent, target molecule, functional group interconversion, disconnection approach, importance of the order of events in organic synthesis. Chemo-selectivity, one group C-C and C-X disconnection (disconnection of alcohols, alkenes, and carbonyl compounds)

Two group C-C & C-X disconnections: 1,3 and 1,5 difunctionalised compounds, α, β-unsaturated carbonyl compounds, control in carbonyl condensation, synthesis of 3,4,5 and 6 membered rings in organic synthesis. Diels- Alder reaction, Connection in retro synthesis

Protecting groups: Protection of hydroxyl, carboxyl, carbonyl, amino groups. Umpolung reagents, definition of umpolung, Umpolung strategy using radical synthesis, acyl anion equivalent, Protection of carbon-carbon multiple bonds. Illustration of protection and deprotection in synthesis.

Organic Reagents: Use of the following reagents in organic synthesis and functional group transformation, Gilman's reagent, lithium diisoproplyamide (LDA), dicyclohexylcarbodimide, timethylsilyl iodide, Woodward and Provost hydroxylation, DDQ, SeO_2, phase transfer catalyst, crown ethers and Merrifield resin, Baker yeast, N-Heterocyclic carbenes,

Name reactions in organic synthesis: Peterson olefination, McMurry, Shapiro reaction, Palladium based reactions- Suzuki, Heck, Negishi, Sonagashira, Hiyama, Stille coupling. Sharpless epoxidation, Claisen, Baylis Hillman reaction, Stork enamine reaction and selective mono and di alkylation via enamines, Buchwald-Hartwig reaction, olefin metathesis, Noyori asymmetric hydrogenation, Ugi and passerine reaction, Domino/tandem/cascade reaction concepts with selected examples

REFERENCES

1.	House, *Modern Synthetic Reaction*, 1973
2.	S. Warren, *Organic Synthesis The Disconnection approach*, Wiley and sons, 2002.
3.	M. B. Smith, *Organic Synthesis,* 4^{th} Edition, Academic press
4.	W. Carruthers, *Modern methods of Organic Synthesis,* Cambridge University Press
5.	Clayden, Greeves, Warren & Wothers, *Organic Chemistry,* Oxford University Press.
6.	Jie Jack li, *Name Reactions,* Springer, 3rd Edn, 2006.
7.	R. R. Carey and R. J. Sundburg, *Advanced Organic Chemistry, Part A and Part B*, Springer, 5^{th}Edn, 2007.

COURSE OUTCOMES (CO)

Upon completing the course, the student will be able to understand

CO1	the concept of retrosynthesis and the terms involved
CO2	about one group and two group disconnections
CO3	the various protection and deprotection of important functional groups
CO4	the use of important reagents in organic synthesis
CO5	about selected name reactions in Organic synthesis

Course Code	**:**	CHPC615
Course Title	**:**	Main Group, Bioinorganic and Nuclear Chemistry
Type of Course	**:**	CHPC603 and CHPC604
Prerequisites	**:**	B.Sc. Chemistry
Contact Hours	**:**	45
Course Assessment Methods	**:**	Continuous Assessment, End Assessment

COURSE LEARNING OBJECTIVES (CLO)

To introduce the students

CLO1	to the rules concerning the main group and TM clusters and isolobal analogy
CLO2	to the inorganic chains, rings, cages and polymers
CLO3	to the role of metal ions in biological process.
CLO4	to the bio-energetic processes and metals in medicine.
CLO5	to the basics of nuclear chemistry and its applications

COURSE CONTENT

Cluster chemistry: Isolobal analogy - extensions and applications - metal–metal bonding - polyhedral boranes and carboranes - STYX notation - Wade-Mingos and Jemmis electron counting rules - heteronuclear clusters - carboranes - heteroboranes - metalloboranes - bonding in P4 and B_4Cl_4 clusters - Transition metal clusters geometric and electronic structure

Main group chemistry: Inorganic chains – rings – cages - polymers - structure and synthesis - boron halides - phosphine-boranes – borazine - phosphorous halides, acids and oxyacids – phosphazenes - sulphur halides - oxo acids of sulphur - S–N heterocycles - chemistry of halogens and noble gases - polyoxometallates - P, Si, S, N & O based polymers, poly-phosphazenes, poly-thiazenes, poly-siloxanes and poly-silanes. Molecular clusters in catalysis, clusters to materials, boron-carbides and metal-borides.

Bioinorganic chemistry-I: Various elements in organisms - vitamin and coenzyme B12 - functions - photosynthesis - dioxygen uptake, transport and storage - hemoglobin and myoglobin - hemerythrin - hemocyanin - catalysis through hemoproteins - electron transfer, oxygen activation and metabolism - cytochrome –iron-sulfur and other non-heme iron proteins - siderophores - ferritin - nickel-containing enzymes - copper-containing proteins-Zinc containing enzymes such as Alcohol dehydrogenase, Carbonic anhydrase, Carboxypeptidase A, Zinc finger proteins, superoxide dismutase (Cu, Zn).

Bioinorganic chemistry-II: Mo, W, V, Cr & Zn containing proteins and enzymes - function and transport of alkali and alkaline earth metal cations - catalysis and regulation of bio-energetic processes by alkaline earth metal ions Mg^{2+} and Ca^{2+} - biological functions of non-metallic inorganic elements - bioinorganic chemistry of quintessentially toxic metals - biochemical behaviour of radionuclides and medical imaging - chemotherapy - cisplatin.

Nuclear chemistry: Mass and charge - nuclear moments - binding energy - mass defect - packing fraction - stability - magic numbers - modes of radioactive decay - rate of radioactive decay - half-life - average life - energetics and types - nuclear fission - liquid drop model - nuclear fusion - essential features of nuclear reactors - tracer techniques - neutron activation analysis - carbon and rock dating - application of tracers in chemical analysis - reaction mechanisms - medicine and industry.

REFERENCES

1.	D. M. P. Mingos and D. J. Wales, *Introduction to Cluster Chemistry,* Prentice Hall, 1990.
2.	T. Chivers, I. Manners, *Inorganic Rings and Polymers of the p-Block Elements,* from Fundamentals to Applications, RSC Publishing, 2009.
3.	J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, *Inorganic Chemistry: Principles of Structure and Reactivity,* Pearson, 5^{th} Edition, 2023.
4.	K. F. Purcell and J. C. Kotz, *Inorganic Chemistry; Cengage Learning,* 3^{rd} Indian reprint, 2017.
5.	N. N. Greenwood and E. A. Earnshaw, *Chemistry of Elements,* Pergaman Press, 1984.
6.	G. L. Miessler, P. J. Fischer and D. A. Tarr, *Inorganic Chemistry,* 5th Edition, Pearson Prentice Hall, New York, 2014.
7.	A. K. Das, M. Das, A. Das, *Fundamental Concepts of Inorganic Chemistry,* 3^{rd} Edition, Vol. 2., CBS Publishers & Distributers Pvt Ltd., 2021.
8.	M. Weller, J. Rourke, T. Overton, F. Armstrong, *Inorganic Chemistry,* 7^{th} Edition., Oxford University Press, UK, 2018.
9.	S. F. A. Kettle, *Physical inorganic Chemistry: A Coordination Approach,* Spektrum Academic Publishers,1996.
10.	F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, *Advanced Inorganic Chemistry,* Wiley, 6^{th} Edition, 2007.

11.	S. J. Lippard and J. M. Berg, *Principles of Bioinorganic Chemistry,* Panima Publishing Company, New Delhi, 1997.
12.	W. Kaim and B. Schewederski, *Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life,* 2nd Edition, John Wiley and Sons, New York, USA, 2013.
13.	Bertini, Gray, Lippard and Valentine, *Bioinorganic Chemistry,* Viva books Pvt. Ltd. 1998.
14.	A. K. Das, M. Das and A. Das, *Bioinorganic Chemistry,* 2nd Edition, Books & Allied (P) Ltd., 2020.
15.	A. K. Das, M. Das, A. Das, *Fundamental Concepts of Inorganic Chemistry,* 3rd Edition, Vol. 1., CBS Publishers & Distributers Pvt Ltd., 2022.
16.	H. J. Arnikar, *Essentials of Nuclear Chemistry,* 4th Edition, New Age International Publishers Ltd., New Delhi, 1995.

COURSE OUTCOMES (CO)

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

CO1	understand the different rules concerning the main group and TM clusters and isolobal analogy
CO2	describe the inorganic chains, rings, cages and polymers
CO3	explain the role of metal ions in biological process.
CO4	understand the bio-energetic processes and metals in medicine.
CO5	elaborate the basics of nuclear chemistry and its applications

Course Code	**:**	CHPC617
Course Title	**:**	Statistical Thermodynamics, Photochemistry, and Surfaces
Type of Course	**:**	PC
Prerequisites	**:**	CHPC605 and CHPC606
Contact Hours	**:**	45
Course Assessment Methods	**:**	Continuous Assessment, End Assessment

COURSE LEARNING OBJECTIVES (CLO)

CLO1	To learn the statistical models of thermodynamic properties of macroscopic systems
CLO2	To understand the principles of photochemistry, surface chemistry and their applications

COURSE CONTENT

Statistical Thermodynamics-I: Maxwell's law of distribution of molecular speeds, derivation of expressions for average, most probable and root mean square velocity. Concept of velocity space and phase space, Combination-laws of probability-microstates for distinguishable and indistinguishable particles. Derivation of Maxwell Boltzmann distribution law - partition functions and their calculation. Expressions for thermodynamic quantities in terms of partition functions-translational, rotational, vibrational and electronic contributions to the thermodynamic properties of perfect gases, Intermolecular forces in imperfect gases. Statistical interpretation of laws of thermodynamics, third law of thermodynamics.

Statistical Thermodynamics II: Limitation of classical statistics - quantum statistics and classical statistics, comparison-heat capacities of gases in general and hydrogen in particular-heat capacities of solids. Einstein and Debye models - Bose Einstein statistics and Fermi Dirac statistics and corresponding distribution functions- applications of quantum statistics to liquid helium, electrons in metal and Planck's radiation law.

