BODOLAND UNIVERSITY

MSc in Chemistry (*Two Year/One Year*) Syllabus under NEP 2020 (w. e. f. 2024–2025)

Approved in the 14th Academic Council Meeting held on 5th July, 2024



DEPARTMENT OF CHEMISTRY BODOLAND UNIVERSITY

Debargaon, Kokrajhar – 783 370 Assam, India

Important Guidelines

- a) There shall be a 2-year Postgraduate (PG) programme for those who have completed the 3-year Bachelor's programme.
- b) For students completing a 4-year Bachelor's programme with Honours/ Honours with Research, there shall a 1-year PG programme.
- c) There may be an integrated 5-year PG programme.
- d) Higher education qualifications leading to a degree/diploma/certificate shall be as described by the NHEQF (National Higher Education Qualifications Framework).
- e) PG framework should be in sync with National Credit Framework (NCrF) for the creditization of all learning and assignment, accumulation, storage, transfer & redemption of credit, subject to assessment. In accordance with the NHEQF, the levels for the PG/Master's programmes are given in the **Table 1**.

Table 1: Credit Distribution

Qualifications	Level	Credits
PG Diploma	6	40
1-Year PG after a 4-year UG	6.5	40
2-Year PG after a 3-year UG	6.5	80

- f) For 2-year PG: Students entering 2-year PG after a 3-year UG programme can choose to do
 - (i) only course work in the 3^{rd} and 4^{th} semester or (ii) course work in the 3^{rd} semester and research in the 4^{th} semester or (iii) only research in the 3^{rd} and 4^{th} semester.

Refer table 2.

 Table 2: Two-year PG Programme

Curricular Con	nponents	Minimum Credits (Two-year PG Programme)				
		Course	Coursework	Research	Total	
		Level		Thesis/	Credits	
				Project		
1 st Year		400	20		40	
(1st & 2nd Seme	(1 st & 2 nd Semester)		20			
Students who exit at the end of 1st year shall be awarded a Postgradu				aduate Diploma		
	Coursework		40		40	
2 nd Year	(or)	500				
(3 rd & 4 th	(3 rd & 4 th Coursework +		20	20	40	
Semester) Research						
	(or)					
	Research]		40	40	

(g) Students entering 1-year PG after a 4-year UG programme can choose to do (i) only coursework or (ii) course work and research or (iii) research. **Refer Table 3**.

Table 3: PG Programme (One Year) for 4-year UG (Hons. / Hons. with research)

Curricular Components		Minimum Credit {PG Programme (One Year) for 4-yr UG (Hons. / Hons. with research)}								
	Course Level									
Coursework		40		40						
Coursework + Research	500	20	20	40						
Research	1		40	40						

- (h) Programmes that are intended to sharpen the students' analytical abilities to optimally solve problems, the curriculum, in general, comprises advanced skills and real-world experience and less of a research component.
- (i) **400-499**: Advanced courses which would include lecture courses with practicum, seminar-based course, term papers, research methodology, advanced laboratory experiments/software training, research projects, hands-on-training, internship/apprenticeship projects at the undergraduate level or First year postgraduate theoretical and practical courses.
- (j) **500-599**: For students who have graduated with a 4-year bachelor's degree. It provides an opportunity for original study or investigation in the major or field of specialization, on an individual and more autonomous basis at the postgraduate level.

Course Structure of PG Programme (MSc) in Chemistry

2-Year PG Programme

SEMESTER I

Paper	Paper Name	Credi	L+T+P	Contact	Internal	Final	Total
Code		ts		Hours	Exam	Exam	Marks
CHMADL	Physical Chemistry-I	4	3+0+1	45+30	30	50+20	100
14014							
CHMADL	Organic Chemistry-I	4	3+0+1	45+30	30	50+20	100
14024							
CHMADL	Inorganic Chemistry-	4	3+0+1	45+30	30	50+20	100
14034	I						
CHMADL	Spectroscopy-I	4	3+1+0	60	30	70	100
14044							
CHMADL	Research	4	3+0+1	45+30	30	50+20	100
14054	Methodology						

SEMESTER II

Paper	Paper Name	Credits	L+T+P	Contact	Internal	Final	Total
Code				Hours	Exam	Exam	Marks
CHMADL	Nanomaterials	4	3+0+1	45+30	30	50+20	100
14064	and Green						
	Chemistry						
CHMSPL	Physical	4	3+0+1	45+30	30	50+20	100
15074	Chemistry-II						
CHMSPL	Organic	4	3+0+1	45+30	30	50+20	100
15084	Chemistry-II						
CHMSPL	Inorganic	4	3+0+1	45+30	30	50+20	100
15094	Chemistry-II						
CHMSPL	Spectroscopy-II	4	3+1+0	60	30	70	100
15104							

2-Year PG/1-Year PG Programme

• Students entering 2-year PG programme after a 3-year UG programme can choose to do

- (A) Only course work in the PG 3rd and 4th semesters (*Total Credits: 40*), or
- (B) Course work in the 3rd semester and research in 4th semester (*Total Credits: 40*), or
- (C) Only research both in the 3rd and 4th semester (*Total Credits: 40*).

• Students entering 1-year PG programme after a 4-year UG programme can choose to do

- (A) Only course work in the 1st and 2nd semesters (*Total Credits: 40*), or
- (B) Course work in the 1st semester and research in 2nd semester (*Total Credits: 40*), or
- (C) Only research both in the 1st and 2nd semester (*Total Credits: 40*).

<u>Option A</u> – Only course work in the 3^{rd} and 4^{th} semesters (2-Year PG)/Only course work in the 1^{st} and 2^{nd} semesters (1-Year PG) (*Total Credits: 40*)

SEMESTER III (2-Year PG)/SEMESTER I (1-Year PG)

Paper Code	Courses	Credits	L+T+P	Contact	Internal	Final	Total
				Hours	Exam	Exam	Marks
CHMSPL	Quantum	4	3+1+0	60	30	70	100
25014	Chemistry						
CHMSPL	Analytical	4	3+1+0	60	30	70	100
25024	Techniques in						
	Chemistry						
CHMSPL	Supramolecular	4	3+1+0	60	30	70	100
25034	Chemistry						
CHMSPL	Literature Survey	4	4	60	30	70	100
25044							
CHMSPL	Practical	4	0+0+4	120	30	70	100
25054							

SEMESTER IV (2-Year PG)/ SEMESTER II (1-Year PG)

Papers	Credits	L+T+P	Contact	Internal	Final	Total
			Hours	Exam	Exam	Marks
Paper 1	4	3+1+0	60	30	70	100
Paper 2	4	3+1+0	60	30	70	100
Paper 3	4	3+1+0	60	30	70	100
Paper 4	4	3+1+0	60	30	70	100
Paper 5	4	0+0+4	120	30	70	100

		Elective Papers
Paper 1	CHMSPL 25064	Reaction Dynamics and Statistical Thermodynamics
	CHMSPL 25074	Organic Synthesis and Heterocyclic Chemistry
	CHMSPL 25084	Inorganic Photochemistry
Paper 2	CHMSPL 25094	Polymer Science
	CHMSPL 25104	Natural Products Chemistry
	CHMSPL 25114	Bioinorganic Chemistry
Paper 3	CHMSPL 25124	Catalysis
	CHMSPL 25134	Medicinal and Bioorganic Chemistry
	CHMSPL 25144	Organometallic Chemistry
Paper 4	CHMSPL 25154	Computational Chemistry
	CHMSPL 25164	Advanced Topics in Organic Chemistry
	CHMSPL 25174	Group Theory and Application
Paper 5	CHMSPL 25184	Physical Chemistry Practical
	CHMSPL 25194	Organic Chemistry Practical
	CHMSPL 25204	Inorganic Chemistry Practical

Example for Code: CHMADL14014

CHM – Subject code (Chemistry) same as UG (NEP)

ADL – Advanced learning

- 1 Year
- 4-Level
- 01 Sequence of paper (Paper Number)
- 4-Credit
- SPL Special learning

<u>Option B</u> – Coursework + Research *i.e.* Course work in the 3^{rd} semester and Research in 4^{th} semester (2-Year PG) / Course work in the 1^{st} semester and research in 2^{nd} semester (1-Year PG) (*Total Credits: 40*)

SEMESTER III (2-Year PG)/ SEMESTER I (1-Year PG)

Paper	Courses	Credits	L+T+P	Contact	Internal	Final	Total
Code				Hours	Exam	Exam	Marks
CHMSPL	Quantum	4	3+1+0	60	30	70	100
25014	Chemistry						
CHMSPL	Analytical	4	3+1+0	60	30	70	100
25024	Techniques in						
	Chemistry						
CHMSPL	Supramolecular	4	3+1+0	60	30	70	100
25034	Chemistry						
CHMSPL	Literature Survey	4	4	60	30	70	100
25044							
CHMSPL	Practical	4	0+0+4	120	30	70	100
25054							

SEMESTER IV (2-Year PG) / SEMESTER II (1-Year PG) Dissertation (CHMDIS 250620)

• Research thesis/Project with minimum 1 conference paper. Peer reviewed research publication should be encouraged.

 $\underline{\mathit{Option}\ C}$ – Only Research i.e. only research both in the 3^{rd} and 4^{th} semesters (2-Year PG) / Only research both in the 1^{st} and 2^{nd} semesters (1-Year PG) ($\mathit{Total\ Credits:}\ 40$) Dissertation (CHMDIS 250140)

• Research thesis/Project with minimum 2 conference papers. Peer reviewed research publication should be encouraged.

SEMESTER I

Course Code: CHMADL 14014 Course Title: Physical Chemistry-I

Credits: 3+0+1

(Theory: 45 Hours, Practical: 30 Hours)

Total Marks: 100 (Theory: 50, Practical: 20, Internal Assessment: 30)

Course Objectives: The aim of this course is to teach students the important topics of physical chemistry viz. chemical thermodynamics and electrochemistry. Moreover, the students will acquire the knowledge of experimental thermodynamics and electrochemistry.

Course Outcomes: The students are expected to learn some advanced topics of chemical thermodynamics and its application. They will also learn about various aspects of dynamic electrochemistry and their applications. After attending this course, the students will be able to understand thermodynamics and electrochemistry. After studying the lab course of this paper, students will be able to know the practical aspects of thermochemistry and electrochemistry.

Unit 1. Chemical Thermodynamics

17 Lectures

Brief review of thermodynamic functions and laws of thermodynamics: Temperature dependence of thermodynamic functions; Experimental determination of thermodynamic functions; Thermodynamic description of mixtures, Gibbs-Duhem equation; Chemical equilibrium; Thermodynamic description of phase transitions, Clapeyron-Claussius equation, Phase diagrams; Thermodynamics of non-ideal systems— fugacity and activity concepts, excess properties.

Thermodynamics of real gases and gas mixtures, fugacity and its determination. Nonideal solutions, activity and activity coefficient- different scales of activity coefficients, electrolytic activity coefficients.

Thermodynamic criteria of phase equilibrium, Gibbs phase rule and its application to three-component systems- triangular plots- water-acetic acid chloroform and ammonium chloride-ammonium sulphate-water system.

Unit 2. Non-equilibrium Thermodynamics

14 Lectures

Difference between equilibrium and non-equilibrium thermodynamics, Criteria of nonequilibrium thermodynamics; uncompensated heat and its relation to other thermodynamic functions, Fluxes and forces- relation between these two quantities, Entropy production in heat transfer, mass transfer in flow of current, in mixing of gases, and in chemical reaction; phenomenological relation: Onsager relation, microscopic reversibility and Onsager reciprocity. Coupled reaction. Thermoelectric effects: Seebeck, Peltier and Thompson effect.

Unit 3. Dynamic Electrochemistry

14 Lectures

Ion-solvent interactions: The Born model-thermodynamic parameters of ion-solvent interactions -structural treatment; the ion-dipole model – its modifications, ion-quadrupole and ion-induced dipole interactions.

Primary solution – determination of hydration number, compressibility method and Viscosity mobility method.

Debye-Húckel theory of ion-ion interactions – derivation, validity and limitations; extended Debye-Húckel-Onsager equation.

The random walk model of ionic diffusion - Einstein-Smoluchowski relation. Electro catalysis-influence of various parameters.

Physical Chemistry-I LAB - CHMADL 14014

30 Hours

Unit 1. Thermochemistry

- (i) Determination of the heat capacity of a calorimeter and hence determination of the enthalpy of solution of NH₄Cl.
- (ii) Determination of heat of hydration of hydrated salt.
- (iii)Determination of integral heat of solution of a salt at two concentrations and hence the heat of dilution
- (iv)Determination of the integral heat of dilution of sulphuric acid.
- (v) Determination of heat of precipitation of BaSO₄.
- (vi)Determination of heat of transition.

