

Dhanamanjuri University

Master of Science in Chemistry

COURSE STRUCTURE OF
✓ 2-YR PG PROGRAMME
(FOUR-SEMESTERS PG PROGRAMME)

AND

1-YR PG PROGRAMME
(2-SEMESTERS PG COURSE)



2026

Department of Chemistry
School of Mathematical and Physical Sciences
Dhanamanjuri University
Imphal-795001
Manipur

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Dhanamanjuri University

Master of Science in Chemistry

COURSE STRUCTURE OF

**2-YR PG PROGRAMME
(FOUR-SEMESTERS PG PROGRAMME)**



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DHANAMANJURI UNIVERSITY

CURRICULUM AND CREDIT FRAMEWORK FOR POST GRADUATE

SL. No.	Programme	Eligibility	Curricular Components	NHEQF Level	Minimum credits	Credit Points (Level × Minimum credits)
1	1-Yr. PG (2-semester PG)	4-Yr. UG (Honours/Honours with Research) with a minimum of 160 credits	1 st Sem: Course Work 2 nd Sem: Course Work & Research	6.5	20 22	273
					42	
2	PG Diploma (2- Semesters PG)	3-Yr. UG with a minimum of 120 credits Or 4-Yr. UG (Honours/Honours with Research) with a minimum of 160 credits	1 st Sem: Course Work 2 nd Sem: Course Work	6	24 18	252
					42	
3	2-Yr. PG (4-Semester PG)	3-Yr. UG with a minimum of 120 credits Or 4-Yr. UG (Honours/Honours with Research) with a minimum of 160 credits	1 st Sem: Course Work 2 nd Sem: Course Work 3 rd Sem: Course Work 4 th Sem: Course Work & Research	6.5	24 18 20 20	273 260
					82	

**COURSE STRUCTURE OF 2-YR PG PROGRAMME
(FOUR-SEMESTERS PG PROGRAMME)**

TOTAL MARKS=2050

TOTAL CREDITS=82

SEMESTER I

Paper Code	Paper Type	Paper Title	Internal Assess. Marks	End-Sem. Marks	Total Marks	No. of Credits
CHE-501	DSC	ANALYTICAL CHEMISTRY	20	80	100	4
CHE-502	DSC	INORGANIC CHEMISTRY-I	20	80	100	4
CHE-503	DSC	ORGANIC CHEMISTRY-I	20	80	100	4
CHE-504	DSC	PHYSICAL CHEMISTRY-I	20	80	100	4
CHE-505	DSC	CHEMISTRY LAB-I	-	100	100	4
CHE-506	DSC	CHEMISTRY LAB-II	-	100	100	4
Total					600	24

- All papers are Core papers to be taken by every student.
- Total credit score is 24.

SEMESTER II

Paper Code	Paper Type	Paper Title	Internal Assess. Marks	End-Sem. Marks	Total Marks	No. of Credits
CHE-507	DSC	INORGANIC CHEMISTRY-II	20	80	100	4
CHE-508	DSC	ORGANIC CHEMISTRY-II	20	80	100	4
CHE-509	DSC	PHYSICAL CHEMISTRY-II	20	80	100	4
CHE-510	DSC	CHEMISTRY LAB-III	-	100	100	4
VAC-001	VAC/AEC			50	50	2
Total					450	18

- Four papers are Core papers to be taken by every student.
- One VAC paper of 2 credits is to be taken by every student.
- Total credit score is 18.

SEMESTER III

Paper Code	Paper Type	Paper Title	Internal Assess. Marks	End-Sem. Marks	Total Marks	No. of Credits
CHE-611	DSC	GROUP THEORY AND ITS APPLICATION IN CHEMISTRY	20	80	100	4
CHE-612	DSC	COMPUTATIONAL CHEMISTRY AND ITS TECHNIQUES	20	80	100	4
CHE-621	DSE	INORGANIC CHEMISTRY SPECIAL-I	20	80	100	4
CHE-622	DSE	INORGANIC CHEMISTRY SPECIAL-II	20	80	100	4
CHE-623	DSE	INORGANIC CHEMISTRY SPECIAL-LAB	-	100	100	4
CHE-631	DSE	ORGANIC CHEMISTRY SPECIAL-I	20	80	100	4
CHE-632	DSE	ORGANIC CHEMISTRY SPECIAL-II	20	80	100	4
CHE-633	DSE	ORGANIC CHEMISTRY SPECIAL-LAB	-	100	100	4
CHE-641	DSE	PHYSICAL CHEMISTRY SPECIAL-I	20	80	100	4
CHE-642	DSE	PHYSICAL CHEMISTRY SPECIAL-II	20	80	100	4
CHE-643	DSE	PHYSICAL CHEMISTRY SPECIAL-LAB	-	100	100	4
Total					500	20

*A third semester student has to –

- (i) Take two Core Theory papers i.e., CHE-611 and CHE-612 as common papers which are compulsory for every student.
- (ii) Opt one of the three sets as Elective (Specialization), with each set consisting of two theory papers and one practical paper:

Set 1: Inorganic Chemistry Special-CHE-621, CHE-622 and CHE-623

Set 2: Organic Chemistry Special-CHE-631, CHE-632, and CHE-633

Set 3: Physical Chemistry Special- CHE-641, CHE-642, and CHE-643

Total no. of credit per student: 20

SEMESTER-IV

Paper Code	Paper Type	Paper Title	Internal Assess. Marks	End-Sem. Marks	Total Marks	No. of Credits
CHE-613	DSC	CHEMICAL BINDING AND ATOMIC SPECTROSCOPY	20	80	100	4
CHE-614	DSC	PHYSICAL METHODS IN CHEMISTRY	20	80	100	4
CHE-624	DSE	INORGANIC CHEMISTRY SPECIAL-III	20	80	100	4
CHE-634	DSE	ORGANIC CHEMISTRY SPECIAL-III	20	80	100	4
CHE-644	DSE	PHYSICAL CHEMISTRY SPECIAL-III	20	80	100	4
CHE-R01	DSC	RESEARCH METHODOLOGY	10	40	50	2
CHE-R02	RESEARCH	RESEARCH WORK (PROJECT/DISSERTATION)	-	150	150	6
Total					500	20

*A fourth semester student has to-

- (I) Take two Core theory papers i.e., CHE-613 and CHE-614 as common papers
- (II) Opt one of the three sets, each set consisting of one Elective paper (Specialization)
 - Set 1: Inorganic Chemistry Special –III CHE-624
 - Set 2: Organic Chemistry Special –III CHE-634
 - Set 3: Physical Chemistry Special-III CHE-644

The student has to continue in the same specialization as in Semester-III

- (III) Take the core Research Components as compulsory papers consisting of two papers CHE-R01 and CHE-R02.

Total number of credit per student is 20.

