MASTER OF SCIENCE IN

CHEMISTRY

SYLLABUS FOR THE
CREDIT BASED FLEXIBLE CURRICULUM

FROM 2022 ONWARDS

Department of Chemistry
National Institute of Technology
Tiruchirappalli – 620 015
Tamil Nadu, India

National Institute of Technology, Tiruchirappalli

Vision, Mission, Core Values and Goals

NIT Tiruchirappalli, through its Vision, Mission and Core Values, defines herself as:

- An Indian institution with world standards.
- A global pool of talented students, committed faculty and conscientious researchers responsive to real-world problems and, through a synergy of education and research, engineer a better society.

VISION

To be a university globally trusted for technical excellence where learning and research integrate to sustain society and industry.

MISSION

- To offer undergraduate, postgraduate, doctoral and modular programmes in multi-disciplinary / inter-disciplinary and emerging areas.
- To create a converging learning environment to serve a dynamically evolving society.
- To promote innovation for sustainable solutions by forging global collaborations with academia and industry in cutting-edge research.
- To be an intellectual ecosystem where human capabilities can develop holistically.

Department of Chemistry

VISION

To be a world-class centre in Basic and Applied Chemistry

MISSION

- To impart and enhance the advanced knowledge and skills of students and professionals to meet the global challenges.
- To offer effective solutions to the industries through research and consultancies.
- To address rural needs through research and ecofriendly solutions.

M.Sc. Chemistry

Programme Educational Objectives

PEO1	Achievement of mastery of chemistry in a foundational level to the current knowledge
PEO2	Development of cognitive research skills at a level required to pursue higher education
PEO3	Understanding of experimentation, observation and data analysis suitable for any Chemistry based industry
PEO4	Familiarity with available instrumentation for conducting specific scientific research
PEO5	To communicate effectively, verbally and written, for the purposes of conveying chemical information to both professional scientists and to the public

Programme Outcomes

PO1	To understand the application of the classical subjects in modern chemistry
PO2	To master factual and experimental knowledge across the principle areas of chemistry
PO3	To demonstrate competence in solving industrial scientific problems through experimental, computational and/or data analysis models
PO4	To indulge in deeper learning of the principles of Organic, Inorganic and Physical Chemistry
PO5	To learn modern analytical and spectroscopic tools and their applications to different disciplines of chemistry
PO6	To design and conduct experiments as well as to analyse and interpret the data
PO7	To work effectively both as an individual and as a collaborative team member
PO8	To learn the interdisciplinary nature of chemistry and to integrate the knowledge with a variety of chemical problems
PO9	To appreciate the importance of goal-setting and to recognize the need for life-long reflective learning.
PO10	To learn, design and demonstrate sustainable industrial reactions within realistic constraints such as economic, environmental, social, ethical, health, safety and productivity

Mapping of Departmental mission statements to PEO's

	PEO1	PEO2	PEO3	PEO4	PEO5
To impart and enhance the advanced knowledge and skills of students and professionals to meet the global challenges	√	√	√	√	√
To offer effective solutions to the industries through research and consultancies	√	√	√	√	√
To address rural needs through research and eco-friendly solutions		√		√	√

Mapping of PO with PEO

	PEO1	PEO2	PEO3	PEO4	PEO5
PO1	√	√	√	√	
PO2	√	√	√	√	√
PO3	√	√	√	√	√
PO4	√	√	√		
PO5	√	√	√	√	
PO6	√			√	√
PO7			√	√	√
PO8		√	√	√	
PO9			√	√	√
PO10	√	√	√	√	√

Curriculum components

Category	Credits
Core courses	36
Elective courses	12
Laboratory	12
Project work	08
Total	68

Curriculum

The total minimum credits required for completing the M.Sc. in Chemistry is 68

SEMESTER 1					
Code	**Course of Study**	**L**	**T**	**P**	**C**
CH 601	Organic Chemistry - Reaction Mechanisms and Their Types	3	-	-	3
CH 603	Coordination Chemistry: Bonding, Reactions and Spectra	3	-	-	3
CH 605	Quantum Chemistry and Group Theory	3	-	-	3
CH 607	Instrumental Methods of Chemical Analysis	3	-	-	3
CH 609	Organic Preparations and Separations Lab	-	-	6	2
CH 611	Inorganic Preparations and Qualitative Analysis Lab	-	-	6	2
	ELECTIVE I	3	-	-	3
		-	-	-	19

SEMESTER II					
Code	**Course of Study**	**L**	**T**	**P**	**C**
CH 602	Stereochemistry, Photochemistry, Pericyclic and Rearrangement reactions	3	-	-	3
CH 604	Organometallic and Bioinorganic Chemistry	3	-	-	3
CH 606	Thermodynamics, Electrochemistry and Kinetics	3	-	-	3
CH 608	Molecular Spectroscopy	3	-	-	3
CH 610	Organic and Inorganic Quantitative Analysis Lab	-	-	6	2
CH 612	Analytical Chemistry Lab	-	-	6	2
	ELECTIVE II	3	-	-	3
		-	-	-	19

SEMESTER III					
Code	**Course of Study**	**L**	**T**	**P**	**C**
CH 613	Synthetic Organic Chemistry	3	-	-	3
CH 615	Main Group Chemistry, Inorganic Spectroscopy and Nuclear Chemistry	3	-	-	3
CH 617	Statistical Thermodynamics, Photochemistry and Surface Chemistry	3	-	-	3
CH 619	Spectroscopy-Applications in Organic Chemistry	3	-	-	3
CH 621	Physical Chemistry Lab	-	-	6	2
CH 623	Spectroscopy Lab	-	-	6	2
	ELECTIVE III	3	-	-	3
	ELECTIVE IV*	3	-	-	3
		-	-	-	22

SEMESTER IV					
Code	**Course of Study**	**L**	**T**	**P**	**C**
CH 614	M.Sc. Project	-	-	-	8
	Total Credits	-	-	-	**68**

ELECTIVES

Code	Course of Study	L	T	P	C
CH 616	Environmental Chemistry	3	-	-	3
CH 622	Catalysis	3	-	-	3
CH 624	Inorganic Rings, Cages and Clusters	3	-	-	3
CH 625	Medicinal Chemistry	3	-	-	3
CH 626	Nano Science and Technology	3	-	-	3
CH 627	Computational Methods in Chemistry	2	-	3	3
CH 628	Natural Products Chemistry	3	-	-	3
CH 629	Polymer Chemistry	3	-	-	3
CH 630	Advanced Heterocyclic Chemistry	3	-	-	3
CH 631	Electronic Structure Methods for Molecular and Solid-State Systems	2	-	3	3
CH 632	Interfacial Chemistry and Sonochemistry	3	-	-	3
CH 634	Lanthanide and Actinide Chemistry	3	-	-	3
CH 635	Fuel cells for Stationary and Automotive Applications	3	-	-	3
	NPTEL, SWAYAM, Coursera, edX Online courses	-	-	-	3
CH 636	Homogeneous Catalysis	3	-	-	3
CH 637	Advanced Bioinorganic Chemistry	3	-	-	3
CH 638	Organometallic Chemistry for Organic Synthesis	3	-	-	3
CH 639	Principles and Applications of Fluorescence Spectroscopy	3	-	-	3
CH 640	Biocatalytic processes in Chemical Industries	3	-	-	3

*Elective IV may be one of elective courses offered by the department or one of the online courses under mathematics and basic sciences category which does not overlap the syllabus.

CH 601	Organic Chemistry- Reaction Mechanisms and Their Types	L	T	P	C
		3	0	0	3

PRE-REQUISITE: NIL

COURSE LEARNING OBJECTIVES

Upon completion of the course the student will be able to understand

- The basics of reaction mechanism and the mechanistic concepts
- The fundamentals of substitution reactions and reactive intermediates
- The addition reactions of C=C and C=O bonds
- The mechanism of elimination reactions and important redox reagents
- The concept of aromaticity and reactions of aromatic compounds

COURSE CONTENT

Reaction mechanism: Definition of reaction mechanism, 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. Addition to carbonyl compounds- 1,2 and 1,4-addition, benzoin, Knoevenegal, Stobbe 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 and Antiaromaticity, Huckel's rule, annulences and heteroannulenes, fullerenes (C60). Other conjugated systems, Chichibabin reaction. 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.

REFERENCE BOOKS

1. M. B. Smith, J. March, *March's Advanced Organic Chemistry*, John Wiley & Sons, 6thEdn, 2007.
2. R. R. Carey and R. J. Sundburg, *Advanced Organic Chemistry, Part A and Part B*, Springer, 5thEdn, 2007.
3. Peter Sykes, *A Guide Book to Mechanism in Organic chemistry*, Orient-Longman, 6th Edn, 1996.
4. P. Y. Bruice, *Organic Chemistry*, Pearson Education, 7th edition, 2013.