Unit 2. Electrochemistry

- (i) Determine the equivalent conductivity of acetic acid at infinite dilution by Kohlrausch's method and hence find the degree of dissociation constant of the acid
- (ii) Compare the relative strength of acetic acid and monochloroacetic acid by conductance measurement.
- (iii)Determine the solubility and the solubility product of a sparingly soluble salt like PbSO₄ or PbI₂ at room temperature by conductance measurement.
- (iv)Determine the degree of hydrolysis and the hydrolysis constant of aniline hydrochloride/sodium acetate.
- (v) Determine the strength of the components of the following mixtures by conductometric titration.
 - (a) Hydrochloric acid and acetic acid.
 - (b) Sulphuric acid and copper sulphate.
 - (c) Hydrochloric acid and potassium chloride.

N.B.: New experiments will be introduced from time to time subject to the availability of chemicals and instrument.

SEMESTER I

Course Code: CHMADL 14024 Course Title: Organic Chemistry-I

Credits: 3+0+1

(Theory: 45 Hours, Practical: 30 Hours)

Total Marks: 100 (Theory: 50, Practical: 20, Internal Assessment: 30)

Course Objectives: The It is aimed to teach students the important concepts of stereochemistry, stereoselective reactions and reactivity and selectivity principles. Moreover, the students will be taught the organic photochemistry.

Course Outcomes: Students will be able to demonstrate/explain the unique features of stereochemistry, stereoselective reactions and reactivity and selectivity principles and will be able to solve related problems. After learning the course, students will acquire the detailed knowledge on organic photochemistry. After studying the lab course of this paper, students will be able to analyse and identify binary organic mixtures and will be able to estimate organic compounds.

Unit 1. Stereochemistry

20 Lectures

Chirality: Concept of chirality, symmetry elements, relative and absolute configuration and their stability.

Two or more chiral centres: Constitutionally unsymmetrical molecules: erythro-threo and syn-anti systems of nomenclature. Constitutionally symmetrical molecules with odd and even number of chiral centers: enantiomeric and meso forms, concept of stereogenic, chirotopic, and pseudoasymmetric centres. R-S nomenclature for chiral centres in acyclic and cyclic compounds.

Axial and planar chirality: Principles of axial and planar chirality. Stereochemical features and configurational descriptors (R, S) for the following classes of compounds: allenes, alkylidene cycloalkanes, spirans, biaryls (buttressing effect) (including BINOLs and BINAPs), ansa compounds, cyclophanes, trans-cyclooctenes.

Prochirality: Chiral and prochiralcentres; prochiral axis and prochiral plane. Homotopic, heterotopic (enantiotopic and diastereotopic) ligands and faces. Identification using substitution and symmetry criteria. Nomenclature of stereoheterotopic ligands and faces. Symbols for stereoheterotopic ligands in molecules with i) one or more prochiralcentres ii) a chiral as well as a prochiralcentre, iii) a prochiral axis iv) a prochiral plane v) propseudoasymmetric centre. Symbols for enantiotopic and diastereotopic face.

Unit 2. Reactivity & Selectivity principles

5 Lectures

Reactivity- selectivity principle— product selectivity, substrate selectivity, chemoselectivity, regioselectivity, stereoselectivity & stereospecificity in substitution, elimination and addition reactions; steric acceleration and steric retardation.

Unit 3. Stereoselective synthesis

8 Lectures

Classification of stereoselective synthesis— diastereoselective, enantioselective & double stereodifferentiating reactions; nucleophilic addition to aldehyde and acyclic ketones- Cram, Felkin and Felkin-Anh model; nucleophilic addition to cyclic ketones.

Asymmetric synthesis—use of chiral reagent, chiral catalyst and chiral auxiliary.

Unit 4. Organic Photochemistry

12 Lectures

General principles of photochemistry; excited state, and photosensitization, photochemical processes—chemiluminescence, Jablonski diagram, chemical and photochemical method of producing singlet oxygen, reactions of singlet oxygen- photooxidation, photostereomutation of cis-trans isomers.

Photochemistry of carbonyl compounds—representation of the excited states of ketones, Norrish type-I and Norrish type-II reactions. Photoreduction of saturated, arylalkyl and α,β -unsaturated ketones and p-benzoquinone; Paterno-Buchi reaction.

Organic Chemistry-I LAB – CHMADL 14024

30 Hours

A. Qualitative Organic Analysis

22 Hours

Binary mixtures of organic compounds, covering compounds with major functional groups, should be given with an objective to train students in qualitative separation by physicochemical methods and identifying the compounds by chemical analysis.

B. Organic Estimation

8 Hours

- I. Number of hydroxy groups in a disaccharide by acetylation.
- II. Percentage purity of carbonyl compounds by 2,4 dinitrophenylhydrazine.
- III. Carboxylic acid by Ag-salt method.
- IV. Glucose & sucrose in a mixture.

N.B.: New experiments will be introduced from time to time subject to the availability of chemicals and instrument.

SEMESTER I

Course Code: CHMADL 14034 Course Title: Inorganic Chemistry-I

Credits: 3+0+1

(Theory: 45 Hours, Practical: 30 Hours)

Total Marks: 100 (Theory: 50, Practical: 20, Internal Assessment: 30)

Course objectives: The aim of this course is to teach students the important topics of chemical bonding, group theory, structure of simple solids, and supramolecular chemistry.

Course outcome: Students will be able to develop a comprehensive understanding of chemical bonding principles, applying them to predict molecular structures and reactivity. Master symmetry concepts in group theory, analysing molecular properties and extending knowledge to the structure of crystalline solids. Gain proficiency in understanding crystal structures and diffraction techniques, correlating structural characteristics with solid properties. Students will get the idea of supramolecular chemistry for a wide range of applications. After studying the lab course of this paper, students will be able to prepare inorganic complexes.

Unit 1. Chemical bonding

17 Lectures

Chemical bonding of simple inorganic covalent compounds-molecular orbital treatments, hybridization; understanding molecular properties from bonding. Molecular orbital theory of homo-and hetero nuclear diatomics, molecular orbitals of Polyatomic molecules, molecular shape in terms of molecular orbitals- Walsh diagrams. Atomic and ionic radii-bond length and bond strength, vanderWaals forces. Hydrogen bonding interactions, effects of hydrogen bonding and other chemical Forces on melting and boiling points and solubility.

Unit 2. Group Theory

8 Lectures

Symmetry elements, symmetry operations, point groups and molecular symmetry, Mulliken's symbol, reducible and irreducible representations, character tables.

Unit 3. Structure of simple solids

12 Lectures

Packing of spheres-hexagonal and cubic close-packing, tetrahedral and octahedral Holes in close-packed structures-metals and alloys, solid solutions. The ionic model For the description of bonding in ionic solids. Characteristic structures of ionic solids -the NaCl and CsCl types, the sphalerite and wurtzite types of ZnS, the NiAs Structure type, Structures of compounds of the type: AB [zinc sulfide (ZnS), nickel arsenide (NiAs)], AB₂ [fluorite (CaF₂), antifluorite (Na₂O), rutile (TiO₂) and layer structures viz., cadmium chloride (CdCl₂) and cadmium iodide, (CdI₂)], the perovskite and spinel structure types of mixed-metal oxides. Importance of ionic radii and the radius ratios in determining structure type among ionic solids. Lattice energy considerations, thermal stability and solubility-of inorganic solids.

Unit 4. Supramolecular Chemistry

8 Lectures

Introduction to supramolecular chemistry, concepts of host guest chemistry, classification, thermodynamics and kinetic stability, non-covalent interactions, molecular recognition, recognition of anionic substrates, Molecular receptors for different types of molecules: Crown ethers, cryptands, cyclodextrins, Calixarenes.

Inorganic Chemistry-I LAB - CHMADL 14034

30 Hours

Preparation and characterization

Preparation of selected inorganic compounds and their physicochemical characterization by elemental analysis, IR and electronic spectrophotometry, magnetic susceptibility measurements, magnetic resonance spectroscopy, solution conductivity measurements, wherever appropriate and possible.

- (i) Complexes with O-donor ligands
 - (a) $A_3M(C_2O_4)_3 M = Al$, Cr, Fe; A = alkali metal
 - (b) VO(acac)₂
 - (c) $Cu_2(OAc)_4(H_2O)_2$
 - (d) Cu(acac)₂
- (ii) Complexes with N donor ligands
 - (a) [Co(NH₃)₅Cl]Cl₂, [Co(NH₃)₅(ONO)]Cl₂, [Co(NH₃)₅(NO₂)]Cl₂
 - (b) $Hg[Co(NCS)_4]$
 - (c) Ni(dmg)₂
 - (d) $NH_4[Cr(NH_3)_2(SCN)_4]$

N.B.: New experiments will be introduced from time to time subject to the availability of chemicals and instrument.

SEMESTER I

Course Code: CHMADL 14044 Course Title: Spectroscopy-I Credits: 3+1+0

(Theory: 45 Hours, Tutorials: 15 Hours)

Total Marks: 100 (Theory: 70, Internal Assessment: 30)

Course Objectives: The aim of this course is to teach students the important concepts and ideas of rotational, vibrational-rotational, IR, NMR, optical and electronic spectroscopy.

Course Outcome: On completion of the course, students will be able to understand and identify/elucidate the basis of different spectroscopic techniques, and demonstrate their various applications in analyzing and interpreting experimental data.

Unit 1. Rotational (microwave) spectroscopy

10 Lectures

- (a) Classification of molecules according to their moments of inertia, rotational energy levels of HCl. Determination of molecular geometry by isotopic substitution effects on pure rotational spectrum. Stark effect, estimation of molecular dipole moments. Spectra of symmetric top and asymmetric top type molecules.
- (b) Rotational Raman spectra anisotropic polarizability. Specific selection rule in Raman spectroscopy. Interpretation of IR and Raman spectra of simple inorganic and organic compounds.

Unit 2. Vibrational-rotational spectroscopy

15 Lecture

- (a) Diatomic molecules force constants. Fundamental vibration frequencies. The anharmonicity of molecular vibrations and its effect on vibrational frequencies, second and high harmonics.
- (b) Vibration-rotation spectrum of HCI P, Q and R branches. Vibrational Raman spectra of diatomic molecules, Overtone and combination bands (H₂O, CO₂).
- (c) Polyatomic molecules (*e.g.* CO₂, NH₃) normal modes vibrations, symmetry of vibrations group theoretical treatment. Elements of normal coordinate analysis for the CO₂ molecule.

Unit 3. IR spectroscopy

8 Lectures

IR spectroscopy – Characteristic bands for different functional groups, change in band frequency due to FGI. Effects of hydrogen bonding on band frequency. Structure elucidation by IR spectroscopy – finger print region and group frequencies – effect of hydrogen bonding (alcohol, keto-enol) and coordination to metal. Problem solving.

Unit 4. NMR spectroscopy

15 Lectures

Chemical shifts and splitting patterns of signals, coupling constant and its distinction from chemical shift - use of coupling constant in structural elucidation. Simplification of spectra by use of shift reagents and high magnetic fields, integration and its use in proton count and molecular ratios - determination of enantiomeric excess. Deuterium exchange technique in the determination of labile hydrogen, spin-decoupling and NOE, ¹³C NMR (DEPT), Complexity of ¹³C NMR spectra and use of spin decoupling in its simplification, CINDP and its applications. Worked out examples using application of NMR. Introduction to Magnetic Resonance Imaging (MRI).

Unit 5. Optical and electronic spectroscopy

12 Lectures

Chiroptical properties: Introduction to CD (Circular Dichroism), ORD (Optical Rotatory Dispersion) and CPE. Applications of CD and ORD - octant rule.

Study of metal-ligand equilibria and Job's method, CD, ORD and MCD of inorganic compounds.

Fluorescence and phosphorescence, Jablonski diagram. Electronic spectra of conjugated, aromatic and coordination compounds - d-d and charge-transfer spectra. Change of molecular shape upon electronic excitation.

UV-visible spectroscopy: λ_{max} and molar absorptivity, factors affecting them. Calculation of λ_{max} - Woodward Fieser's rules.

Photoelectron spectroscopy: Basic principles and applications of PES $(O_2, N_2 \text{ and } N_3^-)$ only, chemical information from ESCA.

SEMESTER I

Course Code: CHMADL 14054 Course Title: Research Methodology Credits: 3+0+1

(Theory: 45 Hours, Practical: 30 Hours)

Total Marks: 100 (Theory: 50, Practical: 20, Internal Assessment: 30)

Course Objectives: This course is introduced to impart knowledge about the basic concepts of research and to provide a road map for conducting research.

Learning Outcomes: After completing this course, students are expected to identify, explain and apply basic concepts of research; acquire information, recognize various issues related to research, lab safety and software/computer-based applications for research.

Unit 1. Research methodology

15 Lectures

Definitions, Purpose of Research, Types of research, Research approaches, Research Methods, Stages of the research process, Background reading & information gathering: Literature survey (different sources of literature survey including online databases), Hypothesis: Identification of Research Problem; Ethical issues in research, Data collection, Data recording and reproducibility, Importance of documentation.