****NOTE:**

1. **INTERNAL ASSESSMENT (20 MARKS) OF THEORY PAPERS IN ALL THE SEMESTERS WILL HAVE THE FOLLOWING COMPONENTS:**
 - (I) Written Test = 10 marks
 - (II) Seminar = 06 marks
 - (III) Attendance = 04 marks
2. **All Practical/lab papers, and VAC/AEC do not have internal assessment.**
3. **Research Paper CHE-R02 which consists of PROJECT/DISSERTATION will be assessed/evaluated as follows:**
 - (i) M.Sc. Project Work/Dissertation = 100 marks
 - (ii) Seminar Presentation and Viva Voce = 50 marks

SEMESTER I

Paper Code: CHE-501

Paper Type: DSC

Paper Name: ANALYTICAL CHEMISTRY

Credit = 4

Marks = 100

Course Objectives

CO1. Understand fundamental principles of analytical chemistry including sampling, evaluation of data, sources of errors, and statistical methods (F, Q, t-tests) to ensure accuracy and precision in qualitative and quantitative analysis.

CO2. Apply spectroscopic techniques (UV-Visible, IR, and Raman) for the identification, characterization, and quantitative analysis of chemical species, including metal complexes, while understanding selection rules and instrumental principles.

CO3. Develop skills in thermal and electroanalytical methods to determine composition and properties of compounds, such as using thermogravimetry for metal estimation and pH-metric, potentiometric, and conductometric titrations for analytical determinations.

CO4. Gain expertise in separation techniques like solvent extraction and chromatography (TLC, HPLC, GLC, LC) for qualitative and quantitative analysis, understanding the underlying mechanisms, efficiencies, and practical applications in complex mixtures.

Unit 1. Qualitative and quantitative aspects of analysis

Tools in analytical chemistry and their applications, Sampling, evaluation of analytical data, errors, accuracy and precision, statistical test of data; F, Q and t-test, rejection of data, and confidence intervals.

Unit 2. Spectroscopy

Origin of spectra, interaction of radiation with matter, fundamental laws of spectroscopy and selection rules, validity of Beer-Lambert's law.

Vibration spectroscopy: Basic principles of instrumentation, sampling techniques. Application of IR spectroscopy for characterization through interpretation of data, Effect and importance of isotope substitution. Introduction to Raman spectra.

UV-Visible Spectrometry: Basic principles of instrumentation, principles of quantitative analysis using estimation of metal ions from aqueous solution, Determination of composition of metal complexes using Job's method of continuous variation and mole ratio method.

Unit 3. Thermal analysis

Thermogravimetric analysis (TA); Differential Thermal Analysis (DTA) and Differential Scanning (DSC): Principles, instrumentation. Applications on thermal methods of analysis in inorganic and coordination compounds, organic compounds, polymers, analytical chemistry, coal and soil analysis, cement industry, refractory materials.

Unit 4. Separation techniques Solvent extraction

Classification, principle and efficiency of the technique. Mechanism of extraction: extraction by solvation and chelation. Technique of extraction: batch, continuous and counter current extractions. Qualitative and quantitative aspects of solvent extraction: extraction of metal ions from aqueous solution, extraction of organic species from the aqueous and nonaqueous media. Chromatography techniques: Classification, principle and efficiency of the technique. Mechanism of separation: adsorption, partition & ion exchange. Development of chromatograms: frontal, elution and displacement methods. Qualitative and quantitative aspects of chromatographic methods of analysis using LC, GLC, TLC and HPLC.

Course Learning Outcomes

By the end of the course, the students will be able to:

CLO1. Demonstrate understanding of qualitative and quantitative analysis, including proper sampling, error analysis, data evaluation, and application of statistical tests (F, Q, t-tests) to ensure accuracy and precision in experimental results.

CLO2. Apply principles of IR, Raman, and UV-Visible spectroscopy for the characterization of compounds, interpretation of spectral data, and quantitative estimation of metal ions and complex composition.

CLO3 Analyse thermal behaviour of compounds using thermogravimetric techniques and determine metal composition; perform pH-metric, potentiometric, and conductometric titrations to identify equivalence points and calculate pK_a values.

CLO4. Employ solvent extraction and chromatographic methods (LC, GLC, TLC, HPLC) for qualitative and quantitative separation and analysis of metal ions and organic species, understanding the underlying principles, mechanisms, and efficiency of each technique.

Essential/Recommended readings

1. Mendham, J., A. I. Vogel's Quantitative Chemical Analysis 6th Ed., Pearson, 2009.
2. Willard, H.H. et al.: Instrumental Methods of Analysis, 7th Ed. Wardsworth Publishing California, USA, 1988.
3. Christian, G.D, Analytical Chemistry, 6th Ed. John Wiley & Sons, New York, 2004.
4. Harris, D.C.: Exploring Chemical Analysis, 9th Ed. New York, W.H. Freeman, 2016.
5. Skoog, D.A. Holler F.J. & Nieman, T.A. Principles of Instrumental Analysis, Saunder College Publications, (1998).
6. Mikes, O. Laboratory Hand Book of Chromatographic & Allied Methods, Elles Harwood John Wiley 1979.
7. Ditts, R.V. Analytical Chemistry; Methods of separation, van Nostrand, 1974.
8. Khopkar, S. M., Basic Concepts of Analytical Chemistry, New Age (Second edition)1998
9. Skoog D.A., Holler F.J., Nieman T.A., Principles of instrumental analysis, 5th Edn., Brooks & Cole (1997). P

Paper Code: CHE-502

Paper Type: DSC

Paper Name: INORGANIC CHEMISTRY-I

Credit = 4

Marks = 100

Course Objectives

- CO1 Explain mechanisms and dynamics of inorganic substitution reactions, particularly in coordination complexes.
- CO2 Familiarize students with the principles, techniques, and applications of radiochemistry and radioisotopes.
- CO3 Develop experimental insight into how modern techniques like G-M and Scintillation counters are used in inorganic chemistry. Create awareness about environmental chemical processes and the impact of pollutants on air, water, and soil.
- CO4 Develop experimental insight into how modern techniques like G-M and Scintillation counters are used in inorganic chemistry.
- CO5 Explore the synthesis, bonding, and reactivity of organometallic complexes, especially those involving CO, NO, N₂ ligands, and metallocene, and to understand their roles in homogeneous catalysis.

Unit 1: Inorganic Reaction-I

Nature of substitution reactions, classification of nucleophilic substitution reaction (ligand substitution reaction), mechanism of ligand substitution reactions, and their reaction profiles (energy profiles). Factors affecting the rate of ligand substitution reactions. Lability and inertness of the octahedral complexes based on VBT and CFT. Acid hydrolysis and base hydrolysis reactions of Co (III) complexes.

Unit 2: Radiochemistry and Applications

Radiochemistry, different types of nuclear reactions, interactions of radiations with matter, Q-energy, cross section, G-M and Scintillation Counters. Typical reactions involved in preparation of radioisotopes (³H, ¹⁴C, ²²Na, ¹³⁷I, ^{99m}Tc and ³²P). Applications of radioisotopes, radio diagnostics and radiopharmaceuticals, physiochemical applications, diffusion coefficients, solubility of substances agricultural and analytical applications, neutron activation analysis and X-ray fluorescence.