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

MAPPING OF COURSE OUTCOME WITH PROGRAMME OUTCOMES

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO1	✓	✓		✓		✓		✓	✓	✓
CO2	✓	✓	✓	✓		✓		✓	✓	✓
CO3	✓	✓		✓	✓	✓		✓	✓	✓
CO4	✓	✓		✓	✓	✓		✓	✓	✓

CH 603	Coordination Chemistry: Bonding, Reactions and Spectra	L	T	P	C
		3	0	0	3

PRE-REQUISITE: NIL

COURSE LEARNING OBJECTIVES

To introduce the students to the theory, bonding, reactions, structure and spectra of coordination compounds. To provide them a brief idea on solid state chemistry and properties of lanthanides and actinides.

COURSE CONTENT

Theories of coordination compounds: VB theory - CFT - splitting of d orbitals in ligand fields and different symmetries - CFSE - factors affecting the magnitude of 10 Dq - 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 - π-bonding and molecular orbital theory - experimental evidence for π-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 - ligand field effects and reaction rates – 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 - Orgel and Tanabe-Sugano diagrams - evaluation of 10 Dq and β for octahedral complexes of cobalt and nickel - charge transfer spectra - magnetic properties of coordination compounds - change in magnetic properties of complexes in terms of spin orbit coupling - temperature independent 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.

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Structure: Structure 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 - caesium chloride - wurtzite - zinc blende - rutile - fluorite - antifluorite - diamond and graphite - spinels (normal and inverse) – perovskite - band theory of solids - dislocation in solids - Schottky and Frenkel defects - electrical properties - insulators, semiconductors and conductors - super conductors.

REFERENCE BOOKS

1. J. E. Huheey, E. A. Keiter and R. L. Keiter, *Inorganic Chemistry: Principles of Structure and Reactivity*, Harper Collin College Publishers, 4th Edition, 1993.
2. F. A. Cotton and G. Wilkinson, *Advanced Inorganic Chemistry*, Wiley Interscience, 4th & 5th Editions, 1998.
3. J. Lewis and R. G. Wilkins, *Modern Coordination Chemistry*, Wiley Interscience, 1960.
4. D. F. Shriver, P. W. Atkins and C. H. Langford, *Inorganic Chemistry*, Oxford University Press, l994.
5. G. L. Miessler and D. A. Tarr, *Inorganic Chemistry*, 3rd Edition, Pearson Prentice Hall, 2005
6. J. E. House, *Inorganic Chemistry*, Elsevier, 2008.
7. C. E. Housecroft and A. G. Sharpe, *Inorganic Chemistry*, Prentice Hall, 2005
8. L.V. Azaroff, *Introduction to Solids*, Mc.Graw hill, New York, 1984
9. R. West, *Solid State Chemistry and its Applications*, John Wiley & Sons, 1984.

COURSE OUTCOME

Upon completing the course, the student will be able to

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

MAPPING OF COURSE OUTCOME WITH PROGRAMME OUTCOMES

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PO10**
CO1	✓	✓		✓		✓		✓	✓	✓
CO2	✓	✓	✓	✓		✓		✓	✓	✓
CO3	✓	✓		✓	✓	✓		✓	✓	✓
CO4	✓	✓		✓	✓	✓		✓	✓	✓

CH 605	Quantum Chemistry and Group Theory	L	T	P	C
		3	0	0	3

PRE-REQUISITE: NIL

COURSE LEARNING OBJECTIVES

To learn the fundamental principles of the properties of matter, energy quantization, its application, symmetry properties of molecules and application of group theory in understanding the molecular properties based on symmetry.

COURSE CONTENT

Quantum Chemistry-I: The failures of classical physics – Black body radiation-photoelectric effect- Bohr's quantum theory, Wave particle duality-Uncertainty principle- Operator algebra, Linear and Hermitian operators, Quantum mechanical postulates, Schrodinger equation and its solution to the problem of a particle in one- and three-dimensional boxes.

Quantum Chemistry-II: Quantum mechanical results for a rigid rotator and simple harmonic oscillator, Solution of Schrodinger equation for harmonic oscillator and rigid rotor. Schrodinger equation for hydrogen atom and its solution-Derivation of Eigen function and Eigen value for hydrogen atom. Term symbols for electronic state in atoms –LS and JJ coupling. The origin of electronic quantum numbers and physical significance - radial probability density-significance of magnetic quantum number with respect to angular momentum.

Quantum Chemistry-III: Hydrogen molecule ion and hydrogen molecule-Pauli's exclusion principle. Born Oppenheimer approximation, Mulliken designation of molecular orbitals.MO theory of bonding, MO treatment of H-bonded systems, ethylene, butadiene and benzene. Approximation methods: Perturbation and variation method, wave functions for many electron atoms – Hartree-Fock SCF method, Slater orbitals.

Group Theory-I: Elements of group theory, definition, group multiplication tables, conjugate classes, conjugate and normal subgroups, symmetry elements and operations, point groups, assignment of point groups to molecules, Matrix representation of geometric transformation and point group, reducible and irreducible representations, construction of character tables, bases for irreducible representation, direct product, symmetry adapted linear combinations, projection operators. Orthogonality theorem - its consequences.

Group Theory-II: Symmetry aspects of molecular orbital theory, planar π-systems, symmetry factoring of Huckel determinants, solving it for energy and MOs for ethylene and 1,4-butadiene, sigma bonding in AX_n molecules, hybridization, tetrahedral, octahedral, square planner, trigonal planar, linear, trigonal bipyramidal systems, hybrid orbitals as linear combination of AOs, electronic spectra, selection rule, polarization electron dipole transition, electronic transitions in formaldehyde, butadiene, configuration interaction, vibrational spectra, symmetry types of normal molecules, symmetry coordinates, selection rules for fundamental vibrational transition, IR and Raman activity of fundamentals in CO_2, H_2O,N_2F_2, the rule of mutual exclusion and Fermi resonance. Metal-metal bond dinuclear systems exhibiting allowed delta-delta transitions etc.

REFERENCE BOOKS

1. N. Levine, *Quantum Chemistry*, Prentice Hall India, 4thEdnm, 1994.
2. A. K. Chandra, *Introductory Quantum Chemistry*, Tata McGraw Hill, 1994.
3. M. S. Gopinathan and V. Ramakrishnan, *Group Theory in Chemistry*, Vishal Publishers, 1988.
4. D. A. McQuarrie, *Quantum Chemistry*, University Science Books, 1983.
5. F. A. Cotton, *Chemical Applications of Group Theory*, Wiley Eastern Ltd., 2ndEdn., 1990.
6. R. K. Prasad, *Quantum Chemistry*, Tata McGraw Hill, 1995.
7. P.W. Atkins, *Physical Chemistry*, Oxford University Press, 6thEdn., 1998.

COURSE OUTCOME

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

CO1	Understand the properties of matter and the wave-particle duality
CO2	Apply the concept of quantization of energy and its modes
CO3	Relate symmetry of the molecules to their properties
CO4	Apply group theory and character table to analyse the molecular properties

MAPPING OF COURSE OUTCOME WITH PROGRAMME OUTCOMES

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PO10**
CO1	✓	✓		✓						
CO2	✓	✓	✓	✓	✓			✓		
CO3	✓	✓	✓	✓	✓					✓
CO4	✓	✓	✓	✓	✓	✓		✓		✓

CH 607	Instrumental Methods of Chemical Analysis	L	T	P	C
		3	0	0	3

PRE-REQUISITE: NIL

COURSE LEARNING OBJECTIVES

To introduce the basic principles, working and applications of Instrumental techniques like Chromatography, Electrophoresis, Potentiometry, spectroelectrochemisty and thermal methods to the I year M.Sc. students.

COURSE CONTENT

Errors in chemical analyses: Accuracy and propagation of errors, Statistical data analysis and evaluation: Confidence intervals, statistical aids to hypothesis testing- analysis of variance and Regression analysis

Separation techniques: Solvent extraction - Methods of extraction and applications of solvent extraction. Chromatography- thin layer chromatography, ion exchange chromatography and size exclusion chromatography –HPLC-outline study of instrument modules. Gas chromatography – basic instrumental set up-carriers, columns, detectors and comparative study of TCD, FID, ECD and NPD. Theory & applications –electrophoresis- theory and applications.

Electroanalytical techniques: Potentiometry - electrode systems, direct potentiometric titrations-null-point potentiometry and applications. Polarography, stripping voltammetry & Amperometric techniques - diffusion currents, Half-wave potentials, construction & characteristics of the DME-quantitative analysis-amperometric titrations and applications of polarography – electrogravimetry and coulometry - coulometry at constant potential, coulometric titrations-conductometric titrations.