Unit 2. Research ethics and Publication

7 Lectures

Presentation of research findings: Elements of research publications; Seminar presentation; Patent; Paper writing; Journal impact factor, h-index; review process.

Unit 3. Laboratory safety

8 Lectures

General health and safety concerns; What to do after splash/cut, Chemical hazards, commonly used hazardous laboratory chemicals (azide, perchlorate, nBuLi, acid chlorides, bromine, cyanide, mercury, etc), Personal protective equipment, Environmental safety issues: Fume hood safety, Safety data sheet, Waste handling, Disposal of chemical and plastic-waste; precautionary measure for the maintenance of laboratory equipment.

Unit 4. Statistical Methods and Computer Applications in Chemistry 15 Lectures

Errors, precision and accuracy; Average Mean Deviation, Standard Deviation, Variance, f-test, t-test, Chi-square Test. Applications of Curve Fitting, Straight Line Fitting, Interpolation

in solving chemical problems. Applications of commonly used Computer Softwares, such as Chemdraw, Chemoffice, Mercury, Origin, Excel, X'Pert HighScore, ImageJ, etc.

Research Methodology LAB – CHMADL 14054

30 Hours

- 1. Use of Chemdraw for drawing chemical structure, Reaction and Reaction Scheme.
- 2. Use of Origin software, Preparation of tables, figures, flowchart, and PowerPoint presentation.
- 3. Application of f-test, t-test, Chi-square Test in data analysis.
- 4. Applications of Curve Fitting, Straight Line Fitting, Interpolation in solving chemical problems.

SEMESTER II

Course Code: CHMADL 14064

Course Title: Nanomaterials and Green Chemistry

Credits: 3+0+1

(Theory: 45 Hours, Practical: 30 Hours)

Total Marks: 100 (Theory: 50, Practical: 20, Internal Assessment: 30)

Course Objectives: Students will be introduced to the nanochemistry and green chemistry.

Course outcome: Students will be able to understand the nanochemistry and its various properties and applications. Moreover, students will be able to explain and compare relationships between Green Chemistry and chemical laboratory and industry for the design of safer processes and chemicals. After studying the lab course of this paper, students will be able to prepare nanomaterials/nanocomposites using different methods, and also will be able to apply green methods for the preparation/synthesis of materials and compounds.

Unit 1. Nanochemistry

25 Lectures

Introduction to Nanoscience and Nanotechnology, influence of nano over micro/macro. 1D, 2D and 3D nanostructured materials, Quantum Dots shell structures, mechanical- physical-chemical properties, Quantum confinement effect and Surface plasmon resonance. Synthesis and modification of nanoparticles: Top-Down and Bottom-Up approach, experimental procedure (coprecipitation, Sol-gel, Hydrothermal, colloidal etc.), Properties of precipitates and precipitating reagents: Colloidal and Crystalline Precipitates, nucleation (homogeneous and heterogeneous), crystal growth, morphology dependence properties. Introduction to surface active agents, types of surfactants. Basic characterizations for structural purity and

morphology study. Applications of metal oxide and semiconductor nanoparticles in catalysis (photocatalysis, electrocatalysis etc.) and energy.

Carbon nanoclusters and nanotubes, application of CNT in fuel cell, catalysis, computer and as chemical sensors. Polymeric nanofibers, supramolecular structures; nanoparticles organized in/on polymer surfaces. Quantum wells, wires and dots. Fullerenes in nanochemistry.

Application of nanomaterials in green reactions and green energy production.

Unit 2. Green Chemistry

20 Lectures

Evolution of Green Chemistry—the background, Tools of green chemistry, Principles of green chemistry. Concept of Atom Economy. Green starting materials, Green reagents, Green solvents (Water, Ionic liquid, Polyethylene glycol, Super Critical Fluids etc.), Green reaction conditions and Green chemical products; solvent free reactions; microwave assisted reactions, sonication.

Waste: production, problems and prevention.

Green chemistry in Catalysis, Health and Environment.

Water oxidation; Conversion of CO₂, Utilising CO₂ as reactant.

Feedstock chemicals, Chemicals from Biomass, Concept of platform molecules. Conversion of biomass to value-added products.

Real World Solutions: Designing for Materials and Energy Efficiency; Designing for Degradation.

Introduction to Sustainability; Aspects of Sustainability Ethics; Designing Sustainable Solutions.

Challenges of Green Chemistry.

Nanomaterials and Green Chemistry LAB – CHMADL 14064

30 Hours

- 1. Synthesis of nanoparticles/nanocomposites by coprecipitation, Sol-gel, Hydrothermal, and colloidal methods and their characterization.
- 2. Green synthesis of metal oxide nanoparticles and their characterization.
- 3. Synthesis of organic compounds by solvent free method, ionic liquid medium and microwave assisted synthesis.
- 4. Mechanochemical method for Hantzsch Pyridine synthesis, Begeneli reaction, Schiff Base reaction, etc.

N.B.: New experiments will be introduced from time to time subject to the availability of chemicals and instrument.

SEMESTER II

Course Code: CHMSPL 15074 Course Title: Physical Chemistry-II

Credits: 3+0+1

(Theory: 45 Hours, Practical: 30 Hours)

Total Marks: 100 (Theory: 50, Practical: 20, Internal Assessment: 30)

Course Objectives: The aim of this course is to teach students the important topics of physical chemistry viz. adsorption & surface chemistry and solid-state chemistry. Moreover, the students will acquire the knowledge of and solid-state reactions as well.

Course Outcomes: The students are expected to learn some advanced topics of adsorption & surface chemistry and solid-state chemistry. After attending this course, the students will be able to learn about adsorption isotherms and defects in solids. They will also learn about various techniques for characterization of solid substances. After studying the lab course of this paper, students will be able to know the practical aspects of adsorption and solid-state chemistry.

Unit 1. Adsorption and Surface Chemistry

15 Lectures

Adsorption of gases on solid surfaces - Langmuir's theory and its limitations. Derivation of BET equation - determination of surface area of an adsorbent, thermodynamics of adsorption processes. Capillary condensation - adsorption in micropores, hysteresis loop. Kinetics of heterogeneous catalysis - Langmuir-Hinshelwood model and Riedel-Eley model. Electrical aspects of surface chemistry, Electro kinetic phenomena, the structure of electrical double layer, Zeta potential and colloidal stability, Measurement of zeta potential. Surfactants – definition and classification, micelle formation and determination of critical micelle concentration. Reverse micelle and its application, solubilization, microemulsion.

Unit 2. Solid State Reactions

15 Lectures

Preparative Methods: Vapour phase transport, preparation of thin films – electrochemical methods, chemical vapour deposition; Crystal growth - Bridgman & Stokbarger methods, zone melting.

Characterization of Solids: Crystal diffraction of X-rays, X-ray diffraction method; Powder method– principles and uses; Scattering of X-rays by crystals – systematic absences; Electron diffraction; Neutron diffraction.

Unit 3. Powder Compact Reactions and Solid-State Defects15 Lectures

Diffusion Model: Parabolic rate law, Jander's rate equation, Kroger-Zeigler equation, Ginstling- Brounshtein rate equation.

Stoichiometric Defects: Equilibrium concentration of point defects in crystals - Schottky defects, Frenkel defects; The photographic process - light sensitive crystals, mechanism of latent image formation, lithium iodide battery.

Non-Stoichiometric Defects: Origin of non-stoichiometry, consequences of non-stoichiometry; Equilibria in non-stoichiometric solids, Color centers: F-centre, electron and hole centre; colour centre and information storage.

Physical Chemistry-II LAB – CHMSPL 15074

30 Hours

Unit 1. Adsorption and Surface Chemistry

- (i) Investigation of the adsorption of oxalic acid from aqueous solution by activated charcoal, examine the validity of Freundlich and Langmuir isotherm, determination of Q_{max} value.
- (ii) Removal of trace metals from aqueous medium using adsorption phenomena.
- (iii)Study of adsorption of iodine from alcoholic solution by charcoal.

Unit 2. Solid State

- (i) Determination of dipole moment of a liquid such as chlorobenzene, chloroform, nitrobenzene etc.
- (ii) Determination of magnetic susceptibility of Mohr's salt at room temperature and hence the magnetic moment.
- (iii) Analysis of a solid sample for determination of interplanar spacing by PXRD studies.

N.B.: New experiments will be introduced from time to time subject to the availability of chemicals and instrument.

SEMESTER II

Course Code: CHMSPL 15084
Course Title: Organic Chemistry–II
Credits: 3+0+1

(Theory: 45 Hours, Practical: 30 Hours)

Total Marks: 100 (Theory: 50, Practical: 20, Internal Assessment: 30)

Course Objectives: The aim of this course is to teach students the important topics of oxidation, reduction, and pericyclic reactions and will be introduced about retrosynthetic analysis.

Course outcome: After learning the course, students will acquire the detailed knowledge on oxidation, reduction reactions, and pericyclic reactions. Students will be able to understand the important concepts of retrosynthesis of organic compounds. After studying the lab course of this paper, students will be able to know the practical aspects of organic preparation,

chromatographic techniques for analytical purpose and will be able to know the extraction and isolation techniques of natural products.

Unit 1. Oxidation reactions

10 Lectures

Allylic oxidation of alkenes— use of chromium trioxide-pyridine complex (Collin's reagent) and selenium dioxide.

Oxidation of alcohols— use of PCC, PDC, Swern oxidation, Mn (IV) oxide, silver carbonate, tetrapropylammonium perruthenate (VII). Oxidation of 1,2-diols - use of periodic acid and Pb-tetraacetate.

Oxidation of carbon-carbon double bonds— perhydroxylation by KMnO₄, OsO₄ (including Sharpless dihydroxylation & epoxidation), oxidation with iodine, silver carboxylate and peroxy acids; introduction to electrooxidation— oxidation of tertiary amines, alkenes and carboxylates.

Unit 2. Reduction reactions

8 Lectures

Use of H₂/Pd-C, LAH, NaBH₄, NaCNBH₃, 9-BBN, Lindlar's catalyst, DIBAL, diimide, alkali metals in liquid ammonia, super hydride and selectrides; chiral reducing agents; Electroreduction- reduction of carbonyl compounds, alkyl halides and nitro compounds.

Unit 3. Pericyclic reactions

15 Lectures

Introduction of pericyclic reactions, MO symmetry; FMO of conjugated polyenes. Woodward- Hoffmann principle of conservation of orbital symmetry, allowed and forbidden reactions, stereochemistry of pericyclic reactions. Cycloaddition reactions |2+2|, |4+2|, |6+2| cycloadditions, stereoselectivity of the reactions. Sigmatropic rearrangements of hydrogen and chiral alkyl group - fluxional molecules, stereoselectivity in Cope and Claisen rearrangements.

1, 3 - dipolar cycloadditions—stereochemistry of the reactions. Electrocyclic reactions and cyclo reversions—stereochemistry of the reactions.

Cheletropic reactions—linear and nonlinear cheletropic rearrangement; theories of cheletropic reactions, stereochemistry of the reactions.

The ene reactions—ene reactions of 1,7—dienes, carbonyl enophiles, retro-ene reaction.

Unit 4. Retrosynthetic analysis

12 Lectures

Basic principles and terminology of retrosynthesis, linear, convergent and divergent synthesis, synthesis, synthesis of aromatic compounds, one group and two group C-X disconnections, One group C-C and two group C-C disconnections, amine and alkene synthesis, important strategies of retrosynthesis, functional group transposition, important functional group interconversions, Umpolung of reactivity.

Protection and deprotection of hydroxy, carboxyl, carbonyl, carboxy amino groups and carbon-carbon multiple bonds; chemo- and regioselective protection and deprotection Illustration of protection and deprotection in peptide and carbohydrate synthesis.

30 Hours

A. Organic Preparation

10 Hours

One-step preparation and analysis with spectroscopic techniques.

- I. Benzyhdrol from benzophenone by reduction in alkaline medium.
- II. Anthraquinone from anthrancene by oxidation with chromium trioxide.
- III. Preparation of *m*-nitro aniline from *m*-dinitro benzene.
- IV. Preparation of methyl orange from aniline.
- V. Preparation of bakelite from phenol.

B. Chromatographic Application

10 Hours

- I. Separation and identification of aromatic nitro compounds present in a binary mixture by TLC.
- II. Separation and identification of amino acids present in a ternary mixture by paper chromatography.

C. Experiments on Natural Products

10 Hours

- I. Soxhlet extraction of carotenoids/chlorophyll from carrot/tomato/papaya/spinach and determination of R_f values by TLC.
- II. Isolation of nicotine from tobacco.
- III. Extraction of milk proteins.
- IV. Extraction of essential oils from orange peels/rose petals/clove/ginger.

N.B.: New experiments will be introduced from time to time subject to the availability of chemicals and instrument.