Unit-3 Organometallic Chemistry-I

Definition and Classification with appropriate examples based on the nature of metal-carbon bond (ionic, s, p, and multicentre bonds). Structures of methyl lithium, Zeiss salt, and ferrocene. EAN rule as applied to carbonyls. Preparation, structure, bonding, and properties of mononuclear and polynuclear carbonyls of 3d metals. p-acceptor behavior of carbon monoxide. Synergic effects (VB approach)- (MO diagram of CO can be referred to for synergic effect to IR frequencies). Synthesis, structure, bonding, and reactivity of complexes with CO, NO, and N₂. Organometallic

reagents in homogeneous catalytic reactions. Metallocene- synthesis of cyclopentadienyl compounds, reaction of ferrocene-like molecules, and structure of cyclopentadienyl compounds.

Unit 4: Environmental Chemistry

Air Pollution: Gases and particulate pollutants formation and their effects. Water Pollution: Toxicity and biochemical effects of arsenic, cadmium, lead, and mercury. Biochemical effects of pesticides-DDT, organophosphate, organochlorine, and malathion; algae nutrients and eutrophication. Water quality parameters DO, BOD, COD, conductivity, pH, alkalinity, and hardness) and its determination; industrial, municipal water treatment processes; and wastewater treatment (primary, secondary, and tertiary). Soil pollution: Industrial and urban waste, agricultural practice, municipal garbage; adjustment of soil acidity, ion-exchange in soil.

Course Learning Outcomes

- CLO1 Describe radiochemistry, apply radioisotope techniques in various fields, and evaluate neutron activation and X-ray fluorescence for elemental analysis.
- CLO2 Explain atmospheric structure and reactivity, assess sources and impacts of pollutants, and evaluate environmental issues related to air, water, and soil chemistry.
- CLO3 Analyse the synthesis, bonding, and reactivity of organometallic complexes involving ligands such as CO, NO, and N₂, and evaluate their roles in homogeneous catalysis and the structure and reactivity of metallocenes like ferrocene.
- CLO4 Explain nucleophilic substitution mechanisms in coordination complexes, interpret their kinetics, and analyze the reactivity of Co (III) complexes using VBT and CFT.

Reference Textbook:

1. Advanced Inorganic Chemistry; F A Cotton, Wilkinson; Wiley International
2. Essential Nuclear Chemistry; H J Arnikar; New Age International
3. Mechanism of Inorganic reactions; F Basolo, R G Pearson; Wiley-Eastern Ltd
4. Principles of Inorganic Chemistry; B R Puri, LR Sharma, K C Kalia; Milestone Publishers and distributors
5. Environmental Chemistry; A K Dey; New age International
6. Environmental Chemistry; H Kaur; Pragati Edn.
7. Environmental Chemistry; P S Sindhu; New Age International

Paper Code: CHE-503

Paper Type: DSC

Paper Name: ORGANIC CHEMISTRY-I

Credit = 4

Marks = 100

COURSE OBJECTIVES (COs)

- CO1.** Analyze the three-dimensional arrangements of atoms in molecules, identify molecular symmetry elements, and understand how these spatial properties dictate physical behavior, spectroscopic activity, and chemical reactivity and Apply stereochemical principles to understand reaction mechanisms (e.g., stereoselectivity and stereospecificity).
- CO2.** Understand the structure and stability of reactive intermediates and also analyse the factors affecting reactivity and rearrangement of reactive intermediates, including neighbouring group participation and molecular rearrangements in acyclic and monocyclic systems.
- CO3.** Explore the generation mechanisms and reaction pathways of carbanions, free radicals, carbenes, nitrenes, and benzyne, and apply the HSAB principle in predicting reactivity. Evaluate the synthetic and mechanistic roles of reactive intermediates in organic chemistry, including ipso-effects, cage effects, and ambident ion reactions.
- CO4.** Utilize light (photons) rather than heat to drive chemical transformations and understanding the interaction between light and matter, reaction mechanisms, and the synthetic application of photoinduced processes in carbonyl groups, alkenes and dienes; photo-induced reactions like Norrish cleavages and Paterno-Büchi reactions, di- π -methane rearrangement, Barton reaction.
- CO5.** To equip students with the conceptual tools to analyse and predict pericyclic reactions, using molecular orbital theory, Woodward-Hoffmann rules, and frontier molecular orbital approaches, covering electrocyclic, cycloaddition, and sigmatropic rearrangements.

Unit.1 Molecular Symmetry and Stereochemistry

Molecular symmetry and chirality, stereogenicity, homotopic, enantiotopic and diastereotopic relationships, pro-chiral relationships Asymmetric synthesis-enantioselective and diastereoselective synthesis, regio-selectivity, stereospecificity, stereoselectivity, molecular dissymmetry and chiroptical properties, CD and ORD curves, Octant rule, resolution of enantiomers. Conformational analysis of acyclic systems and cyclohexane derivatives. Atropisomerism-nomenclature and reactivity, stereoisomerism in biphenyl systems

Unit.2 Study of Reactive Intermediates

Carbocations: Classical and non-classical, structures, stability and reactivity, neighboring group participations, molecular rearrangement in acyclic and monocyclic systems. Carbanions: generation, structure and stability; ambident ions and their general reactions, HSAB principle and its applications. Free radicals: Generation, structure, stability and reactions, Cage effects, Carbenes: Formation and structure, reactions involving carbenes Nitrenes: Generation, structure, and reactions Benzyne: Generation, structure and rearrangements, Ipso-effects.

Unit.3 Photochemistry

General principles, orbitals symmetry consideration related to photochemical reaction, photochemistry of carbonyl groups, Norrish Type I and Type II cleavage, photochemistry of alkenes and dienes, photochemistry of aromatic compounds and cycloaddition, Paterno-Buchi reaction, Barton reaction, Hofmann-Löffler-Freytag Reaction, Photo-Fries rearrangement.

Unit.4 Pericyclic Reactions

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Woodward-Hoffmann correlation diagrams. Frontier molecular orbital and Perturbational molecular orbital approach. Electrocyclic reactions: conrotatory and disrotatory motions. Cycloaddition: antarafacial and suprafacial additions. $4n$ and $4n + 2$ systems, $2 + 2$ addition of ketenes, 1,3-dipolar cycloadditions and cheletropic reactions. Sigmatropic rearrangements. Claisen, Cope and Aza-Cope rearrangements.