Atomic spectrometry: Atomic Absorption Spectroscopy: Principles, instrumentation and applications. Plasma Emission Spectrometry: Instrumentation, Sample Introduction for Plasma Sources, Analytical Measurements and Applications. Inductively Coupled Plasma–mass Spectrometry (ICP–MS): Principles, Instrumentation and Applications. Atomic Fluorescence Spectrometry: Principles and Applications.

Thermal techniques: Thermogravimetry - instrumentation and applications of TG. Differential thermal analysis (DTA) - instrumentation and applications of DTA. Differential scanning calorimetry (DSC) - Instrumentation, applications of DSC and comparison of DTA & DSC. Thermomechanical analysis (TMA) and dynamic mechanical analysis (DMA) - instrumentation, applications of TMA and dynamic mechanical analysis.

REFERENCE BOOKS

1. G. H. Geeffery et al., *Vogel's Text Book of Quantitative Chemical Analysis*, ELBS Edn, 1989.
2. D. A. Skoog, D.M. West, F.J Holler, S.R Crouch, *Fundamentals of Analytical Chemistry*, 8^{th} edition, Thomson Brooks Cole, 2004.
3. F. Rouessac and A. Rouessac, Chemical Analysis: Modern Instrumentation Methods and Techniques, 2^{nd}Edn, John Wiley and Sons.

4. D. A. Skoog, E. J. Holler, S. R. Crouch , *Principles of Instrumental Analysis*, 6th edition, Thomson Brooks Cole , 2007.
5. F. W. Fifield and D. Kealey, *Principles and Practice of Analytical Chemistry*, 2nd Edition, International Book Company, London, 1983.
6. H. H. Willard, L.L. Merrit, J.A. Dean and F.A. Settle, *Instrumental Methods of Analysis*, D, CBS Publishers, New Delhi, 1986.

COURSE OUTCOME

Upon completing the course, the student will be able:

CO1	To know the importance of instrumental techniques and its applications.
CO2	To understand sampling methods of the analytes to be measured.
CO3	To get familiarize with the principles, operation and uses of these instruments in industry.
CO4	To conduct demonstration experiments in industry with real samples.

MAPPING OF COURSE OUTCOME WITH PROGRAMME OUTCOMES

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PO10**
CO1	✓	✓	✓	✓	✓	✓		✓		✓
CO2	✓	✓	✓	✓	✓	✓				✓
CO3	✓	✓	✓	✓	✓	✓				✓
CO4	✓	✓	✓	✓	✓	✓				✓

CH 609	Organic Preparations and Separations lab	L	T	P	C
		0	0	6	2

PRE-REQUISITE: NIL

COURSE LEARNING OBJECTIVES

Upon completion of the course the student will be able to understand:

- To introduce students to various techniques for separation, purification and identification of components in a mixture.
- To introduce the students to have hands on experience to perform various reactions.

COURSE CONTENT

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

REFERENCE BOOKS

1. I. Vogel, Text Book of Practical Organic Chemistry,5th Edn., ELBS, London, l989.
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., l992.

COURSE OUTCOME

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

CO1	Separate the organic mixtures and identify the compounds
CO2	To perform various reactions
CO3	To perform natural product extraction

MAPPING OF COURSE OUTCOME WITH PROGRAMME OUTCOMES

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO1			✓	✓	✓	✓	✓		✓	✓
CO2			✓	✓	✓	✓	✓	✓	✓	✓
CO3			✓	✓	✓	✓	✓	✓	✓	✓

CH 611	Inorganic Preparations and Qualitative Analysis Lab	L	T	P	C
		0	0	6	2

PRE-REQUISITE: NIL

COURSE LEARNING OBJECTIVES

To introduce the students to the semi-micro analysis of mixture of cations and to provide them a brief idea about inorganic preparatory methods.

COURSE CONTENT

Semi-micro analysis (minimum 8 mixture): Analysis of mixture containing two common cations and any two of the following less familiar cations. Tl, W, Se, Te, Mo, Ce, Th, Ti, Zr, V, Be, U and Li.

Synthesis and characterization of any five Compounds:

1. Potassium trioxalatocobaltate, Bromopentamminecobalt(III) chloride
2. Tris(ethylenediammine)chromium(III) chloride, Hexamminecobalt(III)chloride
3. Tris(ethylenediammine)cobalt(III)chloride, *Cis* and *trans*
4. Dichlorobis(ethylenediammine)cobalt(III) chloride and resolution of the *cis* form.
5. Hexamminenickel(II) bromide,
6. Bis(N,N'-bis(*o*-hydroxybenzylidine)ethylenediamine)-*m*-aquodicobalt(II)
7. Dichloro(di-2-pyridylamine)copper(II) and Bis(Di-2-pyridylamine)copper(II) chloride
8. Bis(ethylenediamine)nickel(II) chloride
9. Tris(acetylacetonato)iron(III)
10. Tris(acetylacetonato)manganese(III)

REFERENCE BOOKS

1. V. V. Ramanujam, *Inorganic Semi-micro Qualitative Analysis*, 3rd Edition, National Publishing Company, l990.
2. G. Brauer (Ed.), *Handbook of Preparative Inorganic Chemistry (Vol. I and II),* Academic Press, 1963.

COURSE OUTCOME

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

CO1	learn about the semi-micro analysis of mixture of cations
CO2	learn about the preparation of cobalt compounds
CO3	learn about the preparation of nickel compounds
CO4	learn about the preparation of chromium, manganese and iron compounds

MAPPING OF COURSE OUTCOME WITH PROGRAMME OUTCOMES

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO1	✓	✓	✓	✓	✓	✓	✓	✓		✓
CO2	✓	✓	✓	✓	✓	✓	✓	✓		✓
CO3	✓	✓	✓	✓	✓	✓	✓	✓		✓
CO4	✓	✓	✓	✓	✓	✓	✓	✓		✓

CH 602	Stereochemistry, Photochemistry, Pericyclic and Rearrangement reactions	L	T	P	C
		3	0	0	3

PRE-REQUISITE: CH 601

COURSE LEARNING OBJECTIVES

1. To provide a comprehensive information about the stereochemistry of organic molecules.
2. To introduce the students regarding the fundamentals of photochemistry and various photochemical reactions in detail.
3. The students will be able to plan synthetic routes to complex organic molecules through cycloaddition reactions.
4. The students will 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 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-Fundamentals and applications: 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.

Rearrangements: reactions involving electron deficient, carbon, nitrogen, oxygen centers, emphasis on synthetic utility of these rearrangements. Baker–Venkataraman, Benzilic acid, [1,2]-Meisenheimer, [2,3]-Meisenheimer, Wagner-Meerwein, Pinacol, Demyanov, Dienone-Phenol, Favorskii, Wolff, Meyer–Schuster, Rupe, Schmidt, Neber, Smiles, Truce-Smiles rearrangement.

REFERENCE BOOKS

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, 4th 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 Edn, 2006.
6. B. P. Mundy, M. G. Ellerd, F. G., Jr. Favaloro Name Reactions and Reagents in Organic
7. Synthesis, Wiley-Interscience, 2005.

COURSE OUTCOME

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

CO1	Understand the stereochemistry of organic molecules in detail.
CO2	Solve various problems on photochemical transformations.
CO3	The students will be able to plan synthetic routes to complex organic molecules through cycloaddition reactions.
CO4	Understand the various types of rearrangement reactions and their mechanism.

MAPPING OF COURSE OUTCOME WITH PROGRAMME OUTCOMES

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PO10**
CO1	✓	✓	✓	✓					✓	✓
CO2	✓	✓	✓	✓			✓	✓	✓	✓
CO3	✓	✓	✓	✓			✓	✓	✓	✓
CO4	✓	✓	✓	✓			✓	✓	✓	✓

CH 604	**Organometallic and Bioinorganic Chemistry**	**L**	**T**	**P**	**C**
		3	0	0	3

PRE-REQUISITE: CH 603

COURSE LEARNING OBJECTIVES

The course aims at the detailed interception of bonding concepts in organometallic and bioinorganic chemistry. Mechanistic aspects of several well-known industrial catalytic techniques will be studied. The course also aims at a detailed understanding of bioinorganic chemistry.

COURSE CONTENT

Structure and bonding in organometallics: 18/16 electron rule - metal carbonyls - bonding - nitrosyls - dinitrogen complexes – phosphines - metal alkyls, aryls, hydrides - π-bonding ligands - dihydrogen complexes - agostic bonds - metal–metal bonds - Fischer and Schrock carbenes - structure, bonding & reactivity – metallocenes - electronic structure and bonding in ferrocene - fluxional molecules.