SEMESTER II

Course Code: CHMSPL 15094
Course Title: Inorganic Chemistry-II

Credits: 3+0+1

(Theory: 45 Hours, Practical: 30 Hours)

Total Marks: 100 (Theory: 50, Practical: 20, Internal Assessment: 30)

Course Objectives: Students will be taught about the principles of coordination chemistry, structures and bonding in coordination compounds, synthesis and reactivity of organometallic complexes, and redox chemistry of coordination compounds.

Course Outcomes: Students will be able to demonstrate/explain the unique features of Coordination chemistry, Complexes of π -acceptor ligands and organometallic chemistry,

Reactivity of complexes, Redox chemistry and will be able to solve related problems. By the end of the lab course, students will be able to perform qualitative and quantitative analysis of inorganic compounds confidently. They will be able to demonstrate proficiency in qualitative analysis, accurately identifying unknown ions or functional groups based on characteristic reactions and instrumental techniques.

Unit 1. Coordination Chemistry

15 Lectures

General properties of transition elements, coordination compounds - types of ligands and complexes. Mononuclear complexes - commonly observed coordination geometries and their symmetry properties. Tetragonal, rhombic and trigonal distortions in octahedral complexes. Crystal field theory of bonding in octahedral, tetrahedral and square planar transition metal complexes. Factors affecting crystal field splitting, crystal field stabilization energy, spectrochemical series. Qualitative aspect of Ligand field and MO Theory (for octahedral σ -donor, π - acceptor and π - donor complexes)- electronic spectra— d-d spectra interpretation of spectral behaviour of octahedral and tetrahedral complexes. Charge transfer spectra.

Unit 2. Complexes of π -acceptor ligands and organometallic chemistry 15 Lectures

Synthesis, structure, bonding, and reactivity of transition-metal complexes of π -accepting ligands such as CO, NO, PPh₃. Metal carbonyl hydrides and metal carbonyl clusters. Metalmetal bonding in Re₂Cl₈^{2-.} Complexes containing alkenes and alkynes as ligands- Ferrocene-synthesis, structure, bonding and reactivity, Zeise's salt and comparison of synergic effect with that in carbonyls

Unit 3. Reactivity of complexes

8 Lectures

Stability constants, the chelate effect, labile and inert complexes, mechanism of Substitution reactions in octahedral complexes and associated stereochemical changes, isomerization and racemization of tris-chelate complexes. The trans effect. Electron transfer reactions-outer and inner sphere mechanism.

Unit 4. Redox Chemistry

7 Lectures

Standard electrode potentials, pH dependence of electrode potentials. Redox stability of metal ions in water, oxidation by atmospheric oxygen. Applications of Latimer and Frost diagrams, redox behavior of non-transition elements based on electrode Potential data.

Inorganic Chemistry- II LAB – CHMSPL 15094

30 Hours

Qualitative and Quantitative Analysis

- (a) Separation and determination of two metal ions Cu-Ni, Ni-Zn, Cu-Fe, Mn-Fe *etc.* involving volumetric and gravimetric methods.
- (b) Analysis of ores/alloys, cement and steel, etc.Ores: Hematite, Limestone, Dolomite, Cement, Pyrolusite, and other ores.

Alloys: Brass, Gunmetal, cupronickel, Solder, Bronze, Phosphor Bronze, Steel, Copper concentrate, steel nickel alloy and other alloys.

- (c) Determination of hardness of water.
- (d) Determination of stability constant of $[Zn(NH_3)_4]^{2+}$ and $[Ag (en)]^+$ by Potentiometry.

N.B.: New experiments will be introduced from time to time subject to the availability of chemicals and instrument.

SEMESTER II

Course Code: CHMSPL 15104 Course Title: Spectroscopy–II Credits: 3+1+0

(Theory: 45 Hours, Tutorials: 15 Hours)

Total Marks: 100 (Theory: 70, Internal Assessment: 30)

Course Objectives: Students will be taught about spectroscopic techniques for the purpose of identification of various compounds.

Course Outcomes: Students will be able to understand and apply Mass, NMR including 2-D techniques, ESR, and Mössbauer spectroscopic techniques analytical purposes, interpretation of data, and finally identification of organic and inorganic compounds.

Unit 1. Mass spectrometry

10 Lectures

Mass spectrometry: ionization techniques, isotope abundance, molecular ion, fragmentation processes of different organic molecules, McLafferty rearrangement, deduction of structure through mass spectral fragmentation. Applications of ESI-MS and MALDI-MS. Problem solving.

Unit 2. ESR and Mössbauer spectroscopy

12 Lectures

ESR spectroscopy: Basic principles, factors effecting g-tensors, Dragos rule and Kramers degeneracy, hyperfine splitting in inorganic free radicals and metal complexes, zero field splitting. Applications of ESR to d¹ and d⁹ complexes of various symmetry.

Mössbauer: Basic principles, isomer shift, quadruple splitting, and effect of magnetic field. Application to the study of high-spin and low-spin iron compounds and Sn compounds in various oxidation states and coordination geometries.

Unit 3. NMR spectroscopy

16 Lectures

NMR spectroscopy: Simple application to diamagnetic inorganic compounds, NMR paramagnetic shifts, simple application to paramagnetic compounds. NMR of ¹¹B, ³¹Pand ¹⁹F in inorganic compounds.

2D–NMR. Assignment of ¹H and ¹³C chemical shifts by using 2D COSY, HSQC and HMBC spectra for simple organic molecules and natural products.

Unit 4. Characterization of inorganic molecules

10 Lectures

Applications of IR, Raman, NMR, EPR, Mössbauer, UV-visible, NQR, MS, electron spectroscopy and microscopy in the determination of structure and physical properties of inorganic compounds.

Unit 5. Structure elucidation using various spectroscopic techniques 12 Lectures

Determination of chemical structure of organic compounds by analysing UV-Vis, IR, NMR and Mass Spectrometry data.

SEMESTER III (2-Year PG) / SEMESTER I (1-Year PG)

Course Code: CHMSPL 25014
Course Title: Quantum Chemistry

Credits: 3+1+0

(Theory: 45 Hours, Tutorials: 15 Hours)

Total Marks: 100 (Theory: 70, Internal Assessment: 30)

Course Objectives: The aim of this course is to teach students about quantum mechanics and quantum chemistry. Moreover, the students will acquire the knowledge of applications of quantum mechanics in chemistry.

Course Outcomes: The students are expected to learn different approximation techniques and theories used in quantum mechanics. After attending this course, the students will be able to understand the applications of quantum mechanics in chemistry with respect to chemical bonding. They will also learn about Ab initio calculations and self-consistent field theory.

Unit 1. Basic Principles of Quantum Mechanics

16 Lectures

Wave functions of one-particle and many-particle systems: Born interpretation. Well behaved functions and normalized functions. Schwartz inequality (without derivation). Dynamical variables and quantum mechanical operators- Hermitian operators and their properties.

Eigenvalues and eigenfunctions of quantum mechanical operators, their physical significance.

Schrodinger's wave equation. Orthogonal functions - Schmidt's orthogonalization technique. Expectation values of observable properties. Compatible observables and compatibility theorem.

Incompatible observables and the (generalized) uncertainty principle from Schwartz inequality. Basic ideas about the theory of angular momenta— spin and orbital angular momenta, conservation of angular momenta. General angular momentum operators Jx, Jy, Jz, step-up and step-down operators. Eigenvalues of J₂ and Jz operators. Coupling of orbital and spin angular momenta-theoretical basis of the L-S and j-j coupling schemes.

Unit 2. Approximate Methods of Quantum Mechanics 10 Lectures

Time-independent first-order perturbation theory for (i) non-degenerate and (ii) degenerate systems; applications to the ground and first -excited states of the helium atom. The Variation theorem, linear variation function - Secular equation.

Unit 3. General Theorems in Molecular Quantum Mechanics 10 Lectures

Born-Oppenheimer approximation, separation of electronic and nuclear motion. Hellmann-Feynmann theorem and its chemical applications. The electrostatic theorem and the force field concept in chemistry. Introduction to the molecular electronic Virial theorem. Elementary ideas about Density Functional Theory.

Unit 4. Chemical Bonding

12 Lectures

Term symbols for molecular electronic states, their symmetry classification- ligand field terms. Correlation diagrams and the non-crossing rule.

LCAO-MO theory of simple polyatomic molecules (e.g. BeH₂, H₂O molecule).

Electron theory- Huckel molecular orbital (HMO) method for unsaturated carbon compounds showing chain and ring structures, introduction to extended Huckel theory. HMO treatment of infinite linear polyenes, elements of band theory.

Unit 5. Ab initio and Semi-empirical SCF Theories

12 Lectures

The self-consistent field method, Hartree-Fock theory of closed shell electronic configurations of atoms and molecules. Coulomb and exchange integrals, canonical Hartree-Fock equations, Koopman's theorem (without derivation).

SCF LCAO-MO theory of molecules - Roothan equation.

Semi-empirical SCF theory: Parriser–Parr-Pople approximation.

SEMESTER III (2-Year PG) / SEMESTER I (1-Year PG)

Paper Code: CHMSPL 25024

Paper Title: Analytical Techniques in Chemistry

Credits: 3+1+0

(Theory: 45 Hours, Tutorials: 15 Hours)

Total Marks: 100 (Theory: 70, Internal Assessment: 30)

Course Objectives: Students will be taught about various analytical techniques in chemistry for the purpose of identification of various compounds/materials.

Course Outcomes: Students will be able to understand and apply various analytical and instrumental techniques in chemistry for analytical purposes, interpretation of data, and finally identification of organic/inorganic materials.

Unit 1. Chromatographic methods

18 Lectures

Adsorption, liquid-liquid partition, ion—exchange, paper and thin-layer chromatography (TLC), effect of solvent polarity on retention factor, reagents commonly used in the detection of TLC spots, HPLC, HPTLC, gel permeation chromatography, gas chromatography, flash chromatography, GC-MS and LC-MS.

Unit 2. Electrochemical, Thermal and X-ray diffraction methods 20 Lectures

Electrochemical methods: Coulometry, Polarography, anode-stripping voltammetry, pulse techniques, cyclic voltammetry, electrogravimetry, spectroelectrochemistry.

Thermal methods: TGA, DTA, DTG, DSC: Techniques, Instrumentation, Applications *X-ray methods*: Techniques, Instrumentations, and Applications of Powder XRD and Single Crystal XRD.

Unit 3. Microscopy 14 Lectures

Development of Microscopy, Optical microscopy, Reflectance, Transmittance, Fluorescence Microscopy, CLSM, Ultra-high-resolution microscopy.

Electron Microscopy: Scanning Electron Microscopy (SEM, FESEM) and Transmission Electron Microscopy (TEM, HRTEM): Technique, instrumentation, and applications, EDX, SAED.

Scanning Probe Microscopy (SPM): Atomic Force Microscopy (AFM), STM: Techniques, instrumentation and applications.

Unit 4. Analysis of Metals

8 Lectures

Preparation of sample for trace metal analysis in water, air, soil and plants, extraction and dissolution techniques, microwave digestion, atomic absorption spectroscopy, inductively coupled plasma- mass spectroscopy (ICP-MS), Atomic Emission Spectroscopy (ICP-AES), Optical Emission Spectroscopy (ICP-OES).

SEMESTER III (2-Year PG) / SEMESTER I (1-Year PG)

Paper Code: CHMSPL 25034

Paper Title: Supramolecular Chemistry

Credits: 3+1+0

(Theory: 45 Hours, Tutorials: 15 Hours)

Total Marks: 100 (Theory: 70, Internal Assessment: 30)

Course Objectives: Students will be taught about the concepts of supramolecular chemistry. *Course outcome*: The students will acquire the detailed knowledge and will be able to demonstrate principles, structures, properties and applications of supramolecular chemistry.

Unit 1. Supramolecular Chemistry–I

25 Lectures

Introduction to supramolecular chemistry, concepts of host guest chemistry, classification, thermodynamics and kinetic stability.

Properties of covalent bonds - bond length, inter-bond angles, force constant, bond and molecular dipole moments. Molecular and bond polarizability, bond dissociation enthalpy, entropy, intermolecular forces, hydrophobic effects. Electrostatic, induction, dispersion and resonance energy. Magnetic interactions, magnitude of interaction energy, forces between macroscopic bodies, medium effects. Hydrogen bond, non-covalent interactions, molecular recognition, recognition of anionic substrates.

Principles of molecular association and organization as exemplified in biological macromolecules like enzymes, nucleic acids, membranes and model systems like micelles and vesicles. Molecular receptors and design principles. Crown ethers, Cryptands, cyclophanes, calixeranes, cyclodextrins (CD). CD mediated reactions.

Unit 2. Supramolecular Chemistry-II

15 Lectures

- (a) Molecular recognition: Molecular receptors for different types of molecules including arisonic substrates, design and synthesis of coreceptor molecules and multiple recognition.
- (b) Supramolecular reactivity and catalysis.
- (c) Transport processes and carrier design.
- (d) Supramolecular devices. Supramolecular photochemistry, supramolecular electronic, ionic and switching devices.