COURSE LEARNING OUTCOMES (CLOs):

After successful completion of this course, students will be able to:

- CLO1. Analyze and predict stereochemical and conformational behavior of organic molecules, understand concepts of molecular symmetry and chirality, stereoselective and stereospecific synthesis in complex organic transformations.
- CLO2. Understand and analyze the generation, structure, stability, and reactivity of key reactive intermediates (carbocations, carbanions, free radicals, carbenes, nitrenes, benzyne) and apply this knowledge to predict mechanisms, rearrangements, and reactivity.
- CLO3. Analyse and predict photochemical transformations of alkenes, carbonyls, and aromatic systems using orbital symmetry considerations, and apply key concepts such as Norrish Type I and II reactions, Paternò-Büchi cycloadditions, di- π -methane rearrangement, Barton reaction.
- CLO4. Interpret and predict the outcomes of pericyclic reactions using molecular orbital symmetry, Woodward-Hoffmann rules, and frontier molecular orbital (FMO) approaches, with a focus on electrocyclic, cycloaddition, and sigmatropic rearrangements.

Text Books:

1. Organic Chemistry; J Clayden, N Greeves, S Warren; Oxford
2. Basic Stereochemistry of Organic Molecules, Subrata Sengupta; Oxford
3. Reactive Intermediate Chemistry, Robert A. Moss, Matthew S. Platz, Maitland Jones Jr.; Wiley
4. Introduction to Organic Photochemistry, J. D. Coyle; Wiley
5. Advanced Organic Chemistry; J March; John Wiley & Sons 1992
6. Stereochemistry of Organic Compounds; D Nasipuri; Wiley Eastern Limited
7. Stereochemistry, Conformation and Mechanism; P S Kalsi; New Age International
8. Frontier Orbital Theory and Organic Chemical Reactions; L Flemming; John-Wiley and Sons
9. Conservation of Orbital Symmetry; R B Woodward, R Hoffman; Verely-Chemist Academic Press

Paper Code: CHE-504

Paper Type: DSC

Paper Name: PHYSICAL CHEMISTRY-I

Credit = 4

Marks = 100

COURSE OBJECTIVES (COs):

- CO1. Introduce mathematical tools essential for chemical sciences, enabling students to analyse and interpret experimental data with statistical techniques.
- CO2. Build proficiency in differential and integral calculus, matrix operations and solving systems of linear equations, essential for quantum mechanics, spectroscopy, and thermodynamics.
- CO3. To introduce the fundamental principles of quantum mechanics through black-body radiation, photoelectric effect, wave-particle duality, uncertainty principle, and the concept of wave functions and operators, apply Schrödinger's equation to basic quantum systems such as free particles, particle in a box, rigid rotator, simple harmonic oscillator, and hydrogen atom.
- CO4. To develop an understanding of the mathematical framework of quantum mechanics, including normalization, orthogonality, eigen functions, eigen values, and boundary conditions.
- CO5. To provide conceptual insight into the quantum mechanical description of atoms and molecules

Unit 1 Basic Quantum Chemistry

Introduction to black-body radiation and distribution of energy, photo-electric effect, concept of quantization, wave particle duality (de-Broglie's hypothesis), classical wave equation and Schrodinger equation, wave function and conditions for acceptable wave function, quantization, normalization and orthogonality. Postulates of Quantum mechanics, Linear and Hermitian operators, Commutation of operators. Angular momentum operators, Eigen values and eigen-functions. Commutation rules.

Unit 2 Application to simple system

Some exactly solvable problems: Particle in a box (1-D, 2-D & 3-D). Concept of degeneracy. Tunnelling, Simple Harmonic Oscillator problem and its solution using series solution or factorization method. Schrödinger equation, transformation to spherical polar coordinates. Separation of variables. Spherical harmonics. Discussion of solution. Particle in a ring, sphere, and Rigid rotator model of rotation of diatomic molecule. Hydrogen atom and hydrogen like atoms, ϕ , θ and r -equation, radial plots, Shapes of s, p and d-orbitals.

Unit 3 Multi-electron systems and Approximation methods:

Many-electron system (He), Many electron atoms and their wave functions, symmetrical and anti-symmetrical wave functions. Approximation methods, Variation theorem and linear Variation function. Time independent first order perturbation theory for non-degenerate case, ground state and first excited atom. Application of variation methods and perturbation method to Helium atom,

Unit.4 Molecular Orbital Calculations

The n-electron theory of conjugated molecules, Huckel approximations. Huckel treatment of ethylene, allyl, cyclopropyl, 1,3-butadien, and benzene. Calculation of energy and molecular orbital functions resonance energy/electron densities, charge distribution, bond order and free valence indices. Diagrammatic methods for calculating Huckel energies, energy and wave function for π -system with heteroatom (formaldehyde). Extended Huckel theory and its simple chemical applications, Zero differential overlap, introduction to semi-empirical methods.

COURSE LEARNING OUTCOMES (CLOs):

After successful completion of this course, students will be able to:

- CLO1. Apply statistical methods to interpret and analyse chemical data, perform numerical differentiation and integration.
- CLO2. Use fundamental concepts of calculus to solve chemistry-related problems.
- CLO3. Understand and apply the fundamental concepts of quantum mechanics such as black-body radiation, photoelectric effect, wave-particle duality, uncertainty principle, and Schrödinger equation to describe microscopic systems.
- CLO4. Analyse and solve basic quantum mechanical models including the free particle, particle in a box, simple harmonic oscillator, rigid rotator, and hydrogen atom to determine wave functions, energy levels, and degeneracies.
- CLO5. Interpret the mathematical formalism of quantum mechanics through wave functions, normalization, orthogonality, operators, eigenvalues/eigenfunctions, and spherical harmonics, and relate them to physical significance.
- CLO6. Compare and evaluate quantum mechanical models of bonding (Valence Bond theory and Molecular Orbital theory) for simple diatomic systems such as H_2 and H_2^+ , highlighting their applications and limitations.

TEXT BOOKS:

1. Mathematical Methods in the Physical Sciences, 3ed, by Mary L. Boas, Wiley.
2. Mathematical Methods for Physics and Engineering by Ken F. Riley, Mike P. Hobson, et al. Cambridge.
3. Mathematics for Chemistry and Physics; George Turrell; Academic Press, 2002.
4. Mathematical Methods for Physical and Analytical Chemistry; David Z. Goodson; Willey 2011.
5. Theory and Problems of Vector Analysis; Murray R Spiegel; Schaum's Outline series.
6. Theory and Problems of Matrices; Frank A Jr.; Schaum Publishing Co.
7. Arfken G. B., Weber, H. J., et al., Mathematical Methods for Physicists: A Comprehensive Guide. Elsevier.
8. Pilar F. L. Elementary Quantum Chemistry 2nd Ed., Dover Publication Inc.: N.Y.(2001).
9. McQuarrie, D.A, Quantum Chemistry, Viva Publication.
10. Levin, I. N., Quantum Chemistry; Tata McGraw Hill
11. Atkins, P. W, Friedman, R., Molecular Quantum Mechanics, Oxford University Press
12. McQuarrie, D.A. & Simon, J.D. Physical Chemistry: A Molecular Approach 3rd Ed., Univ. Science Books (2001).