Photochemistry: Absorption and emission of radiation, Franck Condon principle decay of electronically excited states, radiative and non-radiative processes, fluorescence and phosphorescence, spin-forbidden radiative transitions, inter conversion and intersystem crossing. Theory of energy transfer - resonance and exchange mechanism, triplet-triplet annihilation, photosensitization and quenching. Spontaneous and induced emissions. Einstein transition probability- inversion of population - laser and masers. Flash photolysis: Chemi and thermo luminescence.

Adsorption Isotherm: Surface Phenomena, Gibbs adsorption isotherm, types of adsorption isotherms, solid-liquid interfaces, contact angle and wetting, solid-gas interface, physisorption and chemisorption, Freundlich, derivation of Langmuir and BET isotherms, surface area determination. Kinetics of surface reactions involving adsorbed species, Langmuir-Hinshelwood mechanism, Langmuir-Rideal mechanism, Rideal-Eley mechanism.

Surface Analysis: Surface Films, Langmuir-Blodgett films, self-assembled mono layers, collapse pressure, surface area and mechanism of heterogeneous catalysis, phase transfer catalysis. Chemical analysis of surfaces: Surface preparations- spectroscopic surface characterization methods, electron spectroscopy, ion scattering spectrometry, secondary ion scattering microscopy (SIMS)-Auger electron spectroscopy- instrumentation and application. Electron stimulated micro analysis, scanning probe microscopes.

REFERENCES

1.	P. W. Atkins, *Physical Chemistry*, Oxford University Press, 6thEdn., 1998.
2.	D. McQuarie, and J. D. Simmen, *Physical Chemistry*, University Science, 1stEdn., 1998.
3.	S. Glasstone, *Thermodynamics for Chemists*, Affiliated East West Press, 1965.
4.	C. McClelland, *Statistical Thermodynamics*, Chapman and Hall, 1973.
5.	L. K. Nash, *Elements of Classical and Statistical Thermodynamics*, Addison-Wesley, 1970.
6.	K. K. Rohatgi - Mukerjee, *Fundamentals of Photochemistry,* Wiley 1992.
7.	P. K. Ghosh, *Introduction to Photoelectron Spectroscopy,* Wiley Interscience, 1983.

COURSE OUTCOMES (CO)

At the end of the course student will be able to

CO1	apply the principles of statistical mechanics on ensembles of molecules
CO2	understand the association between statistical mechanics and thermodynamics
CO3	apply the theories of light-matter interactions in various photophysical processes
CO4	define and explain surface- and interfacial phenomena

Course Code	**:**	CHPE601
Course Title	**:**	Catalysis
Type of Course	**:**	PE
Prerequisites	**:**	B.Sc. Chemistry
Contact Hours	**:**	45
Course Assessment Methods	**:**	Continuous Assessment, End Assessment

COURSE LEARNING OBJECTIVES (CLO)

To introduce the students

CLO1	to the fundamentals of catalysis
CLO2	to the C-H and C-C activation reactions
CLO3	to the asymmetric catalysis
CLO4	to the photocatalytic reactions
CLO5	to the heterogeneous catalysis

COURSE CONTENT

Fundamentals: Catalyst - activation energy concept - types of catalysis - comparison of homogeneous & heterogeneous catalysis - enzyme catalysis - green catalysis - nano catalysis - autocatalysis - phase transfer catalysis - promoters - poisons - examples.

C-H and C-C activation: Alkene Metathesis-Mechanism- ROMP, SHOP and ADMET- C-H bond Activation-Ziegler-Natta Polymerization of olefins-Telomerization Metallocene catalysts -sigma bond metathesis - Diels -Alder Reaction- Isomeration of Alkenes- Oligomerization - Hydrocyanation - Wacker oxidation - Metal catalyzed liquid phase autoxidation - Asymmetric Catalysis - hydrogeneation- isomerization-epoxidation-hydrolyis - Nitroaldol condensation

Asymmetric Catalysis: Assymetric Hydrogenation – Epoxidation of allylic alcholols – Assymmetric dihydroxylation – Hydroformylation – nitroaldol condensation – Liquid phase autooxidation – cyclo hexane p xylene – Phase Transfer Catalysis – Homo and heterobimetallic complexes in cooperative catalysis – Case studies – Azide Alkyne cycloaddition – Pauson – khand reaction - - hydrosilylation

Photocatalysis: Porphyrins -phthalocyanines and semiconductor as photo catalysts in photolysis reactions - generation of hydrogen by photo catalysts - photocatalytic break down of water and harnessing solar energy - photocatalytic degradation of dyes - environmental applications.

Heterogeneous catalysis: Adsorption isotherms - surface area - pore size and acid strength measurements -porous solids -catalysis by metals - semiconductors and solid acids -supported metal catalysts -catalyst preparation - deactivation and regeneration -model catalysts - ammonia synthesis -hydrogenation of carbon monoxide -hydrocarbon conversion - selective catalytic reduction - polymerization.

REFERENCES

1.	P. H. Emmet, *Catalysis* (Vol I and II), Reinhold, 1954.
2.	M. Schlosser, *Organometallics in Synthesis*, A Manual, John Wiley, 1996.
3.	R. H. Crabtree, *The Organometallic Chemistry Of The Transition Metals*, 7th Ed., Wiley- VCH, 2019.
4.	B. D. Gupta and A. J. Elias, *Basic Organometallic Chemistry: Concepts, Syntheses and Applications*, 2nd Ed., Universities Press (India) Pvt Ltd., 2022.
5.	Ajay Kumar, *Organometallic & Bioinorganic Chemistry*, 5th Ed., Aaryush Education.
6.	L. S. Hegedus, *Transition Metals in the Synthesis of Complex Organic Molecules*, University Science, 1999.
7.	D. K. Chakrabarty and B. Viswanathan, *Heterogeneous Catalysis*, New Age, 2008.
8.	B. Viswanathan, S. Kannan and R.C. Deka, *Catalysts and Surfaces: Characterization Techniques*, Narosa, 2010.
9.	M. Kaneko and I. Okura, *Photocatalysis: Science and Technology*, Springer, 2003.

COURSE OUTCOMES (CO)

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

CO1	learn about the fundamentals of catalysis
CO2	learn about the c-h and c-c activation reactions
CO3	learn about the asymmetric catalysis
CO4	learn about the photocatalytic reactions
CO5	learn about the heterogeneous catalysis

Course Code	**:**	CHPE603
Course Title	**:**	Principles and Applications of Fluorescence Spectroscopy
Type of Course	**:**	PE
Prerequisites	**:**	CHPC609
Contact Hours	**:**	45
Course Assessment Methods	**:**	Continuous Assessment, End Assessment

COURSE LEARNING OBJECTIVES (CLO)

The learning objectives are to enable students to

CLO1	acquire specialized understanding of excited state processes and their timescales
CLO2	become familiar with advanced time-resolved spectroscopic and microscopic tools
CLO3	use spectroscopic methods for kinetic analysis of ultrafast processes
CLO4	understand the development of fluorophores for various practical applications

COURSE CONTENT

Unit I: Introduction to fluorescence – electronic spectroscopy and Jablonski diagram, instrumentation for steady-state fluorescence, intrinsic and extrinsic fluorophores, Stokes shift, fluorescence quantum yield, fluorescence lifetime, time-correlated single-photon counting (TCSPC) system, light sources and detectors for TCSPC, multi-exponential fluorescence decay analysis, radiative and non-radiative decay rates, solvent polarity and environmental factors affecting fluorescence, Lippert-Mataga equation and its application, quenching of fluorescence – theory of static and dynamic quenching, Stern-Volmer equation, application of quenching .

Unit II: Dynamics of solvent and spectral relaxation, time-resolved emission spectra (TRES), solvent dynamics in chemical and biological (proteins, DNA and membranes) systems, red-edge excitation shifts, fluorescence anisotropy - steady-state and time-resolved, anisotropy decay analysis, application of fluorescence anisotropy, rotational diffusion of fluorophores.

Unit III: Overview of excited state dynamic processes affecting fluorescence, excimer formation, excited state reactions, inter-/intra-molecular proton transfer (ESIPT), application of ESIPT probes, steady-state and time-resolved decay for two-state model, photo-induced electron transfer – theory and applications.

Unit IV: Fluorescence resonance energy transfer (FRET) – theory of energy transfers, donor-acceptor systems, distance measurement using FRET, fluorescence sensing, application of FRET in conformational fluctuation and ligand-protein binding studies.

Unit V: Fluorescence correlation spectroscopy – theory and applications, multiphoton fluorescence spectroscopy and microscopy, fluorescence lifetime-imaging microscopy, single molecule fluorescence spectroscopy

REFERENCES:

1.	*Fluorescence Spectroscopy,* by J. R. Lakowicz, Springer, (2006).
2.	Molecular Fluorescence - Principles and Applications by B. Valeur, Wiley-VCH, (2002).
3.	J. M. Hollas, *Modern Spectroscopy*, 4thEdn, John Wiley& Sons, (1992).
4.	C. N. Banwell, *Fundamentals of Molecular Spectroscopy,* 4th Edn. Tata McGraw Hill, (1996).

COURSE OUTCOME

Upon completion of this course, the students will be able to

CO1	learn the basic principles of fluorescence spectroscopy and their applications to chemistry materials and biology
CO2	measure and understand the fluorescence properties of various small molecules and bio-macromolecule that important in sensing and other application
CO3	analyse time-resolved fluorescence data for detailed understanding of the excited state processes
CO4	have understanding of advanced fluorescence spectroscopic and microscopic techniques

Course Code	**:**	CHPE605
Course Title	**:**	Medicinal Chemistry
Type of Course	**:**	PE
Prerequisites	**:**	B. Sc. Chemistry
Contact Hours	**:**	45
Course Assessment Methods	**:**	Continuous Assessment, End Assessment

COURSE LEARNING OBJECTIVES (CLO)

The learning objectives are to enable students

CLO1	to introduce the students in the field of medicinal chemistry
CLO2	to provide the students an idea about the classifications of drugs and structure-activity relationship
CLO3	to get an idea about the antibiotics (synthesis, bio-activity)
CLO4	to be familiar with the structures of enzymes and different types of interactions

COURSE CONTENT

Introduction: History of medicinal chemistry, general mechanism of drug action on lipids, carbohydrates, proteins and nucleic acids, drug metabolism and inactivation, receptor structure and sites, drug discovery development, design and delivery systems, gene therapy and drug resistance.