Unit 3. Dendrimers 20 Lectures

- (a) Introduction, synthesis and characterization of macromolecular materials, including linear, branched, dedrimetric and star polymers.
- (b) Synthetic strategies and structural variations. Mechanical and physiochemical properties of polymer types, Kinetics of living polymerization; applications to nanostructures, templates and advanced devices.
- (c) Host-guest assembly and supramolecular assembly.
- (d) Competitive binding of guest molecules on the surface or in the interior of dendrimers.

(e) Supramolecular structure of dendrimer/surfactant aggregates. Biomedical applications, biosensing, photodynamic theory, dendrimer-based MRI contrasts.

SEMESTER III (2-Year PG) / SEMESTER I (1-Year PG)

Paper Code: CHMSPL 25044
Paper Title: Literature Survey
Credits: 4

Total Marks: 100

{Report (40) + Presentation (10) + Viva voce (20) + Internal Assessment (30)}

Course objective: Students will be introduced to the concepts of literature review on published works.

Learning outcome: Students will be able to understand how to perform literature review on published works and will be able to find out the research gap on a particular area including synopsis writing and solve related issues.

LITERATURE SURVEY OF PUBLISHED RESEARCH IN THE RELEVANT FIELD

Each student will carry out literature survey on an assigned topic under the supervision of a faculty member and shall submit three hardbound copies of a report of **Literature Survey** separately based on published works in one of the following broad fields based on at least 50 relevant up-to-date references for evaluation.

- 1. Inorganic Chemistry
- 2. Organic Chemistry
- 3. Physical Chemistry
- 4. Analytical Chemistry

SEMESTER III (2-Year PG) / SEMESTER I (1-Year PG)

Course Code: CHMSPL 25054

Course Title: Practical Credits: 0+0+4 (Practical: 120 Hours)

Total Marks: 100 (Practical: 70, Internal Assessment: 30)

Course outcomes: By the end of this lab course, students will be able to demonstrate advanced proficiency in synthesis/preparation and characterization organic/inorganic compounds using a variety of analytical techniques. They will be able to apply theoretical knowledge to design experiments, interpret data accurately, and communicate findings effectively. Additionally, students will develop critical thinking skills, adhere to safety protocols, and collaborate effectively with peers, preparing them for successful careers in the field of chemistry.

Unit 1. Organic Chemistry Lab

40 Hours

Two-step preparation, purification using chromatography and analysis with spectroscopic techniques

- I. Benzanilide from benzophenone.
- II. Benzilic acid from benzoin.
- III. Dibenzyl from benzoin.
- IV. Anthranilic acid from phthalic anhydride.

Unit 2. Inorganic Chemistry Lab

40 Hours

- (a) Determine the composition of Fe(III) salicylic acid complex solutions by Job's Method.
- (b) Bioinorganic chemistry- Separate pigments, viz., chlorophyll 'a' and 'b', carotene and xanthophylls from green leaves by paper chromatography and column chromatography
- (c) Analysis of talcum powder for Mg by complexometric titration
- (d) Paper Chromatography: Separation of Group II and III metal ions (Cu²⁺& Fe³⁺) by 1(N) K₄[Fe(CN)₆] solution
- (e) Determination of amount of chlorine in bleaching powder by iodometric method

Unit 3. Physical Chemistry Lab

40 Hours

Students have to perform at least one experiment from section 1 to 6 and two experiments from section 7:

1. Distribution Methods

- i. To determine the formula of copper ammonia complex.
- ii. To determine the formula of silver ammonia complex.

2. Phase Equilibrium

- i. To determine the freezing point curve of two component simple eutectic system.
- ii. To determine the freezing point curve of two component compound forming system.

3. Reaction Kinetics

- i. To study the kinetics of hydrolysis of methyl acetate catalyzed by hydrochloric acid at different temperatures and to determine the thermodynamic parameters.
- ii. To study the influence of ionic strength on the rate of reaction between potassium persulphate and potassium iodide in solution.
- iii. To study the kinetics of reaction between potassium persulphate and potassium iodide in solution at different temperatures and determine the thermodynamic parameters.

4. Viscosity Measurements

- i. To determine limiting viscosity number of polystyrene.
- ii. To determine chain linkage in polyvinyl alcohol from viscosity measurements.
- iii. To determine relative molecular mass of polystyrene from viscosity measurements.

5. Surface Chemistry

- i. To determine the critical micelle concentration (CMC) of sodium lauryl sulphate/N-cetyl N,N,N-trimethyl ammonium bromide (CTAB) from measurements of conductivities at different concentrations.
- ii. To determine the critical micelle concentration (CMC) of sodium lauryl sulphate/ N-cetyl-N,N,N-trimethyl ammonium bromide (CTAB) from measurements of surface tensions at different concentrations.

6. Potentiometry / pH metry

- i. To determine the stability constant of the silver-ammonia complex.
- ii. To determine the transport number of silver and nitrate ions in aqueous solution from the cell potential of the concentration cell with liquid junction potential.
- iii. To determine the substitution constants in Hammett equation for 3-aminobenzoic acid/4-aminobenzoic acid and 3-nitrobenzoic acid/4-nitrobenzoic acid.

7. Spectrophotometry: Interpretation of spectra/data

- i. Interpretation of vibrational-rotational spectra of rigid and non-rigid diatomic molecules.
- ii. Interpretation of electronic spectra of diatomic molecules.
- iii. Interpretation of electronic spectra of simple polyatomic molecules.
- iv. Analysis of XRD pattern of cubic system.
- v. Structure elucidation with a given set of spectra,
- vi. Determination of the degree of un-saturation from molecular formula.
- vii. Systematic interpretation of set of UV-Vis and IR spectra (Identification of the compound based on systematic interpretation of spectral data would be preferred).

N.B.: New experiments will be introduced from time to time subject to the availability of chemicals and instrument.

SEMESTER IV (2-Year PG) / SEMESTER II (1-Year PG)

Course Code: CHMSPL 25064

Course Title: Reaction Dynamics and Statistical Thermodynamics

Credits: 3+1+0

(Theory: 45 Hours, Tutorials: 15 Hours)

Total Marks: 100 (Theory: 70, Internal Assessment: 30)

Course objective: Students will be introduced to the concepts of chemical kinetics, molecular dynamics and fast reaction kinetics. This course is also introduced to impart students with the knowledge of terms and concepts used in statistical thermodynamics, partition functions and theories.

Course outcome: After completion of this course students will be able to describe/examine the concepts and theories of chemical kinetics, the applications of molecular dynamics, fast reactions and the fundamentals of statistical thermodynamics.

Unit 1. Chemical Kinetics

12 Lectures

Steady-state approximation and its applications, Oscillating reactions, chemical Chaos, Belousov-Zhabotinski reaction, straight-chain reaction-hydrogen halogen reactions, alkane pyrolysis, Branching-chain reactions- the hydrogen-oxygen reaction, explosion limits, Enzyme catalyzed reactions, Michaelis-Menten mechanism- Lineweaver-Burk and Eadie plots, enzyme inhibition.

Unit 2. Molecular Reaction Dynamics

12 Lectures

Collisions of real molecules- trajectory calculations, Laser techniques, reactions in molecular beam, -reaction dynamics, Estimation of activation energy and calculation of potential energy surface- the transition state theory (TST) of bimolecular gaseous reactions, statistical and thermodynamic formulations. Comparison between TST and hard-sphere collision theory, Theory of unimolecular reactions- Lindemann theory and its limitations, the kinetics of reactions in solution- diffusion-controlled and chemically controlled reactions, TST of reactions in solution- Bronsted and Bjerrum equation, effect of ionic strength, kinetic salt effect.

Unit 3. Study of Fast Reactions

10 Lectures

Stopped flow technique, temperature and pressure jump methods, NMR studies in fast reactions, shock tube kinetics, relaxation kinetics, Linearized rate equation, relaxation time in single step fast reactions, determination of relaxation time.

Unit 4. Theories of Unimolecular Reactions

06 Lectures

Drawbacks of Lindemann theory- Hinshelwood modification, RRK theory, slaters treatment, RRKM theory.

Unit 5. Statistical Thermodynamics – I

10 Lectures

Basic Terminology: probability, phase space, micro and macro states, thermodynamic probability, statistical weight, assembly, ensemble, The most probable distribution: Maxwell-Boltzmann distribution, quantum statistics: The Bose-Einstein statistics and Fermi- Dirac Statistics. Thermodynamic probability (W) for the three types of statistics. Lagrange's undetermined multipliers. Stirling's approximation, Molecular partition function and its importance.

Applications to ideal gases: The molecular partition function and its factorization. Evaluation of translational, rotational and vibrational partition functions, the electronic and nuclear partition functions. For monatomic, diatomic and polyatomic gases.

Unit 6. Statistical Thermodynamics–II

10 Lectures

Thermodynamic properties of molecules from partition function: Total energy, entropy, Helmholtz free energy, pressure, heat content, heat capacity and Gibb's free energy, equilibrium constant and partition function, Heat capacity of crystals and statistical thermodynamics, Third law of thermodynamics and entropy. Ortho- and para-hydrogen, statistical weights of ortho and para states, symmetry number. Calculation of equilibrium constants of gaseous solutions in terms of partition function, Einstein theory and Debye theory of heat capacities of monatomic solids.

SEMESTER IV (2-Year PG) / SEMESTER II (1-Year PG)

Course Code: CHMSPL 25074

Course Title: Organic Synthesis and Heterocyclic Chemistry

Credits: 3+1+0

(Theory: 45 Hours, Tutorials: 15 Hours)

Total Marks: 100 (Theory: 70, Internal Assessment: 30)

Course Outcomes: After learning the course, students will be able to understand various photochemical organic synthesis, c-c single and double bond formation, application of organometallic compounds in organic synthesis, heterocyclic chemistry and designing organic synthesis.

Unit 1. Photochemistry in organic synthesis

10 Lectures

Photochemistry of carbonyl compounds—representation of the excited states of ketones, photolysis of saturated and β , γ - unsaturated ketones. Photo reduction of saturated, arylalkyl and α , β -unsaturated ketones and p-benzoquinone; Paterno-Buchi reaction, [2+2]-cycloaddition, reactions of singlet oxygen- photooxidation, Ene reaction, synthetic applications of singlet oxygen. Olefinic photochemistry—photostereomutation of cis-trans isomers, optical pumping, [2+2] cycloaddition. Photochemistry of conjugated polyenes – cycloaddition and dimerization of 1,3-butadiene, photochemistry of vision.

Photorearrangements—di- π -methane rearrangement, Photo-Fries rearrangement and photorearrangement of cyclohexadienones, Barton rearrangement, Singlet oxygen photochemistry.

Unit 2. Designing Organic Synthesis

10 Lectures

Concepts in organic synthesis: Overview of Retrosynthetic analysis: connection, disconnection, synthons, protection and deprotection of functional groups.

Retrosynthesis and Synthesis of (Ethoheptazine (analgesic), Piperocaine (local anaesthetic), Choloroquine (antimalarial), diclofenac (non-steroidal anti-inflammatory drug),

Unit 3. Formation of C-C single and double bonds

15 Lectures

Alkylation—importance of enolate anions, alkylation of activated methylene groups, dianion in synthesis, alkylation of ketones, enamine and related reactions; alkylation of thio-and seleno-carbanions; allylic alkylation of alkenes, Michael addition (conjugate addition). Aldol reaction—use of boron and silyl enolates; directed aldol reaction. Synthetic applications of carbene and carbenoids; formation of carbon-carbon bond by addition of free radicals-to alkenes; photocyclization reactions.

Elimination reactions—acid catalysed dehydration of alcohols, solvolytic and base-induced elimination from alkyl halides & sulphones, Hofmann elimination from quaternary ammonium salts. Pyrolytic syn elimination—pyrolyses of carboxylic esters and xanthates (Chugaev reaction) and amine oxides (Cope reaction). Wittig and related reactions—use of stabilized and unstabilized phosphorus ylides, Peterson reaction. Alkenes from sulphones, decarboxylation of lactones, stereoselective synthesis of tri and tetrasubstituted alkenes.

Unit 4. Synthetic application of organometallic and activation of C-H bonds

10 Lectures

Preparation, stability, reactivity and synthetic applications of organo-lithium, tin, copper, zinc, palladium, Mo, Ru, Rh reagents. (emphasis on important name reactions viz. Hofmann-Loeffler-Freytag reactions, Heck Reaction, Suzuki Reaction, Sonogashira Reaction, Negishi Reaction, Stille Reaction, Hiyama Reaction, Kumada Reaction, Buchwald-Hartwig, Mc Murry reaction, Ito oxidation, etc.)