Reaction mechanism and catalysis: Ligand substitution - oxidative addition and reductive elimination - C–H and C–C activation - 1,1 and 1,2-insertion - addition and elimination reactions - homogeneous catalysis - alkene isomerisation – hydrocyanation - hydrogenation of olefins - Wilkinson’s catalyst - assymetric hydrogenation - hydroformylation of olefins-Wacker process - Monsanto acetic acid process - Eastman Halcon process - Fischer-Tropsch process.

Homogeneous catalysis - Grubbs catalyst - olefin metathesis - RCM, ROMP, SHOP and ADMET - Ziegler-Natta polymerization of olefins - Heck reaction - Suzuki coupling - Stille coupling - Sonagashira coupling - Nozaki-Hiyama cross coupling - Ullmann coupling – Pauson-Khand reaction - ene reaction - Dotz reaction - Vollhardt reaction - Murai reaction - Hartwig-Buchwald amination - σ-bond metathesis.

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.

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 bioenergetic 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.

REFERENCE BOOKS

1. G.O. Spessard and G. L. Miessler, *Organometallic Chemistry*, 1st, 2nd and 3rd Editions, Oxford University Press, 2015
2. R.H. Crabtree, *The Organometallic Chemistry of Transition Metals*, 7th Edition, Wiley-VCH, 2019
3. W. Kaim and B. Schwederski, *Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life*, John Wiley, 1994.
4. S. J. Lippard and J. M. Berg, *Principles of Bioinorganic Chemistry*, Panima Publ. Corpn., 2005.
5. J. E. Huheey, E. A. Keiter and R. L. Keiter, *Inorganic Chemistry: Principles of Structure and Reactiv*ity, 4th Edition, Harper Collin College Publishers, 1993.
6. C. Elschenbroich, *Organometallics*, 3rd Edition, Wiley-VCH, 1989.

COURSE OUTCOME

Upon completing the course, the student will be able to

CO1	A understanding of organometallic bonding principles
CO2	Understanding of reaction mechanism in organometallic chemistry
CO3	Understanding of industrially important homogenous catalytic cycles
CO4	Understanding of bioinorganic chemistry

MAPPING OF COURSE OUTCOME WITH PROGRAMME OUTCOMES

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PO10**
CO1	✓	✓		✓	✓			✓		✓
CO2	✓	✓	✓	✓	✓		✓	✓		✓
CO3	✓	✓	✓	✓	✓		✓	✓	✓	✓
CO4	✓	✓		✓	✓			✓		✓

CH 606	**Thermodynamics, Electrochemistry and Kinetics**	**L**	**T**	**P**	**C**
		3	0	0	3

PRE-REQUISITE: NIL

COURSE LEARNING OBJECTIVES

To learn the thermodynamic principles of system in equilibrium and their associated properties. To understand the phases of coexistence in any reaction or equilibrium. To understand the basic principles of electrochemistry, interphases and their applications, the kinetics of reactions.

COURSE CONTENT

Thermodynamics: Third law, thermodynamics, need for it, Nernst heat theorem and other forms of stating the third law. Thermodynamic quantities at absolute zero, apparent exceptions to the third law - thermodynamics of systems of variable composition, partial molar properties, chemical potential, relationship between partial molar quantities, Gibbs Duhem equation and its applications (the experimental determination of partial molar properties not included) - thermodynamic properties of real gases, fugacity concept, calculation of fugacity of real gas, activity and activity coefficient, concept, definition, standard states and experimental determinations of activity and activity coefficient of electrolytes.

Phase rule: colloids and micelles: Phase rule: Three component systems, representation by triangular diagrams, systems of three liquids, formation of one pair of partially miscible liquids, formation of two pairs of partially miscible liquids, solid, liquid phases, eutectic systems-colloids: Distinction between suspension, colloidal solutions and true solutions, lyophilic and lyophobic colloids, Tyndall effect, stability of colloids, coagulation, emulsions, various types. Micelles: Surfactant (amphipathic molecule), micellization, critical micelle concentration, size of micelle, aggregation number, thermodynamics of micellization, solubilisation behaviour of micelles, reverse, micelles.

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 Huckel-Onsager equation for the equivalent conductivity of electrolytes - experimental verification of the equation - conductivity at high field and at high frequency - conductivity of non-aqueous solutions-effect of ion association on conductivity. The electrode-electrolyte interface-electrical double layer-electro capillary phenomena-Lippmann equation - the Helmholtz- Perrin - Guoy-Chapmann and Stern models, electro kinetic 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 - 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 - electro deposition. 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: Simultaneous reactions - opposing, parallel and consecutive reactions, the steady state approximation - theories of reaction rates-transition state theory and collision theory a comparison - enthalpy, entropy and free energy of activation, 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 catalysed reactions - effect of substrate concentration, pH and temperature - determination of Michael's parameters.

REFERENCE BOOKS

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.

COURSE OUTCOME

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

CO1	Relate the thermodynamic properties of the system and the chemical composition.
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.

MAPPING OF COURSE OUTCOME WITH PROGRAMME OUTCOMES

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PO10**
CO1	✓	✓	✓	✓		✓		✓		✓
CO2	✓	✓	✓	✓		✓		✓		✓
CO3	✓	✓	✓	✓		✓		✓		✓
CO4	✓	✓	✓	✓		✓		✓		✓

CH 608	Molecular Spectroscopy	L	T	P	C
		3	0	0	3

PRE-REQUISITE: Should have attended CH 605

COURSE LEARNING OBJECTIVES

To introduce the basic concepts and applications of various molecular spectroscopic techniques to the M.Sc. students.

COURSE CONTENT

Rotational spectroscopy: Interaction of radiation with matter–Spectroscopic Transitions-Einstein coefficients- transition probability- Born-Oppenheimer approximation- selection rules-intensity and width of spectral lines-Fourier transformation- Principal moments of Inertia - Diatomic and polyatomic molecules- selection rules – Diatomic Rigid Rotor – Non Rigid Rotor – Nonlinear poly atomic molecules- Effect of Nulcear 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 - Vibration- Rotation spectroscopy- selection rules- FT- IR 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 – Racah Parameters – Zeeman Effect - Frank Condon principle- Vibronic Tranistions-selection rules- parity, symmetry and spin selection rules-polarization of transitions-Instrumentation and sampling - electronic spectra of conjugated systems Fluorescence Spectroscopy – Jablonski Diagram- Kashas rules- Quenching

Electron spectroscopy: Photoelectric effect, 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*, 4thedn. Tata McGraw Hill, 1996.
3. J. M. Hollas, *Modern Spectroscopy*, 4thEdn, John Wiley& Sons, 1992.
4. P. F. Bernath, *Spectra of Atoms and Molecules*, 2ndEdn, 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*, 2ndEdn, Elsevier, 1984.

COURSE OUTCOME

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

CO1	Fundamentals of interactions of electromagnetic radiation with matter & Rotational spectra of diatomic and polyatomic molecules
CO2	A detailed study Vibrational spectroscopy of polyatomic molecules, Raman effect and Raman spectroscopy
CO3	An understanding of Atomic and Electronic spectroscopy of atoms and molecules
CO4	Fundamentals of photo electron spectroscopy and analysis techniques based on high energy radiation.

MAPPING OF COURSE OUTCOME WITH PROGRAMME OUTCOMES

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PO10**
CO1	✓	✓		✓	✓				✓	
CO2	✓	✓		✓	✓				✓	
CO3	✓	✓		✓	✓				✓	
CO4	✓	✓		✓	✓			✓	✓	

CH 610	Organic and Inorganic Quantitative Analysis Lab	L	T	P	C
		0	0	6	2

PRE-REQUISITE: NIL

COURSE LEARNING OBJECTIVES

To introduce the students to the estimation of metal cations and organic compounds.
To provide them a brief idea about analysis of oils.

COURSE CONTENT

1. Inorganic quantitative analysis:

Analysis involving volumetric and gravimetric estimations of mixtures of cations Cu & Ni; Cu & Zn; Zn & Cu; Fe & Ni; Fe(II) & Fe(III).

2. Organic quantitative analysis:

(a) Estimations:

Estimation of phenol, aniline, ascorbic acid.
Estimation of ketone by volumetric method & gravimetric method.
Estimation of lactose in milk.
Estimation of glucose by Fehling’s method.
Estimation of glucose by Bertrand's method.

(b) Analysis of Oils:

Determination of saponification value of an oil, Determination of acetyl value of an oil, Determination of iodine value of an oil, Determination of acid value of an oil.