Classification: Drugs based on structure or pharmacological basis with examples, synthesis of important drugs such as α - methyl dopa, chloramphenicol, griseofulvin, cephelosphorins and nystatin. Molecular modelling, conformational analysis, qualitative and quantitative structure activity relationships.

General introduction to antibiotics: Mechanism of action of lactam antibiotics and non lactam anti biotics, antiviral agents, chemistry, stereochemistry, biosynthesis and degradation of penicillins - An account of semisynthetic penicillins - acid resistant, penicillinase resistant and broad spectrum semisynthetic penicillins.

Elucidation of enzyme structure: Mechanism, kinetic, spectroscopic, isotopic and stereochemical studies. Chemical models and mimics for enzymes, design, synthesis and evaluation of enzyme inhibitors.

Interactions: DNA-protein interaction and DNA-drug interaction. Introduction to rational approach to drug design, physical and chemical factors associated with biological activities, mechanism of drug action. m-RNA, vaccine development, docking study.

REFERENCES

1.	Wilson, Giswald and F. Doerge, *Text Book of Organic Medicinal and Pharmaceutical Chemistry,* J.B. Lippincott Company, Philadelphia, 1971.
2.	A. Burger, *Medicinal Chemistry,* Wiley Interscience, New York, Vol. I and II, 1970.
3.	*Bentley and Driver's Text Book of Pharmaceutical Chemistry* revised by L.M. Artherden,Oxford University Press, London, 1977.
4.	A. Gringauz, *Introduction to Medicinal Chemistry,* How Drugs Act and Why?, John Wiley and Sons, 1997.
5.	G. L. Patrick, *Introduction to Medicinal Chemistry,* Oxford Univeristy Press, 2001.

COURSE OUTCOMES (CO)

Upon completion of this course, the students will be able to

CO1	know the history and fundamentals of medicinal chemistry
CO2	classify the drugs and relationship between structure and activity.
CO3	understand the bio-mechanism of the antibiotics along with their synthetic routes
CO4	know the structure of enzymes, their activity and different types of interactions in bio-molecules

Course Code	**:**	CHPE607
Course Title	**:**	Nanoscience and Nanotechnology
Type of Course	**:**	PE
Prerequisites	**:**	General Chemistry/Engineering background
Contact Hours	**:**	45
Course Assessment Methods	**:**	Continuous Assessment, End Assessment

COURSE LEARNING OBJECTIVES (CLO)

To introduce the students

CLO1	to describe important physical methods in the field of nanoscience
CLO2	to describe important of structures in the field of nanoscience
CLO3	to describe important experimental tools in the field of nanoscience
CLO4	to familiarize with the applications of nanotechnology in sensors

COURSE CONTENT

Introduction to nanomaterials: Properties of materials & nanomaterials, role of size in nanomaterials, nanoparticles, semiconducting nanoparticles, nanowires, nanoclusters, quantum wells, conductivity and enhanced catalytic activity compared to the same materials in the macroscopic state.

Chemical Routes for Synthesis of Nanomaterials: Chemical precipitation and coprecipitation; Metal nanocrystals by reduction, Sol-gel synthesis; Microemulsions or reverse micelles, myle formation; Solvothermal synthesis; Thermolysis routes, Microwave heating synthesis; Sonochemical synthesis; Electrochemical synthesis; Photochemical synthesis, Synthesis in supercritical fluids.

Nanostructures: Zero-, One-, Two- and Three- dimensional structure, Size control of metal Nanoparticles and their properties: Optical, Electronic, Magnetic properties; Surface plasmon Resonance, Change of bandgap; Application: catalysis, electronic devices.

Structural Characterization: X-ray diffraction, Small angle X-ray Scattering, Optical Microscope and their description, Scanning Electron Microscopy (SEM), Scanning Probe Microscopy (SPM), TEM and EDAX analysis, Scanning Tunneling Microscopy (STM), Atomic force Microscopy (AFM).

Carbon nanostructures: Introduction. Fullerenes, C60, C80 and C240 nanostructures. Properties & applications (mechanical, optical and electrical). Functionalization of carbon nanotubes, reactivity of carbon nanotubes. Nanosensors: Temperature sensors, smoke sensors, sensors for aerospace and defence. Accelerometer, pressure sensor, night vision system, nano tweezers, nano-cutting tools, integration of sensor with actuators and electronic circuitry biosensors.

REFERENCES

1.	T. Pradeep, *Nano: The Essentials, Tata McGraw-Hill*, New Delhi, 2007..
2.	G. Cao, *Nanostructures and Nanomaterials – Synthesis, Properties and Applications*, Imperial College Press, London, 2004.
3.	C. N. R. Rao, A. Muller and A. K. Cheetham, *The Chemistry of Nanomaterials, Volume 1*, Wiley –VCH Verlag GmbH & Co. KgaA, Weinheim, 2004
4.	G. A. Ozin, A. C. Aresnault, L. Cadematriri, *Nanochemistry: A chemical approach to nanomaterials*, RSC Publishing, 2008
5.	Ray F. Egerton, *Physical Principles of Electron Microscopy: An Introduction to TEM, SEM, and AFM*, Springer Publishing, 2005

COURSE OUTCOMES (CO)

At the end of the course student will be able to

CO1	describe important physical methods in the field of nanoscience
CO2	describe important of structures in the field of nanoscience
CO3	describe important experimental tools in the field of nanoscience
CO4	familiarize with the applications of nanotechnology in sensors

Course Code	**:**	CHPE609
Course Title	**:**	Electronic Structure Methods and Modelling
Type of Course	**:**	PE
Prerequisites	**:**	Basic knowledge in quantum chemistry is desirable
Contact Hours	**:**	45
Course Assessment Methods	**:**	Continuous Assessment, End Assessment

COURSE LEARNING OBJECTIVES (CLO)

The learning objectives are to enable students

CLO1	to provide basic knowledge of electronic structure methods for molecular and solid-state systems
CLO2	to use the computational methods to design the materials for potential applications

COURSE CONTENT

Ab initio Methods: The Hatree SCF method – the Hatree-Fock equations – Koopmans' theorem – the Roothaan equations – concept of basis sets, electron correlation and configuration interaction, post Hatree-Fock theories such as MP2, CASSCF, CCSD(T), DMRG etc.

Density Functional Theory: Principles of DFT – the Hohenberg-Kohn theorems – the Kohn-Sam equations – local density approximation (LDA), exchange-correlation functionals – gradient corrected functionals, hybrid functional and range separated hybrid functionals, DFT methods for van der Waals interactions, general performance overview of DFT.

Molecular Properties and Analysis: Predicting molecular geometry, optimization algorithms, potential energy surfaces (PES), frequencies analysis, zero-point energies and thermodynamic corrections, population analysis, natural bond order (NBO) analysis, molecular electrostatic potential, multipole moments, estimation of electron affinity (EA) and ionization potential (IP), computing molecular orbitals energies. Molecules in complex environments – Polarizable Continuum Models (PCM).

Surfaces and Low Dimensional Solids: Modelling strategies of periodic solids – lattice constants optimization, surface reconstruction, computing band structures and band gaps, density of states, quantum confinement effect, electronic structure of 1D and 0D systems, modification of electronic gap – designing of hybrid nanostructures. Quantum mechanical simulation of large systems – density functional tight binding (DFTB) approach.

Electronic Excited States: Time-dependent methods, vertical excitations, computing transition dipole moment, dark and bright states, analysis of natural transition orbitals (NTOs), attachment and detachment densities, properties of charge transfer states. Excited-state optimization, computing emission energy, crossing between potential energy surfaces, conical intersections, electronic couplings between excited states. Applications in LED and Solar cells.

Practical Sessions (Programming, Modelling and Simulation):

1. Bash command and shell scripting and the basic structure of FORTRAN program.
2. Molecular modelling and visualization techniques. Searching for minimum energy structure – geometry optimization and computing the potential energy surface.
3. Frequency calculations – predicting IR spectra, computing normal modes, zero-point energy and thermochemical analysis.
4. Determination of the basis set required to predict the accurate structure, Conventional solution to the basis set superposition error (BSSE) – counterpoise correction.
5. Single point calculations – Mulliken population, NBO analysis, electrostatic potential, multipole moments, IP and EA, energies of HOMO and LUMO.
6. Basic of periodic system calculation – super cell approach, lattice parameter optimization, computing band structure, surface reconstruction, calculation of low dimensional solids.
7. Calculation of excited states properties – computing absorption spectra, visualization and plotting of attachment and detachment densities, characterization of charge transfer states.
8. Excited state geometry optimization – computing the emission energy. Solvent effects.

REFERENCES

1.	Szabo and N. S. Ostlund, *Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory,* Dover Publications Inc., Revised ed. edition, 1996.
2.	P. W. Atkins and R. S. Friedman, *Molecular Quantum Mechanics,* Oxford University Press; Fifth edition, 2012.
3.	I. N. Levine, *Quantum Chemistry,* Pearson; Seventh edition, 2013.
4.	R. G. Parr and W. Yang, *Density-Functional Theory of Atoms and Molecules,* Oxford University Press, 1994.
5.	Kittel, *Introduction to Solid State Physics,* Wiley, Eighth edition, 2012.
6.	J. Cramer, *Essentials of Computational Chemistry: Theories and Models,* Wiley-Blackwell; Second edition, 2004
7.	User’s manual of Gaussian, Q-Chem, SIESTA, DFTB program packages.

COURSE OUTCOMES (CO)

Upon completion of this course, the students will be able to

CO1	explain the most important concepts of electronic structure theory
CO2	understand the structure and reactivity of chemical and biological systems
CO3	discuss the structural and physical properties of solids in different dimensions
CO4	design and optimize the efficient materials for specific potential applications

Course Code	**:**	CHPE611
Course Title	**:**	Natural Products Chemistry
Type of Course	**:**	PE
Prerequisites	**:**	B. Sc. Chemistry
Contact Hours	**:**	45
Course Assessment Methods	**:**	Continuous Assessment, End Assessment

COURSE LEARNING OBJECTIVES (CLO)

The learning objectives are to enable students

CLO1	to introduce the students in the field of natural products and their classifications
CLO2	to provide the students a broad idea about amino acids, steroids, carbohydrates and heterocycles
CLO3	the students will be able get an idea about the antibiotics (synthesis, bio-activity)
CLO4	the students will be familiar with the structures of enzymes and different types of interactions

COURSE CONTENT

Classification of natural products: Chemical structure, classification, structure elucidation based on degradative reactions- Isolation and structural elucidation of selected alkaloids and terpenes- quinine, morphine, and reserpine, citral, juvabione and logiofolene -Insect pheromones.