TEXT BOOKS:

1. Molecular Quantum Mechanics; Peter Atkins Ronald Friedman; Oxford University Press
3. Fundamentals of Quantum Mechanics; James E House
4. Quantum Chemistry; J P Lowe, K A Peterson

5. Principles of Quantum Mechanics as Applied to Chemistry and Chemical Physics; D D Fitts; Cambridge University Press
6. Physical Chemistry; PW Atkins; Oxford University Press
7. Statistical Mechanics 3rd Edn.; R K Patharia, P D Beale; Elsevier
8. Statistical Mechanics; D A McQuarrie; Harpar and Row
9. An introduction to Statistical Thermodynamics; Terrell L Hill; Addison-Wesley Publishing Company Inc.
10. Statistical Thermodynamics, Fundamentals and applications; N M Laurendeau; Cambridge
11. Statistical Thermodynamics; M C Gupta; Wiley Eastern
12. Chemical Kinetics; K J Laidler; McGraw Hill

Paper Code: CHE-505

Paper Type: DSC

Paper Name: CHEMISTRY LAB-I

Credit = 4

Marks = 100

INORGANIC CHEMISTRY PRACTICAL

Learning Objectives:

- Develop students' proficiency in quantitative analytical techniques through hands-on experience in volumetric (redox and complexometric) and gravimetric methods for accurate estimation of components in mixtures, alloys, and minerals.
- Enable students to synthesize coordination and inorganic compounds and to characterize them using physical techniques such as magnetic susceptibility, conductivity, infrared (IR), and UV-Visible spectroscopy for understanding their structural and electronic properties.

Course Learning Outcomes:

- Demonstrate the ability to accurately perform and interpret quantitative estimations using volumetric (redox and complexometric) and gravimetric methods for multi-component mixtures, alloys, or minerals, ensuring precision in analytical chemistry practices.
- Synthesize coordination and inorganic compounds and analyze their structure and bonding using physical characterization techniques such as magnetic susceptibility, conductivity measurements, IR, and UV-Visible spectroscopy.

EXPERIMENTS:

1. Quantitative estimation involving volumetric (redox and complexometric) and gravimetric methods of analysis of two/three components in mixture/alloys/minerals.
2. Preparation and characterization (physical studies, which include magnetic susceptibility, conductivity measurement, IR, UV-Visible) of inorganic compounds.
 - i [Cu(NH₃)₄]SO₄.H₂O
 - ii Ni(DMG)₂
 - iii Prussian Blue
 - iv Turnbull's Blue
 - v [Co(en)₂]Cl₂
 - vi Na₃[Fe(C₂O₄)₃].3H₂O

Reference Textbook:

1. Vogel's Textbook of Quantitative Inorganic Analysis revised; J. Bassett, R.C. Denny, G.H. Jeffery, J. Mendham; ELBS/Longman
2. A Textbook of Macro and Semimicro Qualitative Inorganic Analysis; A.I Vogel; Orient Longman Ltd.
3. Advanced Practical Inorganic Chemistry book; Gurdeep Raj; Meerut: Krishna Prakashan
4. Analytical Chemistry; S.K. Agarwal, Keemti Lal; Meerut: Krishna Prakashan

Paper Code CHE-506
Paper Type DSC
Paper Name CHEMISTRY LAB-II
Credit = 4
Marks = 100

ORGANIC CHEMISTRY PRACTICAL

COURSE OBJECTIVES (COs):

- CO1. Identifying organic compounds of complex nature through physical characteristics and functional group analysis.
- CO2. Performing the separation of binary organic mixtures using appropriate chemical and physical techniques.
- CO3. Conducting confirmatory tests and preparing suitable derivatives for conclusive identification.
- CO4. Applying analytical reasoning and laboratory techniques in organic qualitative analysis with proper safety and documentation.

Experiments:

1. Systematic Qualitative analysis of unknown organic compounds of simple bifunctional groups, e.g., salicylic acid, cinnamic acid, nitrophenols, sulphanilic acid, anthranilic acid, etc.,
2. Identification of an organic compound of complex nature, separation of an organic mixture containing two simple compounds and their identification (complete systematic identification with preparation of derivatives is required)
3. Preparation of simple organic compounds involving not more than two stages. Preparation of TLC plates and separation techniques.
4. Quantitative estimation of protein using Lowry's method. Determine the concentration of the unknown sample.
5. Action of salivary amylase at optimum conditions.
6. Isolation of DNA from E Coli/chicken liver/plant parts etc.
7. Qualitative identification and quantitative estimation of different biomolecules.
8. Other experiments suggested.

Text Books:

1. Vogel's Qualitative Organic Analysis
2. Organic Chemistry Manual

SEMESTER II

Paper Code CHE-507

Paper Type DSC

Paper Name INORGANIC CHEMISTRY-II

Credit = 4

Marks = 100

Learning Objectives:

- Understand the fundamental principles of magnetochemistry, including the classification of magnetic substances, origin of magnetic behaviour, spin-orbit coupling, and the application of crystal field theory to interpret magnetic and optical properties of coordination compounds.
- Explain mechanisms and dynamics of inorganic substitution reactions, particularly in coordination complexes.
- Explain Crystal Field Theory, interpret metal-ligand interactions, discuss the Nephelauxetic effect, and apply Molecular Orbital Theory to coordination complexes.
- Examine metal-ligand equilibria in solution, focusing on the stability constants, chelate effect, distribution diagrams, and the techniques for determining complex composition and stability, including spectrophotometry and pH-metric methods.
- Provide foundational knowledge of nanomaterials, their historical development, and nanoscale phenomena such as surface energy, self-assembly, and quantum effects.

Course Learning Outcomes: On completion a student will be able to-

- Explain nucleophilic substitution mechanisms in coordination complexes, interpret their kinetics, and analyze the reactivity of Co (III) complexes using VBT and CFT.
- Interpret metal-ligand equilibria in solution, including stepwise and overall formation constants, chelate effect, and use of spectrophotometric and pH-metric methods to determine composition and stability of complexes; understand their significance in EDTA titrations and solvent extraction.
- Explain the origin of magnetic properties in coordination compounds, classify magnetic materials, and apply crystal field theory and term symbols to interpret spin states, spin-orbit coupling, and magnetic behaviour, including spin crossover phenomena.
- Differentiate and describe mechanisms of inorganic electron transfer reactions, including one- and two-electron processes, isomerization, racemization, and factors affecting reaction rates in both complementary and non-complementary systems.
- Develop an understanding of nanomaterials and composites, focusing on synthesis, structural control, and applications of inorganic compounds. Explore diverse applications of nanomaterials in catalysis, environmental remediation, and biomedical fields, highlighting structure-function relationships

Unit 1: Magneto Chemistry-1

Classification of magnetic substances, origin of magnetic properties. Spin-orbit coupling, quenching of orbital momenta, temperature-independent paramagnetism, determination of magnetic susceptibility using Guoy's method, Term symbols for metal ions, crystal field theory and its applications to explain magnetic properties of coordination compounds, spin crossover, magnetic and optical properties.