REFERENCE BOOKS

1. A. I. Vogel, *Text Book of Quantitative Inorganic Analysis*, 5th Edition, Longman, 1989
2. A. I. Vogel, *Text Book of Practical Organic Chemistry*, 5th Edition, ELBS, l989.
3. B. B. Dey and M. V. Sitharaman, *Laboratory Manual of Organic Chemistry*, Revised by T. R. Govindachari, Allied Publishers Ltd., 4th Edition, l992.

COURSE OUTCOME

Upon completing the course, the student will be able to

CO1	learn about the volumetric estimation of mixture of cations
CO2	learn about the gravimetric estimation of mixture of cations
CO3	learn about the estimation of organic compounds
CO4	learn about the analysis of oils

MAPPING OF COURSE OUTCOME WITH PROGRAMME OUTCOMES

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO1	✓	✓	✓	✓	✓	✓	✓	✓		✓
CO2	✓	✓	✓	✓	✓	✓	✓	✓		✓
CO3	✓	✓	✓	✓	✓	✓	✓	✓		✓
CO4	✓	✓	✓	✓	✓	✓	✓	✓		✓

CH 612	Analytical Lab	L	T	P	C
		0	0	6	2

PRE-REQUISITE: An understanding of basic Analytical Chemistry.

COURSE LEARNING OBJECTIVES

This course will introduce the students of first year M.Sc. to the principles of analytical chemistry in analysis of substance important in day-to-day life. For examples like water, milk, butter, cement, tea, antacid tablets etc.

COURSE CONTENT

(Any 5 experiments from category 1-6)

1. Water analysis
   a) Determination of chloride content in water
   b) Estimation of dissolved oxygen in water
   c) Determination of hardness in water by EDTA
   d) Determination of total alkalinity of water
2. 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
3. Butter analysis
   a) Estimation of salt in butter
   b) Estimation of fat in butter
   c) Estimation of moisture content in butter
4. Cement analysis
5. Estimation of caffeine from tea
6. Analysis of antacid tablet
7. Determination of phosphoric acid in coke.

REFERENCE BOOKS

1. Manual provided by the department.
2. A. I. Vogel, *Text Book of Quantitative Inorganic Analysis*, 5thEdn, Longman, 1989.

COURSE OUTCOME

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

CO1	Importance of analytical chemistry in the analysis of samples in day-to-day life
CO2	Experimental skills required for analysis will be developed
CO3	Students will be able to carry out independent analyses with the developed skills
CO4	Familiarization of biochemical laboratory practices for analysis of biological samples via demonstrations

MAPPING OF COURSE OUTCOME WITH PROGRAMME OUTCOMES

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO1					✓					
CO2			✓			✓	✓			
CO3							✓	✓		
CO4							✓			✓

CH 613	Synthetic Organic Chemistry	L	T	P	C
		3	0	0	3

PRE-REQUISITE: NIL

COURSE LEARNING OBJECTIVES

Upon completion of the course the student will be able to understand

1. The concept of retrosynthesis and the terms involved
2. About one group and two group disconnections
3. The various protection and deprotection of important functional groups
4. The use of important reagents in organic synthesis
5. 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. Chemoselectivity, 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, 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, Complex metal hydrides, Gilman's reagent, lithium diisoproplyamide (LDA), dicyclohexylcarbodimide, timethylsilyl iodide, Woodward and Provost hydroxylation, DDQ, SeO_2, phase transfer catalyst, crown ethers and Merrifield resin, Wilkinson's catalyst, 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, Barton, Baylis Hillman reaction, Stork enamine reaction and selective mono and di alkylation via enamines, Buchwald-Hartwig reaction, olefin metathesis, Noyori asymmetric hydrogenation, asymmetric organo catalysis, Ugi and passerine reaction, Nazarov reaction.

REFERENCE BOOKS

1. House, *Modern Synthetic Reaction*, 1973.
2. S. Warren, *Organic Synthesis The Disconnection approach*, Wiley and sons, 2002.
3. M. B. Smith, Organic Synthesis, 4th Edition, Academic press
4. W. Carruthers, Modern methods of Organic Synthesis, Cambridge University Press
5. Clayden, Greeves, Warren & Wothers, 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, 5thEdn, 2007.

COURSE OUTCOME

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

MAPPING OF COURSE OUTCOME WITH PROGRAMME OUTCOMES

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO1	✓	✓	✓	✓		✓		✓	✓	✓
CO2	✓	✓	✓	✓		✓		✓	✓	✓
CO3	✓	✓	✓	✓		✓		✓	✓	✓
CO4	✓	✓	✓	✓		✓		✓	✓	✓

CH 615	Main Group Chemistry, Inorganic Spectroscopy and Nuclear Chemistry	L	T	P	C
		3	0	0	3

PRE-REQUISITE: NIL

COURSE LEARNING OBJECTIVES

To introduce the students to the basics of solid-state chemistry and structural paradigms in main group and early transition elements, and their rings, cages and cluster compounds. To give a brief idea on the nuclear chemistry.

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 P_4 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.

IR and Raman spectroscopy: Structural elucidation of simple molecules like N_2O, ClF_3, NO_3^-, ClO_4^- - effect of coordination on ligand vibrations - uses of group vibrations in the structural elucidation of metal complexes of urea, thiourea, cyanide, thiocyanate, nitrate, sulphate and DMSO - applications of Raman spectroscopy.

Electron paramagnetic resonance: Basic principles - electron Zeeman - g-value - hyperfine interaction - anisotropy - application to organic radicals and transition metal complexes - zero field splitting - model system for pulse EPR experiments - ESEEM – HYSCORE - Davies and Mims ENDOR - Mössbauer spectroscopy - principle - recoilless emission and absorption - isomer shift – quadrupolar splitting - hyperfine - magnetic interactions - NQR spectroscopy.

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.

REFERENCE BOOKS

1. H. J. Arnikar, *Essentials of Nuclear Chemistry*, 4th Edition, New Age International Publishers Ltd., New Delhi, 1995.
2. J. D. Lee, *Concise Inorganic Chemistry*, 5th Edition, Chapman and Hall, London, 1996.
3. J. E. Huheey, E. A. Keiter and R. L. Keiter, *Inorganic Chemistry - Principles of Structure and Reactivity*, 4th Edition, Harper Collins, New York, l993.

4. D. M. P. Mingos and D. J. Wales, *Introduction to Cluster Chemistry*, Prentice Hall, 1990.
5. N. N. Greenwood and E. A. Earnshaw, *Chemistry of Elements*, Pergaman Press, 1984.
6. T. Chivers, I. Manners, *Inorganic Rings and Polymers of the p-Block Elements, from Fundamentals to Applications*, RSC Publishing, 2009.
7. K. Nakamoto, *Infrared and Raman Spectra of Inorganic and Coordination Compounds*, Part A & Part B, 2nd Edition, Wiley, 2009.
8. D. N. Sathyanarayana, Handbook of Molecular Spectroscopy, From Radio waves to gamma rays, I.K international Publishing house Pvt. Ltd, 2015
9. J. A. Weil, J. R. Bolton, Electron Paramagnetic Resonance, Elementary Theory and Practical Applications, Wiely-Interscience, 2007.
10. 5. A. Schweigher, G. Jeshcke, Principles of Pulse Electron Paramagnetic Resonance, Oxford University press, 2002.
11. D. P. E. Dickson, F. J. Berry, Ed. Mossbauer Spectroscopy, Cambridge University Press, 1986.

COURSE OUTCOME

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

CO1	learn about isolable analogy and structural paradigms in cluster chemistry
CO2	learn about structure and reactivity of main group compounds
CO3	apply EPR, Mossbauer, IR and Raman spectroscopy for the structural characterization of inorganic compounds
CO4	learn about the basics of nuclear chemistry and its applications

MAPPING OF COURSE OUTCOME WITH PROGRAMME OUTCOMES

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PO10**
CO1	✓	✓		✓			✓	✓	✓	✓
CO2	✓	✓		✓			✓	✓	✓	✓
CO3	✓	✓	✓	✓	✓		✓	✓	✓	✓
CO4	✓	✓		✓	✓		✓	✓	✓	✓

CH 617	Statistical Thermodynamics, Photochemistry and Surface Chemistry	L	T	P	C
		3	0	0	3

PRE-REQUISITE: Nil

COURSE LEARNING OBJECTIVES

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

COURSE CONTENT

Statistical thermodynamics I: Maxwell's law of distribution of molecular speeds, graphical representation, experimental verification - derivation of expressions for average, most probable and root mean square velocity. Concept of velocity space and phase space-perturbation and 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 thermodynamics II: Statistical interpretation of laws of thermodynamics, third law of thermodynamics and apparent expression to it. Quantum statistics: 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.