Amino acids: Synthesis of amino acids-reactions - properties- Amino Acids in Nature: -Amino Acids and their Metabolites in Nature –Structure of proteins- Peptides,

Steroids– classification- Synthesis and structure elucidation of cholesterol, conversion of cholesterol to progesterone- androsterone and testosterone-cortisone- Vitamin D - Nucleic Acids- structure of nucleosides and nucleotides-RNA and DNA, Watsons and Crick model-DNA-drug interaction

Carbohydrates: Determination of configuration- Hudsons rules - Structure of sugars - transformation of sugars, Preparation of alditols, glycosides, deoxysugars. Synthesis of vitamin C from glucose.

Heterocycles: Synthesis, Properties and uses of Five membered heterocyclic ring systems with one or two hetero atoms-Furan, pyrrole, thiophene and thiazole: six membered heterocyclic ring system-Pyridine. Fused heterocyclic ring systems- Indole, quinoline. Biologically important heterocycles: Pyrimidines and purines.

REFERENCES

1.	I. L. Finar, *Organic Chemistry Vol. I & Vol. II*- Pearson Education, 6^{th} Edn.
2.	I. L. Finar, *Organic Chemistry Vol. I & Vol. II*- Pearson Education, 6thedn.
3.	I. Fleming, *Selected Organic Synthesis,* John Wiley and sons, 1982
4.	Atta-ur-Rahman, *Studies in Natural Products Chemistry, Vol.1 and 2,* Elsevier, 1988.
5.	R. Krishnaswamy, *Chemistry of Natural Products; A Unified Approach,* Universities Press.
6.	R. J. Simmonds: *Chemistry of Biomolecules: An Introduction,* RSC

COURSE OUTCOMES (CO)

Upon completion of this course, the students will be able to

CO1	Classify the natural products based on their structures.
CO2	Know various types of amino acids, their structures, and importance.
CO3	Understand the bio-functions of steroids and their structures.
CO4	Get a comprehensive knowledge about carbohydrates and some heterocycles

Course Code	:	CHPE613
Course Title	:	Advanced Heterocyclic Chemistry
Type of Course	:	PE
Prerequisites	:	B. Sc. Chemistry
Contact Hours	:	45
Course Assessment Methods	:	Continuous Assessment, End Assessment

COURSE LEARNING OBJECTIVES (CLO)

The learning objectives are to enable students

CLO1	to introduce the students with major classes of heterocyclic compounds and their chemical properties
CLO2	to familiarize the students about the reactivities of different classes of heterocycles
CLO3	to plan synthetic routes to complex organic molecules containing heterocyclic motifs
CLO4	to be familiar with the major advances and the current state-of-the-art methods in heterocyclic chemistry

COURSE CONTENT

Nomenclature and general synthesis: Systematic Nomenclature for monocycle and fused heterocycles (Hantzsch-Widman system). Common approach to heterocyclic synthesis-cyclisation and cycloaddition routes.

Heterocycles in organic synthesis: Masked functionalities, umpolung, Stork annulation reaction and applications (synthesis of testosterone, estrone, progesterone, ranitidine, lansoprazole and/or recently discovered molecules etc.

Non-aromatic heterocyclics: Conformational aspects of non-aromatic heterocycles. Synthesis, reactivity and importance of the following ring systems. Azirines, Aziridines, Oxiranes, Thiiranes, Diazirenes, Diaziridines, Oxaziridines, Azetidines, Oxetanes and thietanes.

Two heteroatom containing heterocycles: 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.

Larger heterocyclic rings: Introduction to chemistry of azepins, oxepins, thiepins and their analogues; ANRORC and Vicarious nucleophilic substitutions in heterocycles. Synthesis of few heterocyclic natural products.

REFERENCES

1.	T. Gilchrist, *Heterocyclic Chemistry,* Prentice Hall; 3rd edition, 1997
2.	J.A.Joule & K.Mills, *Heterocyclic Chemistry,* Wiley-Blackwell, 2010.
3.	A.R.Katritzky, *Handbook of Heterocyclic Chemistry,* Academic Press; 2 edition, 2000.

COURSE OUTCOMES (CO)

Upon completion of this course, the students will be able to

CO1	identify the commonly used synthetic routes to heterocycles and major advances in the field of heterocyclic chemistry.
CO2	plan synthetic routes to complex organic molecules containing heterocyclic motifs
CO3	be familiar with general synthetic approaches used in drug discovery and synthetic routes to major drugs containing heterocyclic motifs
CO4	critically evaluate heterocyclic chemical literature, present seminars and short reviews in heterocyclic chemistry

Course Code	**:**	CHPE602
Course Title	**:**	Polymer Chemistry
Type of Course	**:**	PE
Prerequisites	**:**	B.Sc. Chemistry
Contact Hours	**:**	45
Course Assessment Methods	**:**	Continuous Assessment, End Assessment

COURSE LEARNING OBJECTIVES (CLO)

The learning objectives are to enable students

CLO1	to the basic concept of macromolecules
CLO2	to the polymerization processes
CLO3	to the polymer stereochemistry
CLO4	to the theories of polymer structure, solutions, and speciality polymers

COURSE CONTENT

Concept of macromolecules: Types of polymers and polymerization. Nomenclature of polymers-based on sources, based on structure (non-IUPAC), IUPAC structure-based nomenclature system, Trade names and non-names. Raw material for the synthesis of polymers. Synthetic schemes. Petroleum and petrochemicals - Naphtha as a source of petrochemicals.

Polymerization processes: Free radical addition polymerization- kinetics and mechanism. Chain transfer. Molecular weight distribution and molecular weight control. Cationic and anionic polymerization: Kinetics and mechanism. Living polymers. Ring opening polymerization. Step growth polymerization - Linear *Vs* cyclic polymerization. Other methods of polymerization- bulk, solution, melt, suspension, emulsion and dispersion techniques.

Polymer stereochemistry: Configuration and conformation. Tacticity. Chiral polymers. Polymer characterization. Molecular weights- Methods for determining molecular weights- static, dynamic, viscometry, light scattering and GPC. Crystalline and amorphous states. glassy and rubbery States. Glass transition temperature and crystalline melting of polymers. Degree of crystallinity-X-ray diffraction. Thermal stability of polymers.

Theories of polymer structure: Models of polymer structure: Freely joined chains. Calculation of end-to-end distances. Kratky-Porod model and concept of chain stiffness. Gaussian chain model. Elastic energy and Bead-spring model. Radius of gyration and asphericity. Polymer in solutions: Flory-Huggins theory and classification of solvents. Phase diagram (UCST and LCST). Binodal and Spinodal regions. Conformation: random coil, solvation, and swelling. Determination of degree of cross-linking and molecular weight between cross-links.

Specialty polymers: Industrial polymers- synthesis, structure, and applications of industrially important polymers. Polymers as aids in organic synthesis. Polymeric reagents, catalysts, substrates. Liquid crystalline polymers-Main chain and side chain liquid crystalline polymers. Phase morphology. Conducting polymers - Synthesis & applications of polyacetylenes, polyanilines, polypyrroles & polythiophenes. Photoresponsive and photorefractive polymers. Polymers in optical lithography-Organic electronic materials- Drug Delivery-Drug carriers-Polymer based nanoparticles.

REFERENCES:

1.	George Odian, *Principles of polymerization*, 4^{th} edition, John Wiley & Sons, Inc., Hoboken, New Jersey, 2004
2.	F.W. Billmayer, *Textbook of Polymer Science*. 3^{rd}Edn, Wiley. N.Y. 1991.
3.	J.M.G Cowie. *Polymers: Physics and Chemistry of Modern Materials*. Blackie. London, 1992.
4.	R.J.Young, *Principles of Polymer Science*, 3^{rd}Edn. , Chapman and Hall. N.Y. 1991.
5.	P.J. Flory. *A Text Book of Polymer Science.* Cornell University Press. Ithacka, 1953.
6.	F. Ullrich, *Industrial Polymers*, Kluwer, N.Y. 1993.
7.	H.G.Elias, *Macromolecules*, Vol. I & II, Academic, N.Y. 1991.
8.	J.A.Brydson, *Polymer chemistry of Plastics and Rubbers*, ILIFFE Books Ltd., London, 1966.

COURSE OUTCOMES (CO)

Upon completion of this course, the students will be able to

CO1	know the classification of polymers and its nomenclature.
CO2	learn the different polymerization methods and kinetics
CO3	learn the theories of polymer structures
CO4	learn the uses of polymers for commercial purposes

Course Code	**:**	CHPE604
Course Title	**:**	Computational Methods in Chemistry
Type of Course	**:**	PE
Prerequisites	**:**	B.Sc. Ancillary Mathematics Background
Contact Hours	**:**	45
Course Assessment Methods	**:**	Continuous Assessment, End Assessment

COURSE LEARNING OBJECTIVES (CLO)

CLO1	Logic of computer programming for solving chemistry related problems.
CLO2	Learning numerical methods for evaluation of experimental data related to chemistry problems.
CLO3	Development of computer assisted molecular design for specific properties.
CLO4	Use of software for analysing structure-activity correlation of chemical compounds.

COURSE CONTENT

C - Syntax: Character set-constants and variables, data types and sizes, declarations, operators - expressions -conditional expressions, precedence and order of evaluation, statements and blocks, if-else, if-else-if and switch statements, while, for and Do - while loops, break and continue statements, Goto and labels, basics of functions and types, header files, recursion,arrays – 1D and 2D, file handling concepts.

Kinetics -solving rate equations, thermodynamics -heats of reactions, heat capacity, entropy, spectroscopy-moment of inertia, wave numbers of stokes and anti-stokes Raman lines, masses of isotopes from rotational and vibrational spectroscopic data - Group theory -Huckel MO calculations of delocalisation energy, hybridisation schemes and symmetries of vibrations in non - linear molecules. Crystallography - d spacings for an orthorhombic crystal, Fourier synthesis of electron density using structure factor, axial angles of a triclinic crystal.