Unit 5. Heterocyclic Chemistry

15 Lectures

Nomenclature, π -excessive and π -deficient heterocycles, Principles of heterocyclic synthesis involving cyclization and cycloaddition reaction. Synthesis and properties of three, four, five, six and seven membered heterocycles containing one, two and three heteroatoms viz., N, O and S (aziridine, oxirane, thiirane, azetidine, oxetane, thietane, pyrazole, isoxazole, isothiazole, imidazole, oxazole and thiazole, pyran, azepine, oxepine, thiepine).

SEMESTER IV (2-Year PG) / SEMESTER II (1-Year PG)

Course Code: CHMSPL 25084
Course Title: Inorganic Photochemistry

Credits: 3+1+0

(Theory: 45 Hours, Tutorials: 15 Hours)

Total Marks: 100 (Theory: 70, Internal Assessment: 30)

Course Outcomes: Students will be able to explore the synthesis, properties, and applications of diverse inorganic materials, alongside investigating the magnetic behavior of transition metal ions in different coordination environments. Additionally, they will be able to analyze the electronic spectra of transition metal complexes, correlating electronic transitions with molecular structure and ligand-field effects. Furthermore, students will delve into the principles of Photoinorganic chemistry, studying photochemical processes and their applications in light-driven reactions, photocatalysis, and photovoltaic devices, contributing to advancements in sustainable energy and environmental remediation.

Unit 1. Inorganic Materials

16 Lectures

Magnetic exchange and exchange coupling phenomena, magnetic materials, molecular magnets, ferrofluids. Crystalline, liquid crystalline and amorphous materials, non-stoichiometric oxides, crystal defects, nano materials. Classification, manufacture and applications of Inorganic fibers, and Inorganic fillers, condensed phosphates, and coordination polymers. Band theory of metals, semiconductors, *p*- and *n*- type semi-conductor. Defect perovskites, high Tc superconductivity in cuprates, preparation and characterization of 1-2-3 materials, application of high Tc materials. Thermoelectric properties – dielectric, ferroelectric, piezo electric materials, solid electrolytes and Fuel Cells.

Unit 2. Magnetic properties of transition metal ion

16 Lectures

Magnetic properties of free ions, spin-only magnetic moments of d^n ions in weak and strong crystal fields of O_h and T_d symmetries, orbital contribution and the effect of spin-orbit coupling, quenching of orbital angular momenta by crystal fields, temperature independent paramagnetism, high-spin low-spin equilibria, Ferromagnetism and antiferromagnetism with examples from metal complexes, Magnetic properties of second and third transition series and the lanthanide elements. Measurement of magnetic susceptibility.

Unit 3. Electronic spectra

10 Lectures

La Porte Selection Rules, Effect of vibronic coupling and spin-orbit coupling, band intensities and band widths, Jahn Teller effect. Spectra of aqueous solutions of $M(H_2O)_6^+$, Spectra of high spin and low-spin ML_6^{n+} complexes, Calculation of 10 Dq and values from spectra, distorted octahedral and tetrahedral complexes, M to L and L to M charge transfer spectra.

Unit 4. Photoinorganic chemistry

18 Lectures

Ligand field and charge transfer states (Thexi and DOSENCO states), Energy dissipation by radiative and non-radiative processes, Jablonski diagram. Photosubstitution on Cr(III) and

Co(II) compounds, cis-trans isomerisation, metal carbonyls. Photoredox reactions of Co(III) complexes, Photo catalysis and solar energy conservation by Ru(bpy)₃²⁺. Photochemical pathways (unimolecular or intramolecular process and bimolecular or intermolecular process), quantum yield, Kasha's rule and Stoke shifts, identification of excited states, examples of main photochemical processes: non-redox processes (photoisomerization, photodissociation, photosubstitution), Photosynthesis reactions (mechanism and salient features of photosynthesis reaction I and II), light harvesting, solar energy conversion, metal ion sensors, chemosensors, artificial photosynthesis.

SEMESTER IV (2-Year PG) / SEMESTER II (1-Year PG)

Course Code: CHMSPL 25094 Course Title: Polymer Science Credits: 3+1+0

(Theory: 45 Hours, Tutorials: 15 Hours)
Total Marks: 100 (Theory: 70, Internal Assessment: 30)

Course Outcome: The students will acquire detailed knowledge about polymers, their synthesis, processing abilities, properties, and structure-property relationship to their applications.

Course Objectives: The main objective of this course is to understand the fundamental concepts of polymerization. To know about various types of polymerization reaction and their mechanisms. To learn the various techniques of polymer synthesis and polymer characterization. To know various applications of biodegradable polymers.

Unit 1. Introduction to Polymers

10 Lectures

Importance, historical background, raw materials and basic nature of polymers. Concept of monomer, repeating unit, degree of polymerization. Classification of polymers Average molecular weight concept. Polydispersity and molecular weight distribution. Measurement of molecular weights: end-group analysis, viscosity, light scattering, osmotic and ultracentrifugation methods.

Unit 2. Polymerization and Kinetics

10 Lectures

Step polymerization, chain polymerization including carbonyl polymerization, Ziegler–Natta coordination polymerization, group transfer polymerization, ring opening polymerization, metathesis polymerization, controlled radical polymerization, supramolecular polymerization, Step copolymerization, chain copolymerization, Types of copolymers, Copolymer equation, Monomer reactivity ratios. Structure and reactivity of monomers and radicals, Alfrey price Qescheme, Block and graft copolymers.

Unit 3. Polymer characterization

10 Lectures

Chromatographic method, Spectroscopic methods, X-ray diffraction study, microscopy, thermal analysis, thermal transition in polymer (Tg, Tm). Physical testing: tensile strength, tear strength, fatigue failure, resilience, hardness, impact and abrasion resistance.

Unit 4. Structure and Properties

10 Lectures

Morphology and order in crystalline polymers-configurations of polymer chains. Crystal structures of polymers. Morphology of crystalline polymers, strain-induced morphology, crystallization and melting.

Polymer structure and physical properties-crystalline melting point Tm – melting points of homogeneous series, effect of chain flexibility and other steric factors, entropy and heat of fusion.

The glass transition temperature Tg: Relationship between Tm and Tg, effects of molecular weight, diluents, chemical structure, chain topology, branching and cross linking.

Unit 5. Polymer Processing

10 Lectures

Plastics, elastomers and fibres. Compounding reinforcing. Processing techniques: two roll mill mixing, internal mixer, calendaring, die casting, rotational casting, film casting, moulding, extrusion, thermoforming, foaming and fibre spinning.

Unit 6. Polymer in Special uses

10 Lectures

High temperature and fire-resistant polymers, Liquid crystal polymers, Conducting polymers, Polyelectrolytes, Biodegradable polymers, Superabsorbent, Self-healing polymer. Use of polymers as lubricating oil additives.

SEMESTER IV (2-Year PG) / SEMESTER II (1-Year PG)

Course Code: CHMSPL 25104 Course Title: Natural Products Chemistry

Credits: 3+1+0

(Theory: 45 Hours, Tutorials: 15 Hours)

Total Marks: 100 (Theory: 70, Internal Assessment: 30)

Course Outcomes: After learning the course, students will be able to understand different types of natural products, their sources and applications. Students will also be able to describe important methods of extraction, their synthesis, and biosynthesis processes.

Unit 1. Chemistry of carbohydrates

13 Lectures

Open chain and ring structure of monosaccharides, Reactions of the anomeric centre, Reactions of hydroxyl groups, Cyclic acetals, Glycosyl activation

Chemical disaccharide formation, Enzymatic disaccharide formation, Introductory chemical glycobiology.

Unit 2. Chemistry of terpenoids

13 Lectures

Introduction to terpenoids, isoprene and biogenetic isoprene rule, Biosynthesis of mono and sesquiterpenoids, discussion on caryophylene, longifolene, santonin, abietic acid, and taxol.

Unit 3. Chemistry of alkaloids

12 Lectures

Introduction to alkaloids, Physiological activity of alkaloids, Discussion on morphine, and reserpine.

Unit 4. Chemistry of porphyrins

12 Lectures

Porphyrin ring and chemistry of heme, oxygen transport by haemoglobin, chemistry of chlorophyll and its role in photosynthesis.

Unit 5. Carotenoids and Vitamins

10 Lectures

General Introduction, Discussion on alpha-, beta- and gamma-carotenes, vitamin-A.

SEMESTER IV (2-Year PG) / SEMESTER II (1-Year PG)

Course Code: CHMSPL 25114
Course Title: Bioinorganic Chemistry

Credits: 3+1+0

(Theory: 45 Hours, Tutorials: 15 Hours)

Total Marks: 100 (Theory: 70, Internal Assessment: 30)

Course Outcomes: Students will be able to identify/elucidate the basis of supramolecular chemistry and ion transport, carrier transport storage and activation of dioxygen, metalloenzymes, electron transfer proteins, metals in medicine and demonstrate their various applications in analyzing and interpreting various questions.

Unit 1. Supramolecular Chemistry and Ion Transport

16 Lectures

Definition and examples of Supramolecules, Self-assembly and membranes, Molecular receptors- Cryptands, Valinomycine, Spherands, Molecular recognition. Interaction of metal ions and metal complexes with DNA.

Supramolecular Transport: Active transport of ions across cell membranes, Selectivity of Na and K with crown ethers, cryptands and ionophores, Na/K pump; Transport of Ca²⁺, Biominerals containing Ca and Fe; Transport and Storage of Iron; Transferrins, Sideraphores, and Ferritin.

Unit 2. Carrier, Transport, Storage and Activation of Dioxygen 14 Lectures

Active site structure and function of oxygen carrying proteins: Metalothionins and Ceruloplasmin. Haemoglobin, Myoglobin, Haemerythrin and Haemocyanine; O_2 binding equilibria and mechanism of cooperativity in Hemoglobin, Design of Model O_2 carriers, Reaction leading to toxicity due to dioxygen. Oxidases and Oxygenase: Catalase, Peroxidase, Superoxide Dismutase, Cytochrome c Oxidase, Cytochrome P-450, and Pyrocatechol Dioxygenase - their biological functions, role of metal and dioxygen reactivity.

Unit 3. Metalloenzymes

10 Lectures

Structure and function of carboxypeptidase A and carbonic anhydrase. Importance of Co(II) substitution in Zn proteins; Structure and function of co-enzyme B₁₂. Role of Ni, Cr and V in enzymes; Molybdenum enzymes, structure and function of Nitrogenase, chemistry of dinitrogen fixation, Xanthine oxidases, Metalloenzymes- Classifications, metallohydrolases, Metallo oxidoreductases, Metallo isomerases, Metallo synthases, Metallolyases, Ligases, the role of metal ions in structural context - selected examples-Heme vs non-heme centers

Unit 4. Electron transfer proteins

10 Lectures

Metalloproteins in the electron transfer chains in membrane, The Cytochromes (*a, b, c* types), Mechanism of electron transfer reactions in proteins; Iron Sulfur proteins—Rubredoxin, Ferredoxin, and HiPIP.

Unit 5. Metals in medicine

10 Lectures

Metal deficiency and disease, toxic effect of metals - Fe and Cu overload, Thalassemia, toxicity due to Hg, As, Cd, and Pd; Chelation therapy (EDTA, BAL, Penicillamine); Gold compounds in Rh. arthritis, Cisplatin with case studies and related Anticancer drugs.

SEMESTER IV (2-Year PG) / SEMESTER II (1-Year PG)

Course Code: CHMSPL 25124 Course Title: Catalysis Credits: 3+1+0

(Theory: 45 Hours, Tutorials: 15 Hours)
Total Marks: 100 (Theory: 70, Internal Assessment: 30)

Course Objectives: The aim of this course is to introduce fundamentals of catalysis and characterization techniques employed in catalysis. A detail idea on the homogeneous, heterogeneous and photocatalysis is also introduced in this course.

Course Outcomes: The students are expected to learn about types of catalysis - comparison of homogeneous & heterogeneous catalysis, photocatalysis and different characterization techniques of solid catalysts.

Unit 1. Homogeneous Catalysis

15 Lectures

Atom transfer and electron transfer processes. Role of transition metal ions with special reference to Cu, Pd, Pt, Co, Ru and Rh, catalysis in non-aqueous media. Rates of homogeneously catalysed reactions, turnover number and frequency. Catalysis of isomerisation, hydrogenation, oxidation and polymerization reactions. Asymmetric catalysis, biocatalysis and metal clusters in catalysis. Phase-transfer catalysis.

Unit 2. Heterogeneous catalysis

15 Lectures

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.

Unit 3. Photocatalysis

10 Lectures

Photocatalytic reactions, general mechanism of photocatalysis, 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.

Unit 4. Characterization of solid catalysts

20 Lectures

Surface area & surface morphology, BET surface area analysis, porosity - pore volume - diameter - particle size, principles and applications of PXRD, SEM, TEM, EDX, XPS, AFM to surface studies - TPD, TPR for acidity and basicity of the catalysts, boundary layer theory - Wolkenstein theory -Balanding's approach.