Surface chemistry I: 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 chemistry II: 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.

REFERENCE BOOKS

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 OUTCOME

Upon completing the course, the student will be able to

CO1	Apply statistics to understand the thermodynamic properties of macroscopic systems.
CO2	Understand the principle and applications of photochemistry.
CO3	Learn the theories of surface chemistry and their applications.
CO4	Use instrumental methods for characterization of chemically active surfaces.

MAPPING OF COURSE OUTCOME WITH PROGRAMME OUTCOMES

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PO10**
CO1	✓	✓	✓		✓	✓		✓		✓
CO2	✓	✓	✓		✓	✓		✓		✓
CO3	✓	✓	✓		✓	✓		✓		✓
CO4	✓	✓	✓		✓	✓		✓		✓

CH 619	**Spectroscopy- Applications in Organic Chemistry**	**L**	**T**	**P**	**C**
		3	0	0	3

PRE-REQUISITE: CH 608

COURSE LEARNING OBJECTIVES

Students will learn the fundamentals of NMR and Mass spectroscopy. They will be able to determine the structure of organic molecules.

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.

REFERENCE BOOKS

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 5thEdn. 2007 & 2013.
4. M. Balci, Basic 1H- and 13C-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,2ndEdn, 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 OUTCOME

Upon completing the course, the student 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

MAPPING OF COURSE OUTCOME WITH PROGRAMME OUTCOMES

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PO10**
CO1	✓	✓			✓	✓	✓	✓	✓	
CO2	✓	✓			✓	✓	✓	✓	✓	
CO3	✓	✓			✓	✓	✓	✓	✓	
CO4	✓	✓			✓	✓	✓	✓	✓	

CH 621	Physical Chemistry Lab	L	T	P	C
		0	0	6	2

PRE-REQUISITE: Nil

COURSE LEARNING OBJECTIVES

To conduct various experiments, to analyse the role of reaction conditions and to interpret the data.

COURSE CONTENT

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.

REFERENCE BOOKS

1. C. Garland, J. Nibler and D. Shoemaker, *Experiments in Physical Chemistry*, McGraw-Hill Education; 8th Edn., 2008.
2. Manual provided by the Department.

COURSE OUTCOME

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.

MAPPING OF COURSE OUTCOME WITH PROGRAMME OUTCOMES

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO1	✓	✓	✓			✓	✓	✓	✓	✓
CO2	✓	✓	✓			✓	✓	✓	✓	✓
CO3	✓	✓	✓			✓	✓	✓	✓	✓
CO4	✓	✓	✓			✓	✓	✓	✓	✓

CH 623	Spectroscopy Lab	L	T	P	C
		0	0	6	2

PRE-REQUISITE: An understanding of basic analytical chemistry & basics of spectroscopy

COURSE LEARNING OBJECTIVES

This course will introduce the students of first year M.Sc. to the principles of spectroscopy and analysis of substance important in day-to-day life.

COURSE CONTENT

(Any 5 experiments from category 1-9)

1. Fabry Perot Etalon- Spacing of Etalon-Finesse and free spectral range
2. Zeeman effect- Analysis of Plank's constant and Bohr magneton
3. Michelson's interferometer- Wavelength of laser, refractive index, magnetostrictive properties of ferromagnetic materials
4. Calculation of extinction coefficient
5. Diffraction gratings- Wavelength of light
6. Photoelectric effect- Planks constant- Work function of material
7. Fluorescence spectroscopy- Excitation and emission, Kashas rule
8. Absorption spectroscopy- Beers law –Deviations-Titrations
9. Polarization of light- Rayleigh scattering-Dichroism and birefringence.
10. Raman Spectroscopy

REFERENCE BOOKS

1. Manual provided by the department.
2. A. I. Vogel, *Text Book of Quantitative Inorganic Analysis*, 5th Edn, Longman, 1989.

COURSE OUTCOME

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

CO1	Importance of spectroscopy and the analysis of samples using this techniques in day-to-day life
CO2	Experimental skills required for analysis will be developed
CO3	Students will be able to carry out independent analyses with the developed skills
CO4	Familiarization of biochemical laboratory practices for analysis of biological samples via demonstrations

MAPPING OF COURSE OUTCOME WITH PROGRAMME OUTCOMES

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO1					✓					
CO2			✓			✓	✓			
CO3							✓	✓		
CO4							✓			✓

CH 616	Environmental Chemistry	L	T	P	C
		3	0	0	3

PRE-REQUISITE: NIL

COURSE LEARNING OBJECTIVES

To introduce the underlying concepts of Environmental Chemistry, various aspects of the four main spheres of earth: Atmosphere, Biosphere, Hydrosphere and Lithosphere, their interactions amongst each other and influence on human beings to the M.Sc. students.

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 –vechicular pollution- green house effect and global warming - climatic changes –ozone- photochemical smog-acid rain - sampling -monitoring – control.

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.

REFERENCE BOOKS

1. H. Kaur, *Environmental Chemistry*, 6^{th} 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 OUTCOME

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

CO1	Familiarize the basics of Environmental chemistry and its numerous facets.
CO2	Find out the important causes of pollution.
CO3	Will work out the analysis data for its control.
CO4	Know the health hazard in day-to-day life.

MAPPING OF COURSE OUTCOME WITH PROGRAMME OUTCOMES

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PO10**
CO1	✓	✓	✓		✓		✓	✓		✓
CO2	✓	✓	✓		✓		✓	✓		✓
CO3	✓	✓	✓		✓		✓	✓		✓
CO4	✓	✓			✓		✓	✓		✓

CH 622	Catalysis	L	T	P	C
		3	0	0	3

PRE-REQUISITE: NIL

COURSE LEARNING OBJECTIVES

To introduce the students to the fundamentals of catalysis and characterization techniques in catalysis. To provide them a brief idea on the homogeneous, heterogeneous and photo 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.

Homogeneous catalysis: Noyori asymmetric hydrogenation -metal mediated C-C and C-X coupling reactions - Heck, Stille, Suzuki, Negishi and Sonogashira, Nozaki-Hiyama, Buchwald-Hartwig, Ullmann coupling reactions - directed orthometalation - metal (Rh, Ir) catalyzed C-H activation reactions and their synthetic utility -copper and rhodium based carbene and nitrene complexes - cyclopropanation - Rh catalyzed C-H insertion and aziridination reactions including asymmetric version -introduction to N-heterocyclic carbene metal complexes. Recent challenges in catalysis such as conversion of methane to methanol, activation of CO_2 etc

Characterization of solid catalysts: Surface area - structure - surface morphology - porosity - pore volume - diameter - particle size - X-ray diffraction - SEM, TEM, X-ray absorption spectroscopy, XPS and Auger spectroscopy to surface studies - TPD, TPR for acidity and basicity of the catalysts - theories - boundary layer theory -Wolkenstein theory -Balanding's approach.

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.

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.

REFERENCE BOOKS

1. P. H. Emmet, Catalysis (Vol I and II), Reinhold, 1954.
2. M. Schlosser, Organometallics in Synthesis, A Manual, John Wiley, 1996.
3. L. S. Hegedus, Transition Metals in the Synthesis of Complex Organic Molecules, University Science, 1999.
4. D. K. Chakrabarty and B. Viswanathan, Heterogeneous Catalysis, New Age, 2008.

5. B. Viswanathan, S. Kannan and R.C. Deka, Catalysts and Surfaces: Characterization Techniques, Narosa, 2010.
6. M. Kaneko and I. Okura, Photocatalysis: Science and Technology, Springer, 2003.

COURSE OUTCOME

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

CO1	learn about the fundamentals in catalysis and characterization techniques
CO2	learn about the homogeneous catalysis
CO3	learn about the heterogeneous catalysis
CO4	learn about the photo catalysis

MAPPING OF COURSE OUTCOME WITH PROGRAMME OUTCOMES

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PO10**
CO1	✓	✓	✓	✓		✓		✓	✓	✓
CO2	✓	✓	✓	✓	✓	✓		✓	✓	✓
CO3	✓	✓	✓	✓		✓		✓	✓	✓
CO4	✓	✓	✓	✓		✓		✓	✓	✓

CH 624	Inorganic Rings, Cages and Clusters	L	T	P	C
		3	0	0	3

PRE-REQUISITE: Bonding theories and structure in organometallic and coordination Chemistry.

COURSE LEARNING OBJECTIVES

This advanced elective course aims at making the students explore the world of inorganic structures and vivid bonding theories which are categorized as non-classical bonding.

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.