Unit-2: Metal Ligand Equilibria in solution

Equilibria involving complexes and their distribution diagram. Formation constant (stepwise and overall). Factors affecting the stability of metal complexes with reference to the nature of the metal ion and ligand, the chelate effect, and its thermodynamic origin. Determination of composition and stability of complex ions in solution by spectrophotometric and pH-metric methods, conditional stability constant, and their importance in complexometric (EDTA) titration and solvent extraction of metal ions.

Unit-3: Inorganic Reaction -II

Electron transfer reactions: definition, types of electron transfer reactions, their characteristics and mechanisms, one-electron and two-electron transfer reactions, factors affecting the rates of direct electron transfer reactions, complementary and non-complementary electron transfer reactions. Isomerization and racemization reactions elementary ideas.

Unit 4: Nanomaterials in Inorganic Chemistry

Introduction to nanoscience, nanostructure and nanotechnology (basic idea), Overview of nanostructures and nano-materials, classification, (cluster, colloid, nanoparticles, and nanostructures -Spheroid, Wire, Rod, Tube, and Quantum Dot); Size dependent properties of nanomaterials (basic idea with few examples only): Quantum confinement, Electrical, Optical (Surface Plasmon resonance), variation in colours (Blue shift & Red shift), Magnetic, thermal and catalytic properties. Synthesis of Nanomaterials: Brief introduction about Top-down and Bottom-up approaches & self-assembly techniques of nanoparticles synthesis, hydrothermal/solvothermal process. Characterization basic idea only: Electron microscopic technique, diffraction technique, photoelectron spectroscopy, zeta potential measurement; and Applications in environmental remediation and biology.

Reference Textbooks:

1. Determination and use of stability constants; A F Martell, R J Motekaitis; Wiley VCH
2. Inorganic Chemistry; James E. House; Elsevier, 2009
3. Chemistry of Complex Equilibria; M T Beck; Van Nostrand Reinhold Company
4. Essential Nuclear Chemistry; H J Arnikar; New Age International
5. Mechanism of Inorganic reactions; F Basolo, R G Pearson; Wiley-Eastern Ltd
6. Principles of Inorganic Chemistry; B R Puri, L R Sharma, K C Kalia; Milestone Publishers and distributors
7. Environmental Chemistry; S E Manahan; Lewis Publishers
8. Organometallic Chemistry; R C Mehrotra, A Singh; New Age International
9. Nanomaterials: An Introduction to Properties, Synthesis and Applications by Emmanuel Craig (Editor)
10. Nanomaterials Chemistry: Recent Developments and New Directions by C. N. R. Rao, Wiley
11. Nano: The Essentials by T. Pradeep, McGraw-Hill Education

Paper Code CHE-508

Paper Type DSC

Paper Name ORGANIC CHEMISTRY-II

Credit = 4

Marks = 100

COURSE OBJECTIVES (COs):

CO1. Develop an in-depth understanding of the reaction mechanism of elimination, nucleophilic substitution, electrophilic aromatic substitution, addition reactions, including nucleophilic acyl substitution, conjugate addition, polymerisation, and umpolung strategies for synthetic applications.

CO2. Enable students to explore the chemistry of five-membered heterocycles with two heteroatoms, six membered heterocycles with two nitrogen heteroatoms, focusing on their synthesis, mechanisms of electrophilic/nucleophilic substitution reactions

CO3. Explore the chemistry of carbohydrates and lipids, emphasizing stereochemistry, reactions, conformational analysis, and their importance in biological recognition and membrane structure.

CO4. Gain insights into the chemical structure and function of biomolecules, including amino acids, peptides, proteins, and nucleic acids, and understand their biological roles and synthetic methodologies.

Unit 1. Reaction Mechanism

Elimination reactions: E1, E2, E1cb and E_i; Saytzeff and Hoffmann elimination, Syn and anti elimination.

Substitution Reactions: S_N¹, S_N², S_Nⁱ, elimination vs substitution; Electrophilic aromatic substitution reactions: Electrophilic substitution to aromatic hydrocarbons: benzene, naphthalene, n-annulene heteroannulene, fullerene (C₆₀).

Addition Reaction: Electrophilic and nucleophilic addition reactions. Syn and anti addition; nucleophilic addition-elimination, reaction of α, β-unsaturated carbonyl compounds (conjugate addition reactions), 1,3-dithiane reactivity, Umpolung effect.

Polymerization: Chain-Growth (Addition) Polymerization, Step-Growth (Condensation) Polymerization, Cationic Polymerization Mechanism, Anionic Polymerization Mechanism.

Unit 2. Five membered heterocycles (2 heteroatoms)

Synthesis of 1,2-azoles and 1,3-azoles, nucleophilic and electrophilic substitution reactions.

Six membered heterocyclic compounds with two heteroatoms: Synthetic methods and reactions- Pyridazines, Pyrimidines, Pyrazines.

Unit 3. Biomolecules-I:

Carbohydrates: Stereochemistry, reaction and conformation of monosaccharides, glycosides, epimerization and mutarotation, polysaccharides: structure and functions, Polysaccharides of

industrial and biological importance, dextran, sialic acids, cell-cell recognition and blood group substances.

Lipids: Classification and biological importance of fatty acids and lipids, stereochemical notations in lipids, properties of lipids aggregates, micelles, bilayer, lysosomes and biological membranes.

Unit 4. Biomolecules- II

Proteins: Structure and properties of essential amino acids, Nomenclature and sequencing of polypeptides, Merrifield polypeptide synthesis, Combinatorial synthesis of peptides, Primary, Secondary and Tertiary structures of proteins.

Nucleic Acids: Structure of nucleic acid bases, nucleosides and nucleotides, DNA organization, replication, transcription, genetic code and protein biosynthesis. polymorphic nature of DNA, multistranded DNA structures, Synthetic DNA- PNA, LNA, UNA

COURSE LEARNING OUTCOMES (CLOs):

After successful completion of this course, students will be able to:

CLO1. Understand and apply the mechanisms of elimination, nucleophilic.electrophilic substitution and addition reactions mechanism including special reactivity such as the Umpolung effect and conjugate addition, with emphasis on regio- and stereoselectivity.

CLO2. Interpret the synthesis and biological roles of azoles and six-membered heterocycles with two heteroatoms and their importance in biomolecules such as coenzymes and vitamins.

CLO3. Explain the stereochemistry, conformation, and biological significance of carbohydrates and lipids, including polysaccharides, fatty acids, and lipid aggregates.

CLO4. Describe the structure and biosynthesis of biomolecules, including amino acids, peptides, proteins, and nucleic acids, and explain synthetic methods like Merrifield and combinatorial peptide synthesis.