SEMESTER IV (2-Year PG) / SEMESTER II (1-Year PG)

Course Code: CHMSPL 25134

Course Title: Medicinal and Bioorganic Chemistry

Credits: 3+1+0

(Theory: 45 Hours, Tutorials: 15 Hours)

Total Marks: 100 (Theory: 70, Internal Assessment: 30)

Course Objectives: The students will be taught to about the chemistry behind the development and activity of pharmaceutical materials, to understand the basic idea of lipid chemistry, and to understand the concept of vitamins and their role.

Course Outcomes: Students will be able to predict a drugs properties based on its structure, will gain the knowledge of mechanism of action and adverse effects of drugs. Students are expected to learn the relationship between drug's chemical structure and its therapeutic

properties. They will learn about lipids and their importance in biological system. They will also understand about their synthesis. They will also learn about different types of vitamins and their synthesis and role in biological system.

Section A: Medicinal Chemistry

Unit 1. Basic concept of medicinal chemistry

5 Lectures

Introduction, targets, Agonist, antagonist, partial agonist. Receptors, Receptor types, Theories of Drug – receptor interaction, Drug synergism, Drug resistance, physicochemical factors influencing drug action. Isosterism and bioisosterism

Unit 2. Antibiotics 6 Lectures

Introduction, Targets of antibiotics action, classification of antibiotics, enzyme-based mechanism of action, SAR of penicllins and tetracyclins, clinical application of penicillins, cephalosporin, Beta lactamase inhibitors, tetracyclines, Current trends in antibiotic therapy.

Unit 3. Antihypertensive agents and diuretics

5 Lectures

Classification of cardiovascular agents, introduction to hypertension, etiology, types, classification of antihypertensive agents, classification and mechanism of action of diuretics, Furosemide, Hydrochlorothiazide, Amiloride.

Unit 4. Analgesics, Antipyretics and Anti-inflammatory Drugs 5 Lectures

Introduction, Mechanism of inflammation, classification and mechanism of action of NSAIDs and SAR of paracetamol, Ibuprofen, Diclofenac, naproxen, indomethacin, phenylbutazone and meperidine

Unit 5. Antidiabetic Agents and antimalarials

8 Lectures

Introduction, Types of diabetics, Drugs used for the treatment, chemical classification, SAR, Mechanism of action, Study the treatment strategy of diabetic mellitus. Chemistry of insulin, sulfonyl ureas

Classification, mechanism of action of drugs employed for the treatment of malaria. Current treatment strategy for malaria.

Unit 6. Drugs for CNS

7 Lectures

CNS Active Drugs, CNS depressants, Hypnotics and Sedatives: Barbiturates, non-barbiturates, amides and imides, glutethimide, benzodiazepines, aldehydes and derivatives, methaqualone and other miscellaneous agents. (Mode of action only)

Anticonvulsants: Barbiturates, hydanatoins, oxazolidinediones, succinimides, bezodiazepines, thenacemide, glutethimide. (Mode of action only)

CNS-Stimulants & Psychoactive Drugs: Analeptics, purines, psychomotor stimulants, sympathomimetics, monamine oxidase inhibitors, tricyclic antidepressants, miscellaneous psychomotor stimulants. Hallucinogens (psychedelics, psychometrics): Indolethylamines, R-phenylethylamines, butyrophenones and other miscellaneous drugs. (Mode of action only)

Unit 7. Computational approach in medicinal chemistry

4 Lectures

Structure activity relationship, concept of QSAR, physicochemical parameters- lipophilcity, partition coefficient, electronic-ionization constants, H-bonding, steric parameters, Isosterism, bioisosterism.

Section B: Bioorganic Chemistry

Unit 1. Biochemistry of Lipids

10 Lectures

Biological importance of fatty acids and lipids, even chain and odd chain fatty acids, saturated and unsaturated fats, ketone bodies. Biosynthesis of fatty acids, triacylglycerols, phospholipids, cholesterol and related steroids; prostaglandins.

Unit 2. Chemistry of Vitamins

10 Lectures

Carotenoids - classification, chemistry of β -carotene, lycopene and canthaxanthin. Synthesis of β -carotene, provitamin A, singlet oxygen quenching and food coloring properties of carotenes. Classification and functional role in biological systems; chemistry of thiamine, riboflavin, retinol, tocopherols, vitamin C and pyridoxine.

SEMESTER IV (2-Year PG) / SEMESTER II (1-Year PG)

Course Code: CHMSPL 25144
Course Title: Organometallic Chemistry

Credits: 3+1+0

(Theory: 45 Hours, Tutorials: 15 Hours)

Total Marks: 100 (Theory: 70, Internal Assessment: 30)

Course outcomes: Students will be able to explain and compare relationships between nature of metal-carbon bonds in transition metal compounds, organometallic complexes and its synthesis and structural properties, organometallics in catalysis and fundamental reactions of organotransition metal complexes.

Unit 1. Nature of metal-carbon bonds in transition metal compounds

20 Lectures

Classification of organometallic compounds, M–C σ bond in metal alkyls, β -hydrogen elimination. Complexes with metal carbon π -bonds - with olefins, mechanism of olefin methathesis (Ring opening metathesis, cross metathesis, ring closing metathesis). Bonding in metal carbocyclic systems cyclopentadienyl and other carbocyclic ligands, MO treatment of bonding in ferrocene based on symmetry properties of the ligand and metal orbitals. Bonding in carbene and carbine complexes.

Unit 2. Synthesis, structure and properties of organometallic complexes

18 Lectures

Olefin complexes, acetylene complexes, complexes formed by polyenes and allylic compounds -synthesis and relevance. Cyclopentadiene and arene metal complexes—general reactions. Bent sandwich compounds, Chemistry of arene sandwich compounds, Transition metal alkyls and ylides complexes, metal carbene and metal carbyne complexes -synthesis and reactivity.

Synthesis of metal carbonyls and metal carbonyl hydrides reactions and synthetic utilities. High nuclearity carbonyl cluster, structures, electron counting schemes and bonding - Wade's rules (isolobal analogy).

Unit 3. Fundamental reactions of organotransition metal complexes 10 Lectures

Ligand co-ordination and dissociation - displacement reaction in square planar complexes, steric and electronic influences of ligands. Oxidative addition and reductive elimination. Insertion reactions- insertion of CO, alkenes. Reaction of co-ordinated ligands- reactions of co-ordinated olefins, acetylenes and arenes.

Unit 4. Organometallics in catalysis

12 Lectures

Homogeneous and heterogeneous catalysis. Polymerization and oligomerization of olefins and dienes. Hydrogenation, hydroformylation, isomerization, metathesis and carboxylation of olefins. Synthesis of acetic acid from methanol, reactions of synthesis gas. Oxidation of olefins by Wacker process, synthesis of acrylates, olefin epoxidation. C-H bond activationhydroxylation and autoxidation - basic idea. Allylic oxidations, deactivation and regeneration of catalysts, (catalytic poisons and promoter), Synthetic gasoline preparation (Fischer Tropsch reaction), Monsanto Acetic Acid process

SEMESTER IV (2-Year PG) / SEMESTER II (1-Year PG)

Course Code: CHMSPL 25154
Course Title: Computational Chemistry

Credits: 3+1+0

(Theory: 45 Hours, Tutorials: 15 Hours)

Total Marks: 100 (Theory: 70, Internal Assessment: 30)

Course Objectives: To provide a good understanding and practice of the various programming languages like BASIC and FORTRAN and impart a thorough knowledge of the empirical and semi-empirical electronic structure calculations, computational background and simulations.

Course Outcomes: The students are expected to learn various programming languages that are required for different types of molecular simulations and electronic structure calculations.

They will be able to write independent programs, correctly compile them and use computer to study molecular electronic structures and molecular modelling.

Unit 1. Chemistry and BASIC Programming

15 Lectures

Principles of BASIC Programming- BASIC expressions, statements, Library functions, Arrays, Functions and subroutines, Algorithm and flow-chart. Programming examples from Chemistry illustrating the principles of BASIC language- calculation of molecular weights, mean activity coefficient, ionic mobilities, ionic strength, reduced mass, molecular velocities, calculation of thermodynamic parameters, average value of rate constants

Unit 2. Chemistry and FORTRAN Programming

15 Lectures

Principles of FORTRAN Programming-Characters, constants and variables, FORTRAN expressions and statements, library functions, Algorithm and flow-chart. Programming examples from Chemistry illustrating the principles of FORTRAN language- calculation of molecular velocities, determination of moment of inertia and internuclear distance from Raman spectra data, critical constants of van der Waals gases, dissociation constant of weak acid.

Unit 3. Numerical methods used in chemistry

15 Lectures

Some illustrative numerical methods in chemistry: Least squares fit, root finding, numerical differentiation, integration and solution of ODE, matrix inversion and diagonalization, interpolation. Pattern recognition techniques and molecular graphics. Basics of electronic structure calculations, Molecular Mechanics, Monte Carlo and Molecular Dynamics simulations.

Unit 4. Computer applications in Chemistry

15 Lectures

Use of some packages to study molecular electronic structures and molecular modelling (GAMESS, MOPAC, molecular dynamics packages, etc. Use of electronic spreadsheets in chemistry. Basic ideas on structure-activity relationships, computational background of molecular modelling: potential energy surfaces, molecular mechanics, MO methods, drug and catalysis design, etc. Development of some simulation programs and use of the internet for chemical information retrieval. Chemoinformatics.

SEMESTER IV (2-Year PG) / SEMESTER II (1-Year PG)

Course Code: CHMSPL 25164

Course Title: Advanced Topics in Organic Chemistry

Credits: 3+1+0

(Theory: 45 Hours, Tutorials: 15 Hours)

Total Marks: 100 (Theory: 70, Internal Assessment: 30)

Course Objectives: The students will be introduced to the recent development in chemistry including Click Chemistry, ionic liquids, organic electronics, energy and mechanochemistry. Course Outcomes: Students will be able to learn the role of click chemistry in organic synthesis, predict the synthetic route of various useful chemicals from simple molecules. They will also learn the basics of ionic liquids and its application in green chemistry approaches in organic chemistry, get the idea of organic chemistry in impending electronic industry, learn about the renewable energy and role of organic chemistry in biofuels and have a concept of mechanochemistry and how it will be applied in organic chemistry.

Unit 1. Click chemistry

10 Lectures

Basic principle of click chemistry, Cu(I)- catalyzed Azide - Alkyne Click Chemistry reaction (CuAAC), Strain-promoted Azide - Alkyne Click Chemistry reaction (SPAAC), Strain-Promoted Alkyne-Nitrone Cycloaddition (SPANC), Tetrazine - Alkene Ligation, Reactions of Strained Alkenes; Other applications of click chemistry.

Unit 2. Platform chemicals

10 Lectures

Basic concept; different types of platform chemicals, their source and preparation; Chemistry of 5-Hydroxymethylfurfural, 2.5-Furandicarboxylic acid, alkyl glycosides, glucaric acid, Nacetylglucosamine, etc. in the preparation of chemicals.

Unit 3. Ionic liquids in chemistry

10 Lectures

Definition, composition, application in green chemistry as: solvent, electrolytes, pharmaceuticals, biopolymer processing, reprocessing of nuclear fuel, tribology, waste recycling, solar thermal energy. Challenges of ionic liquids.

Unit 4. Organic electronics

10 Lectures

Introduction of organic electronics, historical milestones, Chemistry of organic light emitting diodes, organic field-effect transistors, organic semiconductors, challenges of organic electronics, etc. Prospects of organic electronics in industries.

Unit 5. Bioenergy and biofuels

10 Lectures

Introduction, types, production and application of biofuels- ethanol, cellulosic ethanol, biodiesel, renewable hydrocarbons, biogases, etc. Challenges of biofuels.

Unit 6. Organic Mechanochemistry

10 Lectures

Basic of mechanochemistry; Application of mechanochemistry in functional group transformation, catalytic process, photochemical reaction, etc.

SEMESTER IV (2-Year PG) / SEMESTER II (1-Year PG)

Course Code: CHMSPL 25174
Course Title: Group Theory and Application
Credits: 3+1+0

(Theory: 45 Hours, Tutorials: 15 Hours)
Total Marks: 100 (Theory: 70, Internal Assessment: 30)

Course Outcomes: Students will learn about the fundamental principles of group theory, including symmetry operations and representations, and their applications in molecular symmetry and spectroscopy. Additionally, they will understand the chemical applications of group theory, focusing on its role in predicting molecular properties.

Unit 1. Basics of group theory

12 Lectures

Representation of symmetry operators by matrices, representation of groups - reducible and irreducible representations, the Great orthogonality theorem and properties of irreducible representations, Character tables Mulliken notations.

Unit 2. Application of group theory

12 Lectures

Transformation properties of atomic orbitals, the Direct Product Representations, construction of Hybrid orbitals for AB_n molecules, construction of symmetry adapted linear combinations (SALCs) and MOs of simple AB_n molecules. Selection rules for electronic and vibrational spectroscopy.