REFERENCE BOOKS

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 OUTCOME

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

CO1	Study different rules concerning the metal clusters
CO2	Have a clear understanding of the structural paradigms in chemistry and isolobal analogy
CO3	Study the inorganic heterocyclic systems of main group elements
CO4	A detailed study of inorganic polymers

MAPPING OF COURSE OUTCOME WITH PROGRAMME OUTCOMES

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PO10**
CO1	✓	✓			✓					
CO2	✓	✓			✓					
CO3	✓	✓			✓					
CO4	✓	✓			✓					

CH 625	Medicinal Chemistry	L	T	P	C
		3	0	0	3

PRE-REQUISITE: NIL

COURSE LEARNING OBJECTIVES

1. To introduce the students in the field of medicinal chemistry
2. To provide the students an idea about the classifications of drugs and structure-activity relationship.
3. The students will be able get an idea about the antibiotics (synthesis, bio-activity)
4. The students will 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.

REFERENCE BOOKS

1. I. 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 OUTCOME

Upon completing the course, the student 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

MAPPING OF COURSE OUTCOME WITH PROGRAMME OUTCOMES

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO1	✓	✓	✓	✓	✓	✓			✓	✓
CO2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO3	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
CO4	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓

CH 626	Nanoscience and Nanotechnology	L	T	P	C
		3	0	0	3

PRE-REQUISITE: Students with appropriate Chemistry/Engineering background may be permitted to enroll

COURSE LEARNING OBJECTIVES

To impart the basic knowledge on nanoscience and nanotechnology which includes the exotic properties of materials at nanoscale, various techniques available for the processing and characterization of nanostructured materials, applications in selected fields such as 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.

REFERENCE BOOKS

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 OUTCOME

Upon completing the course, the 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

MAPPING OF COURSE OUTCOME WITH PROGRAMME OUTCOMES

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PO10**
CO1	✓	✓						✓	✓	✓
CO2	✓	✓						✓	✓	✓
CO3	✓	✓						✓	✓	✓
CO4	✓	✓						✓	✓	✓

CH 627	**Computational Methods in Chemistry**	**L**	**T**	**P**	**C**
		2	0	3	3

PRE-REQUISITE: B.Sc. Ancillary Mathematics Background

COURSE LEARNING OBJECTIVES

To learn the logic of computer programming, numerical methods of evaluation of experimental data and apply them for solving chemistry related problems. The Lab training will equip the students with molecular modelling, and the prediction of molecular properties using software.

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 modeling 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

REFERENCE BOOKS

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, ChemOffice Ultra and Gauss View.

COURSE OUTCOME

Upon completing the course, the 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

MAPPING OF COURSE OUTCOME WITH PROGRAMME OUTCOMES

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PO10**
CO1	✓	✓	✓	✓	✓	✓		✓		✓
CO2	✓	✓	✓	✓	✓	✓		✓		✓
CO3	✓	✓	✓	✓	✓	✓		✓		✓
CO4	✓	✓	✓	✓	✓	✓		✓		✓

CH 628	**Natural Products Chemistry**	**L**	**T**	**P**	**C**
		3	0	0	3

PRE-REQUISITE: NIL

COURSE LEARNING OBJECTIVES

1. To introduce the students in the field of natural products and their classifications.
2. To provide the students a broad idea about amino acids, steroids, carbohydrates and heterocycles.
3. The students will be able get an idea about the antibiotics (synthesis, bio-activity)
4. 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

Aminoacids: 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.

REFERENCE BOOKS

1. I. L. Finar, Organic Chemistry Vol. I & Vol. II- Pearson Education, 6thedn.
2. F. A. Carey and R. J. Sundberg, (Eds) 3rd Edition, Part B. Plenum/Rosetta, 1990.
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 OUTCOME

Upon completing the course, the student 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

MAPPING OF COURSE OUTCOME WITH PROGRAMME OUTCOMES

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PO10**
CO1	✓	✓	✓	✓					✓	✓
CO2	✓	✓	✓	✓			✓	✓	✓	✓
CO3	✓	✓	✓	✓			✓	✓	✓	✓
CO4	✓	✓	✓	✓			✓	✓	✓	✓

CH 629	Polymer Chemistry	L	T	P	C
		3	0	0	3

PRE-REQUISITE: NIL

COURSE LEARNING OBJECTIVES

To introduce the basic concept of macromolecules, polymerization processes, polymer stereochemistry, theory of polymer soultions and speciality polymers to the M.Sc. students.

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.

Polymer solutions: Flory-Huggins theory. Chain dimension-chain stiffness. End-to-end chain distance of polymers. Conformation-random coil, solvation and swelling. Determination of degree of cross linking and molecular weight between cross links. Industrial polymers-synthesis, structure and applications of industrially important polymers.

Specialty 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 & polythiophines. Photoresponsive and photorefractive polymers. Polymers in optical lithography-Organic electronic materials- Drug Delivery-Drug carriers-Polymer based nanoparticles.

REFERENCE BOOKS

1. George Odian, Principles of polymerization, 4th edition, John Wiley & Sons, Inc., Hoboken, New Jersey, 2004.
2. F.W. Billmayer, *Textbook of Polymer Science*. 3rdEdn, 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*, 3rdEdn. , 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 OUTCOME

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

CO1	Classification of polymers and its nomenclature.
CO2	Polymerization methods
CO3	Polymerization kinetics
CO4	Uses of polymers for commercial purposes

MAPPING OF COURSE OUTCOME WITH PROGRAMME OUTCOMES

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PO10**
CO1	✓	✓	✓	✓	✓	✓		✓		✓
CO2	✓	✓	✓	✓	✓	✓				✓
CO3	✓	✓	✓	✓	✓	✓				✓
CO4	✓	✓	✓	✓	✓	✓				✓

CH 630	Advanced Heterocyclic Chemistry	L	T	P	C
		3	0	0	3

PRE-REQUISITE: NIL

COURSE LEARNING OBJECTIVES

1. To introduce the students with major classes of heterocyclic compounds and their chemical properties.
2. To familiarize the students about the reactivities of different classes of heterocycles.
3. The students will be able to plan synthetic routes to complex organic molecules containing heterocyclic motifs.
4. The students will 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.

REFERENCE BOOKS

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 OUTCOME

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

CO1	Familiar with commonly used synthetic routes to heterocycles and major advances in the field of heterocyclic chemistry.
CO2	be able to plan synthetic routes to complex organic molecules containing heterocyclic motifs
CO3	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

MAPPING OF COURSE OUTCOME WITH PROGRAMME OUTCOMES

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PO10**
CO1	✓	✓	✓	✓		✓	✓		✓	✓
CO2	✓	✓	✓	✓		✓	✓	✓	✓	✓
CO3	✓	✓	✓	✓		✓	✓	✓	✓	✓
CO4	✓	✓	✓	✓		✓	✓	✓	✓	✓

CH 631	Electronic Structure Methods for Molecular and Solid State Systems	L	T	P	C
		2	0	3	3

PRE-REQUISITE: Basic knowledge in quantum chemistry is desirable.

COURSE LEARNING OBJECTIVES

Introduction to electronic structure methods (quantum chemical approach) for molecular and solid-state systems and their use in designing the efficient 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.

REFERENCE BOOKS

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 OUTCOME

Upon completing the course, the student 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

MAPPING OF COURSE OUTCOME WITH PROGRAMME OUTCOMES

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PO10**
CO1	✓		✓	✓			✓	✓		
CO2		✓	✓	✓			✓	✓		✓
CO3			✓	✓			✓	✓		
CO4			✓	✓			✓	✓		✓

CH 632	Interfacial Chemistry and Sonochemistry	L	T	P	C
		3	0	0	3

PRE-REQUISITE: Students with appropriate Chemistry/Engineering background may be permitted to enrol.

COURSE LEARNING OBJECTIVES

The course represents the fundamentals and applications of various advanced physical and chemical unit operations and processes for controlling drinking water quality.

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

REFERENCE BOOKS

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 completing the course, the student 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

MAPPING OF COURSE OUTCOME WITH PROGRAMME OUTCOMES

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PO10**
CO1	✓	✓	✓	✓			✓	✓		✓
CO2	✓	✓	✓	✓			✓	✓		✓
CO3	✓	✓	✓	✓			✓	✓		✓
CO4	✓	✓	✓	✓			✓	✓		✓

CH 634	Lanthanide and Actinide Chemistry	L	T	P	C
		3	0	0	3

PRE-REQUISITE: NIL

COURSE LEARNING OBJECTIVES

The student will be able to in detail understand the chemistry and reactivity of lanthanides and actinides, their properties and applications.

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 – naming.

REFERENCE BOOKS

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 edition, 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 and R. L. Keiter, *Inorganic Chemistry: Principles of Structure and Reactivity*, Harper Collin College Publishers, 4th Edition, 1993.