Solving polynomial equations - Newton -Raphson method, solutions of simultaneous equations - Gauss elimination, Jacobi iteration and matrix diagonalisation, numerical differentiation and integration - Simpson’s rule, trapezoidal rule- determination of entropy, solution of differential equations -Runge-Kutta method- theory and application to thermodynamics, linear and non-linear curve fitting.

Force field and electronic structure methods-force field energy and parameterization, electronic structure methods- SCF techniques, semi-empirical methods, basis sets and their classification, density functional theory and methods.

Geometry convergence: energy convergence, dipole moment convergence, vibrational frequencies convergence, bond dissociation curve, angle bending curve, transition state modelling using Chemoffice and Gaussian software- demo on docking software.

Computational Chemistry Lab Experiments

1. Curve fitting for Beer Lamberts law
2. Normalized radial wave function for 1s atomic orbital of hydrogen atom
3. Radial distribution function for 1s atomic orbital
4. Simulation of potentiometric titration plots
5. Computation of energy gap based on particle in 1D models, plot of its wave function and probability density
6. Single point energy of water - comparison based on equipartition principle and quantum principles
7. Single point energy of formaldehyde, visualization of molecular orbitals
8. Evaluation of NMR properties of butane, trans 2-butene and 2-butyne
9. Geometry optimization of ethylene and comparison with fluoro ethylene
10. Geometry optimization and MO energy of ethylene, butadiene and hexatriene, crotonaldehyde - types of electronic transitions, transition dipole evaluation

REFERENCES

1.	Balagurusamy, *Programming in C*, Tata McGraw Hill, 1997
2.	K. V. Raman, *Computers in Chemistry*, Tata McGraw Hill, 1993.
3.	F. Jensen, *Introduction to Computational Chemistry*, John Wiley & Sons, 2003.
4.	M. K. Jain, *Numerical Methods for Scientific and Engineering Computation*, Wiley Eastern Ltd, 1995.
5.	User manuals of Gaussian09, Chem Office Ultra and Gauss View.

COURSE OUTCOMES (CO)

At the end of the course student will be able to

CO1	develop c program for any chemistry problem.
CO2	apply numerical methods to evaluate experimental data.
CO3	conceive the suitable force field methods and parameterization for force field energy.
CO4	carry out geometry optimization, energy calculation using software

Course Code	**:**	CHPE606
Course Title	**:**	Interfacial Chemistry and Sonochemistry
Type of Course	**:**	PE
Prerequisites	**:**	B. Sc. Chemistry
Contact Hours	**:**	45
Course Assessment Methods	**:**	Continuous Assessment, End Assessment

COURSE LEARNING OBJECTIVES (CLO)

The learning objectives are to enable students

CLO1	to describe important physical methods in the field of Advanced Oxidation Processes
CLO2	to describe importance of sonochemistry
CLO3	to describe importance of ozonation
CLO4	to familiarize with the applications of sonochemistry

COURSE CONTENT

Fundamentals and background of advanced oxidation processes (AOPs): The role of hydroxyl radicals and their generation. Reaction kinetics and degradation mechanisms of organic pollutants by hydroxyl radicals. The effects of process parameters and scavenging media on degradation efficiency. Removal of specific pollutants in aqueous media; biodegradability enhancement and toxicity reduction. Practical application of AOPs for water and wastewater treatment; opportunities and limitations.

UV light based (photochemical and photocatalytic) AOPs for water treatment: common oxidants and catalysts and their alternatives. Fenton reaction. Alternative catalysts for Fenton reaction. Types of homogeneous and heterogeneous Fenton and photo-Fenton processes; influencing parameters, reaction kinetics and mechanisms. The role of ligands in modified photo-Fenton processes. Iron catalysts in heterogeneous Fenton processes; sources and supports.

Sonochemistry: Sound properties, Bubble formation, Ultrasound, principles of sonochemistry and acoustic cavitation. Interfaces and Bubbles, Sonoluminescence, Bubble Temperature Estimation Homogeneous (liquid-phase) and heterogeneous (solid surface-liquid, particle liquid and liquid-liquid) reactions. Reactor configurations; batch and flow systems.

Ozonation: background and fundamentals, reaction kinetics and mechanisms. Application of homogeneous and heterogeneous catalytic ozonation in water treatment. Combined application of ultrasound with ozone and/or UV light; synergistic and antagonistic effects.

Sonochemical synthesis and properties: of functional polymers and core-shell architectures and their applications in food and biomedical applications. Synthesis of functional materials using sonochemistry

REFERENCES

1.	T. J. Mason, J. P. Lorimer, *Sonochemistry: Theory, Applications and uses of Ultrasound in Chemistry,* Harword, Chichester, UK, 1988.
2.	M. Ashokkumar, S. Anandan, *Handbook of Ultrasonics and Sonochemistry,* Springer – 2016.
3.	*Water Quality and Treatment: A Handbook of Community Water Supplies,* Fifth Edition AWWA, McGraw-Hill, 1999.

COURSE OUTCOME

Upon completion of this course, the students will be able to

CO1	describe important physical methods in the field of Advanced Oxidation Processes
CO2	describe importance of sonochemistry
CO3	describe importance of ozonation
CO4	familiarize with the applications of sonochemistry

Course Code	**:**	CHPE608
Course Title	**:**	Lanthanide and Actinide Chemistry
Type of Course	**:**	PE
Prerequisites	**:**	B. Sc. Chemistry
Contact Hours	**:**	45
Course Assessment Methods	**:**	Continuous Assessment, End Assessment

COURSE LEARNING OBJECTIVES (CLO)

To introduce the students

CLO1	to the lanthanides and their extraction
CLO2	to the lanthanide Chemistry and spectroscopy
CLO3	to the organometallic chemistry of lanthanides and actinides
CLO4	to the actinides and their extraction
CLO5	to the electronic and magnetic properties of actinides

COURSE CONTENT

Unit I: Lanthanides: Occurrence – Ores- Extraction and separation – The Lanthanide contraction – Electronic configuration – shapes of f – orbitals – ionization energies – simple binary compounds of lanthanides

Unit II: Lanthanides: Coordination chemistry – Coordination numbers – stability and oxidation states - Magnetic Properties – Electronic Spectra – Luminescence Spectra – NMR Applications – and Imaging- EPR Spectroscopy including lanthanide based Single-ion Magnets.

Unit III: Organolanthanide Chemistry: Stability -+3 oxidation state – Alkyls and aryls – Cyclopentadienyls – hydrides- other oxidation states and their organometallic complexes – carbonyl compounds of Sc-Y &Pr

Unit IV: Actinides: Occurrence – Synthesis – Extraction and isolation – Characteristics of the actinides – reduction potentials – relativistic effects – binary compounds of actinides – coordination chemistry of actinides – stability – structure, coordination number and Magnetic properties of actinide compounds including Uranium, Np and Pu.

Unit V: Actinides: Electronic and magnetic properties of actinides – spectra –
Organoactinides – cylopentadienyls- carbonyls – synthesis of transactinides – nomenclature.

REFERENCES

1.	S. Cotton, *Lanthanide and Actinide Chemistry,* John Wiley & Sons, 2006
2.	J. J. Katz, G.T. Seaborg and L.R. Morss (eds), *The Chemistry of the Actinide Elements*, 2nd Ed., Chapman and Hall, 1986.
3.	J. A. McCleverty and T. J. Meyer (eds), *Comprehensive Coordination Chemistry II*, Elsevier, Amsterdam, 2004.
4.	N. M. Edelstein (ed.), *Lanthanide and Actinide Chemistry and Spectroscopy*, Vol. 131. ACS Symposium Series, 1980.
5.	A. A. Cotton & G. Wilkinson, *Advanced Inorganic Chemistry*, John Wiley & Sons, 1988.
6.	J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, *Inorganic Chemistry: Principles of Structure and Reactivity*, Pearson, 5th Edition, 2023.

COURSE OUTCOMES (CO)

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

CO1	learn about the lanthanides and their extraction
CO2	understand the lanthanide chemistry and spectroscopy
CO3	learn about the organometallic chemistry of lanthanides and actinides
CO4	learn about the actinides and their extraction
CO5	learn about the electronic and magnetic properties of actinides

Course Code	**:**	CHPE610
Course Title	**:**	Fuel cells for Stationary and Automotive Applications
Type of Course	**:**	PE
Prerequisites	**:**	Problem-solving skill
Contact Hours	**:**	3
Course Assessment Methods	**:**	Continuous Assessment, End Assessment

COURSE LEARNING OBJECTIVES (CLO)

CLO1	Theoretical principles of various fuel cell systems and PEM fuel cell in particular.
CLO2	Learning on the power demand of fuel cells for specific kinds of stationary and automotive applications.
CLO3	Optimization of components for high efficiency of PEM fuel cell.
CLO4	Evaluation of overall environmental and cost benefits of fuel cells.

COURSE CONTENT

Overview of energy fundamentals: Fossil fuels for Automotive applications, Renewable energy technologies, technical fundamentals and Elements of hydrogen economy, Transition from fossil fuel based to hydrogen economy.

Introduction to fuel cells: Basic operating principles of Fuel Cells, Types- PEM fuel cells, Solid oxide fuel cells, Alkaline fuel cells, Phosphoric acid fuel cells, Molten carbonate fuel cells.

PEM Fuel Cell: Components, Electrolyte, electrodes, Gas Diffusion Layer and Membrane Electrode Assemblies, Assembly of PEM Fuel cell and its performance at various operating conditions.

Fuel Cell Performance: Effect of temperature, partial pressure, Fuel Cell assembly and Evaluation under stationary and simulated Automotive Operating Conditions, Analysis of Experimental Results. fuel cell and storage devices/energy conversion devices.

Durability and Cost aspects: Life cycle cost analysis for Stationary and Automotive applications. Economic and social aspects of PEM Fuel Cells for automotive applications, Future of Hydrogen Roadmap, Sustainable energy economy.

REFERENCES

1.	Kerry-Ann Adamson, *Stationary Fuel Cells: An overview*, Elsevier, Oxford, 2007.
2.	Mathew M. Mench, *Fuel Cell Engines*, John Wiley & Sons, New Jersey, 2008.