Unit 3. Chemical applications of Group Theory

18 Lectures

Molecular vibrations, molecular vibration of symmetrical AB₂ (bent) molecules, symmetry of normal modes of ethylene. Binding in water molecule, symmetries of molecular orbitals and electronic configuration. Vanishing matrix elements.

Unit 4. Ligand Field Theory

18 Lectures

The d wave functions (orbitals), Crystal field potential, Symmetry aspects of d orbital splitting by ligands. Electron repulsion in many electron atoms, Free ion terms for d^n configurations, Electron repulsion parameters, spin - orbit coupling, Effect of weak crystal field on O_h symmetry on the S, P, D and F terms, Free ions in strong crystal fields. Term

energy level diagram for d^n configurations in O_h and T_d symmetries, Tanabe-Sugano diagrams. Influence of the d-configuration on the geometry and stability of complexes. MO theory of complex compounds, LGO and MOs of ML_6 and tetrahedral complexes.

SEMESTER IV (2-Year PG) / SEMESTER II (1-Year PG)

Course Code: CHMSPL 25184
Course Title: Physical Chemistry Practical
Credits: 0+0+4

(Practical: 120 Hours)

Total Marks: 100 (Practical: 70, Internal Assessment: 30)

Course Objectives: This is a special laboratory course introducing some experimental and theoretical experiments of physical chemistry. The objective of the course is to introduce two types of experiments. The objective of first type is involved with basic physical chemistry such as chemical kinetics, theoretical chemistry, thermodynamics, photochemistry etc. The objective of second type of experiments is to introduce students to some modern techniques of analysis such as spectrophotometry, electrochemical analysis and surface chemistry.

Course outcomes: After completing this course, the students will understand physical chemistry from experimental point of view. Moreover, they will learn some modern methods of analysis required in different area of research.

Unit 1. [Minimum 10 experiments, at least 3 experiments from each section, a, b, c]

- (a) Experiments on Chemical Kinetics:
- 1. Determination of the temperature coefficient and energy of activation of acid hydrolysis of methyl acetate, using least squares calculation.
- 2. Study of the autocatalytic reaction between oxalic acid and KMnO₄ and determination of the order of the reaction.
- 3. Study of the decomposition kinetics of the formation of complex between sodium sulphide and sodium nitroprusside spectrophotometrically. Determination of the rate constant and order of the reaction.
- 4. Study of the kinetics of the reaction between peroxydisulphate and potassium iodide and to find the influence of ionic strength on the rate constant.
- 5. Study of the kinetics of oxidation of ethanol by chromium (VI) and to find the rate constant of the reaction. Also find the order of the reaction by half-life period method.

- 6. Study of the double exponential time dependence of the reduction of Cr (VI) by glutathione in an aqueous medium and to obtain the rate constants of the process. (EPC, Halpern Ex. No. 23, 381).
- 7. Determination of the rate constants for the α-chymotrypsin-catalyzed hydrolysis of an ester. (EPC, Halpern Ex. No. 24, 395).
- 8. Determination of the relative strength of two acids (HCl and H₂SO₄) by studying the hydrolysis of an ester (methyl acetate/ ethyl acetate). [Yadav, 288].
- 9. Investigation of the inversion of cane sugar in presence of HCl and H₂SO₄ and hence determination of the relative strengths of the two acids.

(b) Experiments on Conductometric Titrations:

- 1. Determination of the equivalent conductivity of acetic acid at infinite dilution by Kohlrausch's method and hence to find the degree of dissociation constant of the acid.
- 2. Comparison of the relative strength of acetic acid and monochloroacetic acid by conductance measurement.
- 3. Determination of the degree of hydrolysis and hydrolysis constant of aniline hydrochloride /sodium acetate.
- 4. Determination of the strength of the components of the following binary mixture by conductometric titration.
 - (i) Hydrochloric acid and acetic acid
 - (ii) Sulphuric acid and copper sulphate
- 5. Determination of the amount of each component of the following ternary mixture by conductometric titration. Hydrochloric acid, acetic acid and copper sulphate
- 6. Determination of the degree of hydrolysis and hydrolysis constant of CH₃COONa of NH₄Cl by conductance measurement.

(c) Experiments of Spectrophotometry:

- 1. Verify Beers law and determine concentration of
 - (i) K₂Cr₂O₇ (ii) Organic dyes like methylene blue, Rhodamine B (iii) CuSO₄
- 2. Determination of the concentration of chromium and manganese in a mixture of dichromate and permanganate by spectrophotometric method.
- 3. Determination of the composition of iron salicylic acid complex spectrophotometrically by Job's method of continuous variation.
- 4. Investigation of the complex ion formation between Ni²⁺ and o-phenanthroline by Job's method.
- 5. Investigation of the reaction between acetone and iodine by colorimetry.
- 6. Determination of the refractive index of a given liquid by Abbe refractometer and to find the molar and specific refractions.

Unit 2. [Minimum 5 experiments, at least 1 experiment from each section, a, b, c]

- (a) Experiments on pH metric Titrations
- 1. Determination of the dissociation constant of acetic acid/oxalic acid by using Hendersen's equation.

- 2. Finding the amount of the components of the following mixtures using pH metric titration: Hydrochloric acid + Oxalic acid
- 3. Determination of the pH of a buffer solution by using quinhydrone electrode.
- 4. Potentiometric estimation of strength of solutions of hydrochloric acid and acetic acid individually and a mixture of the two using standard sodium hydroxide solution.
- 5. Titration of ferrous ammonium sulphate against potassium dichromate potentiometrically and determination of the standard electrode potential of the ferrous/ferric system.

(b) Electrochemical experiments: Cyclic voltammetry

- 1. Cyclic voltammetry of a standard solution at different scan rates and calculation of redox potential ofelectro-active species.
- 2. Determination of diffusion coefficient from cyclic voltammetry
- 3. Determination of Electrode surface area from Cyclic voltammetry
- 4. Determination of rate of heterogeneous electron transfer from cyclic voltammetry
- 5. Chronocoulometry of a redox dye and determination of amount adsorbed on to the electrode surface
- (c) Adsorptio-desorption on porous materials, Equilibrium study, kinetic study, thermodynamic studies
- 1. Adsorption of dye on activated carbon and analysis of result by different adsorption models.
- 2. Determination of adsorption kinetics of dye on activated carbon.
- 3. Determination of desorption kinetics of dyes from adsorbents
- 4. Determination of thermodynamic quantities ΔH , ΔS and ΔG of dye adsorption on activated carbon.

Unit 3. [Minimum 5 experiments, at least 1 experiment from each section, a, b]

- (a) Experiments of Theoretical Chemistry
- 1. Least squares fitting and plotting linear and exponential graphs using computer.
- 2. Potential energy diagram of hydrogen molecule ion with the help of fortran programming.

(b) Miscellaneous Experiments

- 1. Determination the molar mass of a polymer by viscometric method.
- 2. Study of the variation of surface tension of a solution of n-propyl alcohol/ethanol with concentration and determination of the limiting cross-sectional area of the alcohol molecule.
- 3. Determination of the partial molar volume of methanol/ethanol/formic acid by graphical method by determining the densities of solutions at different concentrations.
- 4. Determination of the influence of NaCl, naphthalene and succinic acid on the critical solution temperature of phenolwater system using 0.5, 1 and 1.5 % concentrations.
- 5. Determination of the Van't Hoff factor for an electrolyte by cryoscopic method.
- 6. Determination of the percentage composition of binary mixture of non-electrolyte (urea and glucose) by cryoscopic method.

- 7. Study of the variation of solubility of Ca(OH)₂ in NaOH solution and hence to determine its solubility product.
- 8. Determination of the equilibrium constant of the reaction: $KI + I_2 = KI_3$ by distribution method.
- 9. Determination of the formula of the complex formed between Cu²⁺ and NH₃ by distribution method.

SEMESTER IV (2-Year PG) / SEMESTER II (1-Year PG)

Course Code: CHMSPL 25194 Course Title: Organic Chemistry Practical

Credits: 0+0+4 (Practical: 120 Hours)

Total Marks: 100 (Practical: 70, Internal Assessment: 30)

Course Outcomes: The students are expected to learn laboratory skills for preparation of organic compounds via coupling reaction, diazotization reaction, Click chemistry method and synthesis of heterocyclic compounds. After studying the lab course of this paper, students will be able to know the characterization of organic compounds using various spectroscopic techniques.

Unit 1. Coupling reaction, purification and characterization of the product using various spectroscopic techniques.

30 Hours

- a. Heck Reaction
- b. Suzuki Reaction
- c. Sonogashira Reaction
- d. Stille Reaction

Unit 2. Preparation of organic compounds using Click chemistry method and their purification & characterization using spectroscopic techniques. 30 Hours

Unit 3. Synthesis of heterocyclic compounds, purification and characterization using spectroscopic techniques.

30 Hours

- a. Quinoline
- b. 2-Phenyl indole
- c. 1,2,3,4-Tetrahydrocarbazole
- d. 5-Hydroxy-1,3-benzoxal-2-one

Unit 4. Synthesis using diazotization reaction, purification and characterization using spectroscopic techniques.

30 Hours

- a. p-Chlorotoluene
- b. o-Chlorobenzoic acid
- c. p-Iodonitrobenzene

N.B.: New experiments will be introduced from time to time subject to the availability of chemicals and instrument.

SEMESTER IV (2-Year PG) / SEMESTER II (1-Year PG)

Course Code: CHMSPL 25204

Course Title: Inorganic Chemistry Practical Credits: 0+0+4

(Practical: 120 Hours)

Total Marks: 100 (Practical: 70, Internal Assessment: 30)

Course Outcomes: By the end of this lab course, students will be able to synthesize and characterize a range of inorganic compounds, including molecular frameworks, metal oxide nanoparticles, chemically synthesized metal oxide nanoparticles, and zeolites, using advanced laboratory techniques. They will gain proficiency in interpreting characterization data to determine the structural and chemical properties of these materials. Additionally, students will develop critical thinking skills, problem-solving abilities, and experimental design expertise, preparing them for further research or professional work in areas such as materials science, catalysis, environmental science, and nanotechnology.

Synthesis and characterization using various analytical techniques

- (a) Synthesize of an inorganic Supramolecular complex (molecular frameworks)
- (b) Synthesis of transition metal oxide nanoparticles by hydrothermal method
- (c) To determine UV-Vis characterization of chemically synthesized metal oxide (ZnO, SnO₂) nanoparticles
- (d) Synthesis and characterization of co-crystals of 5, 7, 7, 12, 14, 14-hexmethyl-1, 4, 8, 11- tetraazacyclo tetra deca-4, 1, 1-dinene with perchloric acid
- (e) Ligand synthesis for multimetal complex: Preparation of bis- (N,N-disalicylidene ethylenediamine) μ-aquo-dicobalt
- (f) Synthesis and characterization of bispyridine iodide nitrate
- (g) Synthesis of zeolites and its characterization.

N.B.: New experiments will be introduced from time to time subject to the availability of chemicals and instrument.

SEMESTER IV (2-Year PG) / SEMESTER II (1-Year PG)

• Research thesis/ Project with minimum 1 conference paper. Peer reviewed research publication should be encouraged.

Course Code: CHMDIS 250620
Course Title: Research Project/Dissertation
Total Credit: 20

Duration: Six Months (*One Semester*)
Total Marks: 500 (Internal Assessment: 30%)

Course Outcomes: The students would be able to demonstrate and plan scientific research, and implement it within a reasonable time-frame. It is expected that after completing this project/dissertation, students will learn to work independently and how to keep accurate/readable record of their experimental works. In addition, students will be able to handle laboratory equipment and chemicals, and utilize sophisticated instruments for analysis, data collection and interpretation. Moreover, students will learn how to perform literature review and will be able to critically examine research articles, find out research gap and improve their scientific writing/communication and be able to disseminate their work by attending conferences.

2-Year PG/1-Year PG Programme

<u>Option C</u> – Only Research i.e. only research both in the 3^{rd} and 4^{th} semesters (2-Year PG) / Only research both in the 1^{st} and 2^{nd} semesters (1-Year PG) (*Total Credits: 40*)

SEMESTER III & IV (2-Year PG) / SEMESTER I & II (1-Year PG)

• Research thesis/Project with minimum 2 conferences papers. Peer reviewed research publication should be encouraged.

Course Code: CHMDIS 250140 Course Title: Research Project/Dissertation Total Credit: 40

Duration: One Year (*Two Semester*)
Total Marks: 1000 (Internal Assessment: 30%)

Course Outcomes: The students would be able to demonstrate and plan scientific research, and implement it within a reasonable time-frame. It is expected that after completing this project/dissertation, students will learn to work independently and how to keep accurate/readable record of their experimental works. In addition, students will be able to handle laboratory equipment and chemicals, and utilize sophisticated instruments for analysis, data collection and interpretation. Moreover, students will learn how to perform literature review and will be able to critically examine research articles, find out research gap and improve their scientific writing/communication and be able to disseminate their work by attending conferences.

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