Text Books:

1. Advanced Organic Chemistry; J March; John Wiley & Sons 1992
2. Modern Synthetic Reactions; H O House; W A Benzamin; New York and Menlo Park, California
3. Outlines of Biochemistry; E S Cohn, R K Stumpf; Wiley Eastern
4. Organic Chemistry; J Clayden, N Greeves, S Warren; Oxford
5. Heterocyclic Chemistry Synthesis, Reactions and Mechanism, R K Bansal; Wiley-Eastern, New Age International

Paper Code CHE-509

Paper Type DSC

Paper Name PHYSICAL CHEMISTRY-II

Credit = 4

Marks = 100

COURSE OBJECTIVES (COs):

- CO1. Understand the interaction between electromagnetic radiation and matter through the time-dependent Schrödinger equation, transition moment integral, and Einstein coefficients.
- CO2. To understand atomic structure and spectra, term symbol, coupling schemes. Rotational spectra of molecules.
- CO3. Gain fundamental knowledge of UV-Vis and IR spectroscopy, including electronic transitions, selection rules, solvent effects, and interpretation of functional group vibrations and Raman spectra.
- CO4. Explore the principles and applications of fluorescence spectroscopy, including fluorescence lifetime, quantum yield, quenching mechanisms, and relevant instrumentation.

Unit 1 Atomic and Rotational Spectroscopy:

Atomic spectroscopy: Elements of atomic spectroscopy; electron spin and space quantization, orbital and spin angular momentum. Coupling of angular momenta; Spin-orbit coupling (angular momentum operators) Russell-Saunders coupling, LS-coupling, JJ coupling. Hund's rule, equivalent and non-equivalent orbitals, Atomic term symbols and spectroscopic states (microstates), multiplet structure; atomic spectra of one-electron and two-electron systems; magnetic properties of atoms, normal Zeeman effect.

Rotational spectroscopy: Rotational spectra of diatomic and linear molecules; rigid rotator; selection rules, intensities of spectral lines, determination of bond lengths of diatomic and linear triatomic molecules, isotopic substitution effect.

Unit 2 Vibrational and Infrared Spectroscopy:

Vibrational spectroscopy: Harmonic and anharmonic oscillators; Morse potential energy functions; vibrational energy level of a diatomic molecules; Zeropoint energy; selection rule and spectral transitions. Vibrational spectra: P, Q, R branches; overtones, hot bands, and combination bands. Fermi resonance, hydrogen bonding.

Infrared spectroscopy: General outlines on instrumentation and sample handling for infrared spectroscopy, Selection rules, types of infrared bands: fundamental, overtones, and combination bands; Fermi resonance, characteristic of different functional group frequencies and interpretation of IR spectra.

Unit 3 Electronic Spectroscopy:

Electronic transitions and selection rules, relative energies of the excited states; effect of solvent effects on electronic transitions

Born-Oppenheimer approximation, vibrational coarse structure, Frank-Condon principle and electronic spectra of diatomic molecules., Frank-Condon overlap integral, Dissociation, Pre-

dissociation, fluorescence and phosphorescence, photoelectron spectroscopy, calculation of electronic transitions of polyenes using free electron model, photoelectron spectra of simple molecules, Electron Spectroscopy of Chemical Analysis (ESCA), Auger electron spectroscopy, charge transfer spectra.

Unit 4 Mossbauer and Fluorescence Spectroscopy

Mossbauer Spectroscopy: Principles of Mossbauer Effect, isomer shift, quadruples splitting, magnetic hyperfine interaction, applications of Mossbauer spectroscopy.

Fluorescence Spectroscopy Phenomenon of Fluorescence, and characteristics of fluorescence, life-time and quantum yields; Fluorescence quenching: Stern-Volmer equation, mechanism and dynamics; fluorescence anisotropy. Instrumentation and applications.

Text Books:

1. High Resolution NMR; E Beaker; Academic Press.
2. Fundamental of Molecular Spectroscopy; C N Banwell; Tata McGraw Hill.
3. Organic Spectroscopy; W Kemp; Educational Low-Price Book Scheme and Tata McMillan Press Ltd.
4. Ultraviolet and Visible Spectroscopy; C N Rao; Butterworth
5. Spectroscopy Identification of Organic Compounds; R.M. Silverstein, G C Bassler; John-Wiley and Sons Inc.
6. Spectroscopy of Organic Compounds; P S Kalsi; New Age International
7. Physical Methods in Chemistry; R S Dargo; Saunders College Publishers.
8. Spectroscopic Methods of Organic Chemistry; D H Williams, Tata-McGraw Hills
9. Instrumental Analysis; D A Skoog, F J Holler; S R Crouch; Brooks/Cole

Paper Code CHE-510
Paper Type DSC
Paper Name CHEMISTRY LAB-III
Credit = 4
Marks = 100

PHYSICAL CHEMISTRY PRACTICAL

Experiments:

1. Determination of surface excess concentration and critical micelle concentration (CMC) of a given surfactant using tensiometer (**Instrument (s) or Technique (s) to be used: Tensiometer**)
2. Construction of a ternary phase diagram for a three-component system-water, acetic acid, and benzene/toluene/chlorobenzene/CCl₄/cyclohexane/ethylenediamine; and study the effect of at least two different concentrations of NaCl/KCl for the same composition (**Instrument (s) or Technique (s) to be used: Acid-base titration**)
3. Determination of order of reaction for saponification of ethyl acetate by NaOH and hence its rate constant. Also study the effect of the presence of NaCl/KCl at least two different concentrations (**Instrument (s) or Technique (s) to be used: pH meter, Acid-base titration**)
4. Determination of critical micelle concentration (CMC) and counter ion binding of an anionic surfactant in presence of an ionic salt such as NaCl or KCl (**Instrument (s) or Technique (s) to be used: Conductometer, Conductometric titration**)
5. Determination of acid-base dissociation constant of a given weak acid in water and in presence of an organic solvent (**Instrument (s) or Technique (s) to be used: pH meter, Acid-base titration**)
6. To find the strength of HCl and acetic acid in a mixture of both by titrating it against NaOH solution (**Instrument (s) or Technique (s) to be used: pH meter, Acid-base titration**)
7. To find out the complexation of ferric ion-thiocyanate complex by Job's method (**Instrument (s) or Technique (s) to be used: UV-Visible spectrophotometer**)
8. Determination of acid and basic dissociation constant (pK_a and pK_b) of an amino acid, and hence the isoelectric point of the acid with the help of pH meter (**Instrument (s) or Technique (s) to be used: pH meter, Acid-base titration**)
8. To study the formation of complex formed between Fe²⁺ ion and o-phenanthroline by Job's method (**Instrument (s) or Technique (s) to be used: UV-Visible spectrophotometer**)
9. To study and evaluate the oscillatory strength of the electronic spectra of diiodine (I₂) in various solvents using a UV-Visible spectrophotometer (**Instrument (s) or Technique (s) to be used: UV-Visible spectrophotometer**)
10. To plot the potential energy curve of hydrogen molecule by Hartree Fock method using STO-3G and 3-21G basis sets (**Instrument (s) or Technique (s) to be used: Computational calculation employing principle of quantum chemistry with help of quantum mechanical software like ORCA or Gaussian**)
11. To determine Peak Width at Half Max (PWHM), silver atom per silver nanoparticle and concentration of silver nanoparticle using spectrophotometer (**Instrument (s) or Technique (s) to be used: UV-Visible spectrophotometer**)
12. Prepare gold nanostructures by reducing auric chloride with tea extract in presence of CTAB as capping agent, and characterize spectrophotometrically (**Instrument (s) or Technique (s) to be used: UV-Visible spectrophotometer**)
13. Prepare CdS nanoparticles and record their UV/Vis spectra (**Instrument (s) or Technique (s) to be used: UV-Visible spectrophotometer**)