3.	James Larminie and Andrew Dicks, *Fuel Cell Systems Explained*, John Wiley & Sons, New Jersey, 2008.

COURSE OUTCOMES (CO)

At the end of the course student will be able to

CO1	apply the fundamental laws governing conversion from chemical to electrical energy.
CO2	understand the need to switch from hydrocarbon economy to hydrogen economy, specifically in the transportation sector.
CO3	select the right type of fuel cell for specific application.
CO4	quantify performance related parameters, such as power density, operational life and cost.

Course Code	:	CHPE612
Course Title	:	Inorganic Rings, Cages and Clusters
Type of Course	:	PE
Prerequisites	:	B.Sc. Chemistry
Contact Hours	:	45
Course Assessment Methods	:	Continuous Assessment, End Assessment

COURSE LEARNING OBJECTIVES (CLO)

To introduce the students

CLO1	to different rules concerning the main group element containing clusters
CLO2	to different rules concerning the transition element containing clusters
CLO3	to a clear understanding of the structural paradigms in chemistry and isolobal analogy
CLO4	to the inorganic homo and heterocyclic systems of main group elements
CLO5	to the inorganic polymers in detail

COURSE CONTENT

Main group clusters: Geometric and electronic structure, three - four and higher connect clusters, the closo-, nido-, arachno- borane structural paradigm, Wade-Mingos and Jemmis electron counting rules, clusters with nuclearity 4-12 and beyond 12.

Transition metal clusters: Low nuclearity metal carbonyl clusters and 14n+2 rule, high nuclearity metal carbonyl clusters with internal atoms, structure, synthesis and reactivity-capping rules. Application of metal clusters in Supramolecular chemistry, Molecular machines. and Metal-organic Frameworks.

Isolobal analogy: Heteronuclear clusters-carboranes and heteroboranes - metal clusters - structural prediction of organometallic clusters-main group transition metal clusters: Isolobalanalogs of p-block and d-block clusters-interstitial systems-cubanes and zintl clusters.

Inorganic homo & heterocycles: Synthesis, structure and reactivity- structural variety& properties of borazines and phosphazenes, borides, carbides, silicides, nitrides, phosphides, oxides and sulphides of transition elements, multiple bonds and cluster variety of transition metals.

Inorganic rings and polymers: Definition, variety and merits, P, Si, S, N & O based polymers, poly-phosphazenes, poly-thiazenes, poly-siloxanes and poly-silanes. Molecular clusters in catalysis, clusters to materials, boron-carbides and metal-borides.

REFERENCES

1.	D. M. P. Mingos and D. J. Wales, *Introduction to Cluster Chemistry*, Prentice Hall, 1990.
2.	N. N. Greenwood and E. A. Earnshaw, *Chemistry of Elements*, Pergaman Press, 1984.
3.	I. Haiduc & D. B. Sowerby (Eds.), *Inorganic Homo-and Heterocycles* Vols. 1 & 2, Academic Press, 1987.
4.	J. E. Mark, R. West & H. R. Allcock, *Inorganic Polymers*, Academic Press, 1992.
5.	T. P. Fehlner, J. F. Halet and J-Y. Saillard, *Molecular Clusters: A Bridge to Solid-State Chemistry*, Cambridge University Press, 2007.
6.	P. Braunstein, L. A. Oro, P. R. Raithby, Ed. *Metal Clusters in Chemistry*, John Wiley and sons, 1999.
7.	T. Chivers, I. Manners, *Inorganic Rings and Polymers of the p-Block Elements, from Fundamentals to Applications*, RSC Publishing, 2009.

COURSE OUTCOMES (CO)

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

CO1	study different rules concerning the main group element containing clusters
CO2	study different rules concerning the transition element containing clusters
CO3	have a clear understanding of the structural paradigms in chemistry and isolobal analogy
CO4	study the inorganic homo and heterocyclic systems of main group elements
CO5	study the inorganic polymers in detail

Course Code	**:**	CHPE614
Course Title	**:**	Advanced Bioinorganic Chemistry
Type of Course	**:**	PE
Prerequisites	**:**	B.Sc. Chemistry
Contact Hours	**:**	45
Course Assessment Methods	**:**	Continuous Assessment, End Assessment

COURSE LEARNING OBJECTIVES (CLO)

To introduce the students

CLO1	to the metal ions in life
CLO2	to the metalloenzyme chemistry
CLO3	to the electron transport phenomena in body
CLO4	to the bio-organometallic catalysis

COURSE CONTENT

Unit I: Essential and trace metal ions in biology and their distribution, thermodynamic and kinetic factors for the presence of selected metal ions; bioligands- amino acids, proteins, nucleic acids, nucleotides and their potential metal- binding sites; special ligands - porphyrins, chlorin and corrin.

Unit II: Enzymes- Nomenclature and classification, chemical kinetics, the free energy of activation and the effects of catalysts kinetics of enzyme catalyzed reactions- Michaelis-Menten constant- effect of pH, temperature on enzyme reactions, factors contributing to the catalytic efficiency of enzymes. O2 binding and activation by heme, non-heme and copper proteins – MMO & RNR, tyrosinase; DβM, PHM, Cytochrome c oxidase with Cytochrome P450 alpha ketalglutarate dependent enzymes. Iron transport and storage proteins in bacterial and mammalian systems – siderophores, transferrin, ferritin.

Unit III: Electron transport proteins – redox properties, organic- redox protein cofactors – FAD, NAD, FMN, ubiquinone; blue copper proteins, cytochromes, iron- sulfur proteins – rubredoxin, ferridoxins, HIPIP; electron transport chain (ETC) in respiration, nitrogen-fixation and photosynthesis.

Unit 1V: Nitrogen-cycle enzymes: Mo in N, and S-metabolism by Mo-pterin cofactors and Mo- Fe-cofactors. NOx reductases, sulfite oxidase, xanthine oxidase, nitrogenase, P and

M- clusters in nitrogenase, transition-metal-dinitrogen complexes and insights into N2 binding, reduction to ammonia.

Unit V: Mn in photosynthesis and O2 evolution: Photosystem I and II – chlorophyll, oxygen evolving complex (OEC), 4Mn-cluster and O2 evolution. Non-redox enzymes with Mg, Zn, Ni: urease, peptidases and phosphatases and their structure and function. Carbonic anhydrase and carboxy peptidase. Applied bioinorganic chem–metals in medicine, anti-cancer agents–cisplatin, radiopharmaceuticals (Tc), diagnostic (Gd in MRI) and therapeutic agents. Toxicity of Hg, Cd, Pb and As and chelation therapy.

REFERENCES

1.	S. J. Lippard and J. M. Berg, *Principles Of Bioinorganic Chemistry*, Univ. Sci. Books, 1994.
2.	D. E. Fenton, *Biocoordination Chemistry: 25*, Oxford Chemistry Primers, 1995.
3.	W. Kaim, B. Schwederski and A. Klein, *Bioinorganic Chemistry - Inorganic Elements in the Chemistry of Life: An Introduction and Guide*, 2nd Ed., A Wiley Text Book Series, 2013.
4.	M. Weller, J. Rourke, T. Overton, F. Armstrong, Inorganic Chemistry, 7th Ed., Oxford University Press, UK, 2018.
5.	Bertini, Gray, Lippard and Valentine, *Bioinorganic Chemistry* – Viva books Pvt. Ltd. 1998.
6.	A. K. Das, M. Das and A. Das, Bioinorganic Chemistry, 2nd Ed., Books & Allied (P) Ltd., 2020.
7.	Ajay Kumar, *Organometallic & Bioinorganic Chemistry*, 5th Ed., Aaryush Education.

COURSE OUTCOMES (CO)

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

CO1	understand and analyse the metal ions in life
CO2	understand and analyse the metalloenzyme chemistry
CO3	understand and analyse the electron transport phenomena in body
CO4	understand and analyse the bio-organometallic catalysis

Course Code	**:**	CHPE616
Course Title	**:**	Organometallic Chemistry for Organic Synthesis
Type of Course	**:**	PE
Prerequisites	**:**	B.Sc. Chemistry
Contact Hours	**:**	45
Course Assessment Methods	**:**	Continuous Assessment, End Assessment

COURSE LEARNING OBJECTIVES (CLO)

To introduce the students

CLO1	to various synthetic strategies
CLO2	to the reaction mechanisms in advanced synthesis
CLO3	to the organometallic based organic synthesis
CLO4	to different named reactions

COURSE CONTENT

Unit I: Organo zinc and copper reagents, preparation using transmetallation, functionalized zinc and copper reagents, synthetic applications in conjugate addition and allylic and propargylic substitution reactions.Organo tin reagents, hydrostannation reaction and synthetic utility of vinylstannanes and allylstannanes in addition and substitution reactions.

Unit II: Organoboron and aluminium reagents, alkyl and aryl derivatives, synthesis and examples of applications in C-C bond forming reactions. Organotitanium and zirconium reagents, metallocene complexes in C-C bond forming reactions. Addition to enynes and diynes, hydrozirconation, metallocycle formation and their synthetic utility.

Unit III: Metal (W, Cr, Rh, Ru, Mo) carbene complexes, Fischer, Schrock and Grubbs type carbene complexes, comparison of their stability and reactivity, reactions of Fischer carbene complexes and their synthetic utility, Dötz reaction, simple and cross metathesis reactions, ring opening, ring closing metathesis in organic synthesis, examples from macrocycles synthesis. Copper and rhodium based carbene and nitrene complexes, cyclopropanation, Rh catalysed C-H insertion and aziridination reactions including asymmetric version. Introduction to N-heterocyclic carbene metal complexes. Metal (Fe, Cr, Mo, Ni, Co, Rh) carbonyl compounds in organic synthesis.

Unit IV: C-C bond forming. Cyclooligomerization of alkenes, enynes and alkynes, Vollhardtreaction. Carbonylation and decarbonylation reactions and hydroformylation reaction. Metal (Fe, Pd) ene, diene and dienyl complexes, metal complexes as protecting groups, activation towards nucleophilic addition reaction and rules governing such additions, synthetic utility. p-allyl palladium, nickel and iron complexes, synthesis and their synthetic utility.