COURSE OUTCOME

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

CO1	Learn about Lanthanides and their extraction
CO2	Understand Lanthanide Chemistry and spectroscopy
CO3	Learn about actinides and their extraction
CO4	Learn about actinides and their extraction

MAPPING OF COURSE OUTCOME WITH PROGRAMME OUTCOMES

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO1	✓	✓		✓	✓			✓		✓
CO2	✓	✓		✓	✓			✓		✓
CO3	✓	✓		✓	✓			✓		✓
CO4	✓	✓		✓	✓			✓		✓

CH 635	Fuel cells for Stationary and Automotive Applications	L	T	P	C
		3	0	0	3

PRE-REQUISITE: This course is open to students from all science and engineering backgrounds. Students should have a basic understanding of electrochemistry, electronics, physics and engineering principles. Some problem-solving skill will be required.

COURSE LEARNING OBJECTIVES

The main objective of this course is to give a theoretical and practical overview of various fuel cell systems and PEM fuel cell in particular analysing the power demand for specific kinds of stationary and automotive applications, and the overall environmental and cost benefits.

COURSE CONTENT

Unit I: 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.

Unit II: 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.

Unit III: 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.

Unit IV: 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.

Unit V: 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.

REFERENCE BOOKS

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 OUTCOME

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

CO1	Understand and be able to 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	Understand and be able to select the right type of fuel cell for specific application.
CO4	Understand the advantages and disadvantages of fuel cell systems to sustain the automotive sector of a modern society and be able to quantify related performance parameters, such as power density, operational life and cost.

MAPPING OF COURSE OUTCOME WITH PROGRAMME OUTCOMES

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PO10**
CO1	✓	✓						✓		
CO2	✓	✓					✓		✓	✓
CO3	✓	✓	✓	✓	✓	✓				✓
CO4	✓	✓	✓	✓		✓			✓	✓

CH 636	Homogeneous Catalysis	L	T	P	C
		3	0	0	3

PRE-REQUISITE: NIL

COURSE LEARNING OBJECTIVES

To introduce the students to the fundamentals of homogeneous catalysis and individual case studies.

COURSE CONTENT

Unit I: Alkene isomerization- Hydroboration-Hydrocyanation- Hydroformylation of olefins-Wacker-smidt Synthesis- Monsanto Acetic Acid process- - BASF process - Water - Gas Shift reaction - Fischer - Tropsch Reaction -Eastman Halcon process- Fischer-Tropsch process

Unit II: 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

Unit III: 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 -

Unit IV: Noyori asymmetric hydrogenation - metal mediated C-C and C-X coupling reactions - Heck, Stille, Suzuki, Negishi and Sonogashira, Nozaki-Hiyama, Buchwald-Hartwig, Murai reaction-Ullmann coupling reactions - directed ortho metalation - metal (Rh, Ir) catalyzed C-H activation reactions and their synthetic utility - copper and rhodium based carbene and nitrene complexes - cyclopropanation - Rh catalyzed C-H insertion and aziridination reactions including asymmetric version - introduction to N-heterocyclic carbene metal complexes.

Unit V: Chemical Industry and Homogeneous Catalysis- Feed Stocks and Definitions- Reactor Design - Stirred Tank- Tubular-Membrane reactors - Mass transfer & Heat Transfer in multiphase reactions - Catalyst recovery - Effluent & Waste disposal-Heterogenization or immobilization - Biocatalysis and Enzyme- immobilzation methods- Cytochrome P450 - Catalysis under super critical conditions - Ferrocene as a Gasoline and Fuel Additive

REFERENCE BOOKS

1. S. Bhadhuri, D. Mukesh, Homogeneous Catalysis - Mechanisms and Industrial Applications, Wiley Interscience, 2000.
2. B. Cornliss, W. A. Herrmann Applied Homogeneous Catalysis with Organometallic Compounds, 2nd Edition, Wiley-VCH, 2002.
3. P. W. N. M. van Leeuwen, Homogeneous Catalysis - Understanding the Art, Kluwer Academic Publishers, 2004.
4. C. Elschenbroich, Organometallics, 3rd Edition, Wiely-VCH.

5. D. Astruc, Organometallic Chemistry and Catalysis, Springer, 2007.
6. P. Kalck, Homo- and Hetero-bimetallic Complexes in Catalysis, Springer, 2016.

COURSE OUTCOME

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

CO1	homogeneous catalysis fundamentals
CO2	Understanding individual reaction cycles
CO3	Asymmetric Catalysis
CO4	Understanding bio organometallic catalysis

MAPPING OF COURSE OUTCOME WITH PROGRAMME OUTCOMES

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PO10**
CO1	√	√	√	√		√		√	√	√
CO2	√	√	√	√	√	√		√	√	√
CO3	√	√	√	√		√		√	√	√
CO4	√	√	√	√		√		√	√	√

CH 637	**Advanced Bioinorganic Chemistry**	**L**	**T**	**P**	**C**
		3	0	0	3

PRE-REQUISITE: NIL

COURSE LEARNING OBJECTIVES

To introduce the students to the advanced bioinorganic chemistry techniques and biological systems.

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.

REFERENCE BOOKS

1. Principle of Bioinorganic chemistry – Lippard and Berg, Univ. Science Books, 1994.
2. Biocoordination chemistry – Fenton, Oxford chemistry primer, 1995.
3. Bioinorganic chemistry: Inorganic perspective in the chemistry of Life, Kaim and Schwederski, 1994.
4. Inorganic chemistry – Shriver, Atkins, and Langford, 1994.
5. Bioinorganic Chemistry – Bertini, Gray, Lippard and Valentine Viva books Pvt. Ltd. 1998.

COURSE OUTCOME

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

CO1	Understanding the metal ions in life
CO2	Metalloenzyme chemistry
CO3	Electron transport phenomena in body
CO4	Understanding bio-organometallic catalysis

MAPPING OF COURSE OUTCOME WITH PROGRAMME OUTCOMES

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PO10**
CO1	✓	✓	✓	✓		✓		✓	✓	✓
CO2	✓	✓	✓	✓	✓	✓		✓	✓	✓
CO3	✓	✓	✓	✓		✓		✓	✓	✓
CO4	✓	✓	✓	✓		✓		✓	✓	✓

CH 638	**Organometallic Chemistry for Organic Synthesis**	**L**	**T**	**P**	**C**
		3	0	0	3

PRE-REQUISITE: NIL

COURSE LEARNING OBJECTIVES

To introduce the students to the advanced Organometallic Chemistry for Organic Synthesis.

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.

REFERENCE TEXT BOOKS

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 OUTCOME

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

CO1	Various synthetic strategies
CO2	Reaction mechanisms in advanced synthesis
CO3	Organometallic based organic synthesis
CO4	Different named reactions

MAPPING OF COURSE OUTCOME WITH PROGRAMME OUTCOMES

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PO10**
CO1	√	√	√	√		√		√	√	√
CO2	√	√	√	√	√	√		√	√	√
CO3	√	√	√	√		√		√	√	√
CO4	√	√	√	√		√		√	√	√

CH 639	Principles and Applications of Fluorescence Spectroscopy	L	T	P	C
		3	0	0	3

PRE-REQUISITE: Understanding of Theory and Fundamentals of Molecular Spectroscopy.

COURSE LEARNING OBJECTIVES

To introduce the students to the basics of Fluorescence spectroscopy and its applications in day-to-day life.

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*, 4thedn. 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

MAPPING OF COURSE OUTCOME WITH PROGRAMME OUTCOMES

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PO10**
CO1	✓	✓	✓		✓		✓	✓		✓
CO2	✓	✓	✓		✓		✓	✓		✓
CO3	✓	✓	✓		✓		✓	✓		✓
CO4	✓	✓		✓	✓		✓	✓		✓

CH 640	Biocatalytic processes in Chemical Industries	L	T	P	C
		3	0	0	3

PRE-REQUISITE: NIL

COURSE LEARNING OBJECTIVES

To introduce the underlying concepts industrial microbiology in chemistry and food related industry. Understand different concepts of Fermentation related techniques applicable to 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 OUTCOME

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

CO1	Familiarize the basics industrial microbiology
CO2	Application of microbial techniques in chemical synthesis
CO3	Understanding biocatalysis
CO4	Understanding the applications of microbiology in chemistry

MAPPING OF COURSE OUTCOME WITH PROGRAMME OUTCOMES

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PO10**
CO1	✓	✓	✓		✓		✓	✓		✓
CO2	✓	✓	✓		✓		✓	✓		✓
CO3	✓	✓	✓		✓		✓	✓		✓
CO4	✓	✓			✓		✓	✓		✓