Unit V: Various Wacker type oxidation and cyclization reactions including asymmetric version. Metal (Co, Zr) alkyne complexes, protection of triple bond, C-C bond forming reactions such as Pauson-Khand reaction, alkyne cyclotrimerization and oligomerization reaction. Metal (Cr, Fe, Ru) arene complexes, synthesis and structure. Activation of arene nucleus and side chain. Nucleophilic substitution and addition of arene. Metal (Rh, Ir) catalyzed C-H activation reactions and their synthetic utility.

REFERENCES

1.	Schlosser, M., *Organometalllics in Synthesis, A manual,* John Wiley, New York, 1996.
2.	Hegedus, L.S.; *Transition metals in the synthesis of complex organic molecules,* second edition, University Science, Book, CA, 1999.
3.	Astruc, D.; *Organometallic Chemistry and Catalysis,* Springer Verlag, 2007.
4.	Davies, S. G.; *Organotransition metal chemistry: Applications to organic synthesis,* Pergamon Press, New York, 1986.

COURSE OUTCOMES (CO)

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

CO1	analyse various synthetic strategies
CO2	understand the reaction mechanisms in advanced synthesis
CO3	evaluate the organometallic based organic synthesis
CO4	identify the different named reactions

Course Code	:	CHPE618
Course Title	:	Environmental Chemistry
Type of Course	:	PE
Prerequisites	:	B.Sc. Chemistry
Contact Hours	:	45
Course Assessment Methods	:	Continuous Assessment, End Assessment

COURSE LEARNING OBJECTIVES (CLO)

To introduce the students

CLO1	to the basics of Environmental chemistry and its numerous facets.
CLO2	to the important causes of pollution.
CLO3	to the analysis data for its control.
CLO4	to the health hazard in day-to-day life.

COURSE CONTENT

Environmental pollution: Structure of atmosphere- bio geological cycles -oxygen -nitrogen – carbon – phosphorous –sulphur - bio distribution of elements- air pollutions- reactions in atmosphere- primary pollutants -air quality standards - analysis of CO, nitrogen oxides, sulphur oxides, hydrocarbons and particulate matter - particulate pollution - control methods –vehicular pollution- green-house effect and global warming - climatic changes –ozone- photochemical smog-acid rain - sampling -monitoring – control – sustainability – NET ZERO – carbon neutrality.

Water pollution: Hydrological cycle- chemical composition - sea water composition -water quality criteria for domestic and industrial uses - BIS and WHO standards - ground water pollution-surface water pollution- lake and river water- eutrophication- marine pollution- water pollutants - biodegradability of detergents –pesticides- endosulfan and related case studies, microplastics.

Water treatment: Principles of water and waste water treatment -aerobic and anaerobic treatment -industrial waste water treatment -heavy metal pollution-hard water - softening - purification of water for drinking purposes - water treatment for industrial use - electrodialysis - reverse osmosis- other purification methods - chemical specification of elements.

Water analysis: Colour - odour - conductivity - TDS - pH - acidity - alkalinity - chloride- residual chlorine - hardness- trace metal analysis- elemental analysis -ammonia - nitrite -nitrate

- fluoride - sulphide - phosphate -phenols - surfactants - BOD - COD - DO - TOC-nondispersive IR spectroscopy- anode stripping - ICP - AES - Chromatography-ion selective electrodes-neutron activation analysis.

Soil pollution: Soil humus - soil fertility- inorganic and organic components in soil -acid -base and ion exchange reactions in soils -micro and macro nutrients -waste and pollutants in soil-introduction to geochemistry- solid waste management- treatment and recycling- soil analysis-radioactive pollution- disposal of radioactive waste.

REFERENCES

1.	H. Kaur, *Environmental Chemistry,* 6th Edn, PragathiPrakashan, Meerut, 2011.
2.	K. H. Mancy and W. J. Weber Jr. Wiley, *Analysis of Industrial Waste Water,* Interscience New York, 1971.
3.	L. W. Moore and E. A. Moore, *Environmental Chemistry,* McGraw Hill Publication, New York, 2002.
4.	S. M. Khopkar, *Environmental Pollution Analysis,* New Age International (P) Ltd, 1993.
5.	C. Baird, *Environmental Chemistry,* W. H. Freemand and Company, 1995.

COURSE OUTCOMES (CO)

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

CO1	familiarize the basics of environmental chemistry and its numerous facets.
CO2	find out the important causes of pollution.
CO3	work out the analysis data for its control.
CO4	know the health hazard in day-to-day life.

Course Code	**:**	CHPE620
Course Title	**:**	Biocatalytic processes in Chemical Industries
Type of Course	**:**	PE
Prerequisites	**:**	B.Sc. Chemistry
Contact Hours	**:**	45
Course Assessment Methods	**:**	Continuous Assessment, End Assessment

COURSE LEARNING OBJECTIVES (CLO)

The learning objectives are to enable students

CLO1	to familiarize the basics industrial microbiology
CLO2	to the application of microbial techniques in chemical synthesis
CLO3	to the understanding biocatalysis
CLO4	to the understanding the applications of microbiology in chemistry

COURSE CONTENT

Unit I: Industrial microorganisms: Differentiation between procaryotes and eucaryotes; Bacteria, Yeast, Molds and Actinomycetes – Cell Structure and Function – Metabolism. Bioprocessing -Fermentation Techniques: Screening procedures; Detection and assay of fermentation products; Fermentation media – down-stream processing product regulation and safety – Bioreactors Design and operation.

Unit II: Microbial production of Vitamins (vitamin B_{12}, Riboflavin); Amino acids (Glutamic acid, Lysine); Organic acids (citric acid, Acetic acid and lactic acid- Production of microbial enzymes-Proteases, Amylases, single cell protein Application of immobilized enzymes – Prodcution of Organic Acids and amino acids. – production of Alkaloids – steroids and Vaccines.

Unit III: Manufacture of food and beverage fermentations – Alcohol based fermentation industries -Production of Vinegar- Manufacture of Bread- Manufacture of Dairy products- Fermented food products - Microbial production of antibiotics – Penicillin, Streptomycin, Microbial transformation of steroids and sterol, Fermentation of hydrocarbon – Production of anti tumor agents.

Unit IV: Microbial contamination and spoilage Bio deterioration of textiles, paper, leather, wood, and rubber -Spoilage of milk, alcoholic beverages, fruits --Spoilage of meat, poultry, eggs and fish. Conversion of Renewable resources to Biofuels and fine chemicals. – Waste treatment in industry.

Unit V: Prevention and control of microorganisms in industry – Fundamentals, control by physical agents and chemical agents. Microbial Enzymens in Industry– Biocatalysts – Immobilized enzymes and immobilized cells – Mining microbiology

REFERENCES

1.	Sanjai Saxena, *Applied Microbiology,* Springer, 2015.
2.	M. J. Waites, N. L. Morgan, J. S. Rockey, G. Higton, *Indisutrial Microbiology, An Introduction,* Blackwell Science, 2001.
3.	EMT El-Mansi, C. F. A. Bryce, B. Dahhou, S. Sanchez, A. L Demainm A. R. Allman, Ed, *Fermentation microbiology and biotechnology,* 3rd Edn, CRC Press, 2012.
4.	Anantha Narayan R. and C.K.Panicker, *"Textbook of Microbiology"* Orient, Longman, New Delhi, 1980.
5.	Akoenova L. and Lisovskaya, *"Microbiology",* Mir Publishers, Moscow, 1980
6.	Bull M.J.: *"Industrial Microbiology",* Elsevier Scientific Publishing Co., New York, 1982.
7.	Barrow W. *"Textbook of Microbiology",* W,B.Saunders Cor, Philadelphia, Ed. 20.
8.	L. E Casida, *"Industrial Microbiology",* 1984.
9.	Thomas D Brock. Katherine M.Brock and David M. Ward. *"Basic Microbiology": with applications.* Prentice Hall, 1986.

COURSE OUTCOMES (CO)

Upon completion of this course, the students will be able to

CO1	familiarize the basics industrial microbiology
CO2	understand the application of microbial techniques in chemical synthesis
CO3	understand the biocatalysis
CO4	understand the applications of microbiology in chemistry

Course Code	:	CHPE622
Course Title	:	Photoredox- and Electro-Catalysis
Type of Course	:	PE
Prerequisites	:	B.Sc. Chemistry
Contact Hours	:	45
Course Assessment Methods	:	Continuous Assessment, End Assessment

COURSE LEARNING OBJECTIVES (CLO)

The learning objectives are to enable students

CLO1	to introduce the students with modern strategies in organic synthesis.
CLO2	to familiarize the students about the reactivities of organic molecules under light and electrochemical cell
CLO3	to plan synthetic routes to complex organic molecules following photo- /electro-catalysis
CLO4	to be familiar with the major advances and the current state-of-the-art methods in organic chemistry.

COURSE CONTENT

Effect of light on organic molecules – Fundamentals of photo redox catalysis – Light Matter interaction – Electronic transitions – Jablonski diagram – Excitation and Relaxation process – Mechanistic Pathway – Oxidative and Reductive quenching cycle

Photocatalyst – Organic photocatalyst –Inorganic photocatalysts – Metal complex and semiconductors – General mechanism – Light absorption – Excited state dynamics – Typical reaction pathway – Single electron transfer (SET) – Applications –Dual photo redox catalysis

Different types of organic transformations using photo redox catalysis – C-H activation – Cross coupling reaction – α Amination of carbonyl compounds – Antimarkovnikov hydroamination of alkene – Reductive dehalogenation – Ritter's decarboxylative arylation

Theory of Electrocatalysis – Electrochemical cell – Electron transfer – Overpotential – Mechanism at Electrode surface – Types of electrocatalysis – Direct and Indirect – Homogeneous electrocatalysis – Heterogeneous electrocatalysis – Photoelectrocatalysis – Bioelectrocatalysis – Types and properties of electrocatalyst – Metallic and non-metallic electrocatalyst

Organic Transformations using electrocatalysis – Oxidative coupling reaction – C-H activation – Cross coupling reactions – Kolbe electrocatalysis – Shono oxidation – Hofer Moest reaction

REFERENCES

1.	*Visible Light Photocatalysis in Organic Chemistry,* by Corey Stephenson, Tehshik Yoon, David W. C. MacMillan, Print ISBN:9783527335602 |Online ISBN:9783527674145 |DOI:10.1002/9783527674145, Publisher: Wiley-VCH Verlag GmbH & Co. KGaA
2.	*Electrochemistry in Organic Synthesis: by Lutz Ackerman.* **ISBN:** 9783132442122; Publisher: Thieme chemistry (SOS).

COURSE OUTCOMES (CO)

Upon completion of this course, the students will be able to

CO1	familiarize with the modern strategies in organic synthesis.
CO2	understand the reactivities of organic molecules under light and electrochemical cell
CO3	plan synthetic routes to complex organic molecules following photo- /electro-catalysis
CO4	know the major advances and the current state-of-the-art methods in organic chemistry

Course Code	**:**	CHPE624
Course Title	**:**	Multiscale Simulation Methods
Type of Course	**:**	PE
Prerequisites	**:**	B.Sc. Chemistry
Contact Hours	**:**	45
Course Assessment Methods	**:**	Continuous Assessment, Practical, End Assessment

COURSE LEARNING OBJECTIVES (CLO)

To introduce the students

CLO1	to the fundamentals of molecular dynamics techniques.
CLO2	to the mesoscale simulation methods.
CLO3	to the methodologies of enhanced sampling techniques.
CLO4	to the application of big-data analysis in chemistry and biology.
CLO5	to the practical applications of computational chemistry and biology.

COURSE CONTENT

Atomistic Simulation: Importance of computational chemistry in predicting molecular properties. Limitations. Basics of Monte-Carlo (MC) technique. Statistical mechanical basics of molecular dynamics (MD). Molecular mechanics and force fields (polarizable, and non-polarizable). Ewald summation and PPPM method. Periodic boundary and cut-off methods. Integration schemes. Velocity-verlet algorithm. Partial charge and RESP charge calculations. Temperature and Pressure baths. Time-correlation and autocorrelation functions. Potential energy landscape: determination of minima and saddle points for complex molecular systems. Normal mode analysis. Basic concepts of hybrid QM/MM simulation and reactive force fields. Examples of MD simulation with water models.

Mesoscale Simulation: *Coarse-grain models:* advantages and disadvantages. Explicit vs Implicit solvents. Brownian and Langevin dynamics. Multiparticle collision dynamics. Dissipative particle dynamics. *Lattice models:* Ising model. Magnetization and curie temperature. Partition function in 1D and 2D (no derivation). Lattice Boltzmann method.

Enhanced sampling methods: Free-energy calculation using MD simulation. Harmonic model of PEL minima. Accelerated MD. MC-MD techniques. Parallel tempering. Hamiltonian replica exchange. Flat histogram methods: Wang-Landau sampling, Metadynamics. Steered

MD and umbrella sampling. Reweighting method: weighted histogram analysis method (WHAM). Free-energy perturbation theory (no derivation). Markov state modelling.

Big-data analysis: *Cheminformatics:* Chemical databases. SMILES, InChi representation. Molecular descriptor and similarity. Drug-protein docking methods. Virtual screening. Drug-likeness and druggability. *Bioinformatics:* Homology modelling. Biological databases (EMBL, Swiss-Prot, PDB, Genome): handling and retrieval. FASTA sequence format. Sequence alignment. Scoring methods. Multiple sequence alignment. Secondary structure prediction. Computational methods of gene prediction.

Practical:

1. Preparation and visualization of molecular structure using Avogadro and VMD.
2. Equilibrating a random distribution of Lennard-Jones particles in LAMMPS.
3. Simulation of TIP3P water model and calculation of physical properties using LAMMPS.
4. Preparation and simulation of a protein using GROMACS.
5. Principle component analysis using GROMACS.
6. Sequence alignment using BLAST.
7. Homology modelling using SWISS-PDB and validation with PRO-CHECK.
8. Drug-protein docking using Autodock and identification of active sites.

REFERENCE

1.	D. Frenkel and B. Smit, *Understanding Molecular Simulation: From Algorithms to Applications*, Oxford Academic Press (1996)
2.	C. J. Cramer, *Essentials of Computational Chemistry: Theories and Models*, John Wiley & Sons, 2002.
3.	D. C. Young, *Computational Chemistry: A Practical Guide for Applying Techniques to Real World Problems*, Wiley Interscience, 2001
4.	F. Jensen, *Introduction to computational chemistry*, Wiley, NY, 2007.
5.	P. Allen and D. J. Tildesley, Computer Simulations of Liquids, Oxford, 1987
6.	R. Leach**,** Molecular Modelling: Principles and Applications, Pearson Education, 2001.
7.	Mount D., *Bioinformatics: Sequence and Genome Analysis*, Cold Spring Harbor Laboratory Press, New York. 2004
8.	Baxevanis, A.D. and Francis Ouellellette, B.F., *Bioinformatics- a Practical Guide to the Analysis of Genes and Proteins*, Wiley India Pvt Ltd. 2009

9.	Andrew R. Leach and Valerie J. Gillet, *An Introduction to Chemoinformatics*, Springer Publisher
10.	Thomas Engel and Johann Gasteiger, *Applied Chemoinformatics - Achievements and Future Opportunities*, Wiley-VCH publisher.

COURSE OUTCOMES

Upon completing the course, the student will be able to

CO1	understand the fundamentals of molecular dynamics techniques.
CO2	understand the mesoscale simulation methods.
CO3	understand the methodologies of enhanced sampling techniques.
CO4	understand the application of big-data analysis in chemistry and biology.
CO5	understand the practical applications of computational chemistry and biology.

Course Code	:	CHPE626
Course Title	:	Semiconductor process integration and skills development by Virtual Fabrication
Type of Course	:	PE
Prerequisites	:	Nil
Contact Hours	:	45
Course Assessment Methods	:	Continuous Assessment, End Assessment

COURSE LEARNING OBJECTIVES (CLO)

To enable the students to:

CLO1	Understand the semiconductor manufacturing ecosystem
CLO2	Understand the advantages of microfabrication and scaling
CLO3	Seamlessly relate circuit abstraction with device cross-section and mask layout.
CLO4	Module-level understanding of advanced CMOS FinFET process
CLO5	Use SEMulator3D® Software for semiconductor process development

COURSE CONTENT

Silicon semiconductor unit processes: Silicon wafers and their purity (grade), roughness, size, and orientation. Manufacturing process from Silicon dioxide to Si wafer. Wafer modification: doping, diffusion, implantation, native-oxide (SiO2) growth, Deposition: APCVD, LPCVD, MOCVD, PECVD, ALD, PVD, electroplating, Etch: Wafer RCA cleaning, wet etch, dry etch, isotropic versus anisotropic etch, and Chemical-mechanical processing.

Semiconductor manufacturing ecosystem: Differences between design, fabrication, packaging, system manufacturing and product. Advantages of microfabrication and scaling, Relating circuit abstraction with device cross-section and mask layout, Lithography, resolution limit, evolution from i-line to EUV, multiple patterning (SADP and SAQP).

Modules of CMOS (Complementary Metal-Oxide-Semiconductor) FinFET processes-1: Isolation module: Advantages and challenges of STI versus LOCOS, Device architecture: Planar to FinFET, use of SiGe and strain, Gate module: SiO2 versus Hi-k dielectrics, polysilicon versus metal gate, gate-first versus gate-last, integration challenges of replacement metal gate. Well & junction module: Basics of implantation, source-drain and well implants, other implants.

Modules of CMOS FinFET processes-2: Contact module: contact resistance issues of simple metal-silicon contact, metal silicides, salicidation, evolution from Ti to Co to Ni silicide. Interconnect module: Need for multiple metal layers, RC delay, challenge of electromigration, evolution from Al vs Cu, Damascene and dual-Damascene process, W plugs and via, Intermediate dielectric: Need for ILD, low-k due to RC delay, SiO2 to SiOF to SiOC to porous SiOC, material and integration challenges, 3D-NAND fabrication process

Working knowledge of SEMulator3D software to solve integration challenges: Implementation of a basic layout by importing layout files or creating one in the layout editor. Simulation of the process flow of a FinFET device and analysis of output. Extraction of cross-sectional images and geometric parameters.

Assignment 1: Creation of a layout of NMOS, PMOS and inverter

Assignment 2: LOCOS isolation verses Shallow Trench Isolation (STI)

Assignment 3: Gate-First versus Gate-Last

Assignment 4: Spacer and multiple patterning

Assignment 5: Replacement metal gate

Assignment 6: Implantation & Silicidation

Assignment 7: Damascene

Assignment 8: Dual-Damascene

Assignment 9: PlanarFET vs FinFET inverter

References:

1	James D. Plummer, Peter B. Griffin, Integrated Circuit Fabrication: Science and Technology, Cambridge Univ Press, 2022

2	Ulrich Hilleringmann, Silicon Semiconductor Technology: Processing and Integration of Microelectronic Devices, Springer Vieweg; 1st edition, 2023
3	Parasuraman Swaminathan, Semiconductor Materials, Devices and Fabrication, Wiley, 2017
4	Richard C. Jaeger, Introduction to Microelectronic Fabrication, Pearson, 2nd edition, 2001
5	Stephen A. Campbell, The Science and Engineering of Microelectronic Fabrication, Oxford Univ Press, 2nd edition, 2001
6	Sorab K Ghandhi, VLSI Fabrication Principles: Silicon and Gallium Arsenide, Wiley-Interscience Publication, 2nd edition, 2008
7	Milton Ohring, Materials Science of Thin Films Deposition and Structure Academic Press, 2nd Edition, 2002
8	Chris Mack, Fundamental Principles of Optical Lithography: The Science of Microfabrication, John Wiley & Sons, Ltd, 2007
9	SEMulator3D® Software help manual

Online Resource:

1. http://www.tf.uni-kiel.de/matwis/amat/elmat_en/index.html by Prof. Dr. Helmut Föll

COURSE OUTCOME

Upon completing the course, the student will be able to:

CO1	Understand the semiconductor unit processes required for process integration
CO2	Relate circuit abstraction with device cross-section and mask layout, and multiple patterns
CO3	Have Module-level understanding of CMOS FinFET process
CO4	Analyse material and integration challenges in advanced CMOS FinFET
CO5	Demonstrate semiconductor skills development through SEMulator3D®