***Note: In Practical exam, one question from each section is compulsory.**

1. Experimental Physical Chemistry; F A Bettelheim
2. Experimental Physical Chemistry; G P Matthews
3. Experimental Physical Chemistry; F Daniels
4. Experimental Physical Chemistry; A Halpern and G McBane
5. Experimental Physical Chemistry; D P Shoemaker, C W Garland, and J W Nibler
6. Physical Chemistry Practical; S K Maity, N K Ghosh

SEMESTER-III

Paper Code CHE-611

Paper Type DSC

Paper Name GROUP THEORY AND ITS APPLICATION

Credit = 4

Marks = 100

Course Objectives:

Course Learning Outcomes:

Unit 1 Introduction to Symmetry:

Symmetry elements and symmetry operations, subgroups, classes, similarity transformation. Products of symmetry operations, point groups, mathematical requirement and classification. Systematic assignment of molecular point groups (Schoenflies notation): Low symmetry groups (C_1 , C_s , C_i), High symmetry groups (T_d , O_h , I_h), Special symmetry groups (C_{nv} , C_{nh} , D_n , D_{nh} , D_{nd}). Group generators, symmetry of Platonic solids. Relationship between symmetry and physical properties (polarity, chirality, optical activity). Matrix Representation of Symmetry elements and point groups, (C_{2v} , C_{3v} , C_{4v}), transformation matrices, Reducible and irreducible representations, Definition and significance of characters. The Great Orthogonality Theorem (GOT) and its consequences, Properties of irreducible representations (IRs), Construction of character tables for simple point groups (C_{2v} , C_{3v} , C_{2h} , D_{3h} , C_{4v}), Mulliken's symbol, Direct product, standard reduction formula.

Unit 2 Applications of group theory:

Symmetry of normal modes of molecules, cartesian and internal co-ordinate methods, normal mode analysis of C_{2v} , C_{3v} , D_{4h} (ML_4), T_d (ML_4) and O_h (ML_6) structures and their infra-red and Raman activity. Hybrid orbitals and hybridization schemes for σ and π bonding, analysis of symmetry allowed combination of atomic orbitals in case of tetrahedral, and octahedral structures. Projection operator and development of Symmetry Adapted Linear Combination of Atomic Orbitals theory, Molecular orbitals theory of coordination compounds: σ and π -bonding in octahedral complexes, Formation of Ligand group orbitals (LGOs), construction of energy correlation diagrams in O_h .

Unit 3 Molecular Spectroscopy-I

Symmetry of molecular electronic states, selection rules for electronic transitions (Laporte selection rule, spin selection rule), symmetry aspects of charge transfer spectra. (ii) Symmetry rules for inorganic reactions, and construction of correlation diagrams, Tanabe-Sugano and Orgel diagrams, analysis of electronic spectra of transition metal complexes.

Unit 4 NMR Spectroscopy

¹H NMR Spectroscopy : NMR phenomenon and theory of nuclear magnetic resonance; chemical shift and factors affecting chemical shifts; integration and proton counting; chemical and magnetic equivalence; first- and second-order spectra; spin-spin coupling and coupling constants; Pascal's triangle; factors influencing coupling constants; A₂, AB, AX, AMX, ABX, and ABC spin systems; D₂O exchange; shift reagents; effect of chiral centers; applications of ¹⁹F and ³¹P NMR; structure elucidation of organic compounds using ¹H NMR spectroscopy. Explain with appropriate examples.

¹³C NMR Spectroscopy

Introduction to ¹³C NMR spectroscopy; correlation charts for ¹³C chemical shifts; proton-coupled and proton-decoupled ¹³C spectra; carbon-deuterium coupling; Nuclear Overhauser Effect (NOE); structural applications of ¹³C NMR; Explain with appropriate examples.

Structural Elucidation of Organic Compounds: Application of UV-Vis, MS, IR and NMR spectroscopic techniques for solving structure of organic molecules. Explain with appropriate examples.

Paper Code CHE-612

Paper Type DSC

Paper Name COMPUTATIONAL CHEMISTRY AND ITS TECHNIQUES

Credit = 4

Marks = 100

I. *Computer programming in Python:*

Basic Python Usage, Strings, Lists and Loops, Comparisons and Flow Control, Functions, Data Structures, File Input/Output, Use of numerical packages- NumPy, SciPy, Matplotlib, SymPy, and pandas. Writing Python program with examples from chemistry- kinetics of formation of ozone in the stratosphere, radial part of orbital wave-function and its probability distribution on two scale, Simulated fundamental band in the IR spectrum of $^1\text{H}^{35}\text{Cl}$, Solving then pi-electron energy of 1,3-butadiene and other examples.

II. *Numerical methods:*

Least Square Fitting, Finding roots of an equation, Iterative method, and Successive bisection method, Method Of false position and Newton-Raphson method. Curve fitting by least square principle; Interpolation, Numerical differentiation and integration, trapezoidal method, Simpson's 1/3 rule; Runge-Kutta method for solving differential equations.

III. *Ab-initio methods:*

Hartree-Fock (HF) and post-HF methods; Density functional theory; Configuration Interactions, semi-empirical methods. Gaussian Basis Sets, Extended Basis Sets. *Molecular simulation methods:* Molecular Mechanics (MM), force field, Molecular Dynamics (MD) and QM/MM or MD Simulation, geometry optimization; energy and frequency calculations; thermochemistry, kinetics, spectroscopic properties; molecular dynamics etc.

IV. *Use of computational and simulation software:*

(i) .gjf (ii) .pdb (iii) .mol (iv) .cif. Introduction to visualization software: (i) Chem Draw (ii) ChemsSketch (iii) Gauss View (iv) Avogadro. Basic geometrical description of molecules: (i) Cartesian coordinate and (ii) Z-matrix. GAUSSIAN, GAMESS, GROMACS, AUTO DOCK, Gaussview, pymol, VMD, Avogadro. QUANTUM EXPRESSO, LAMMPS, OPENFOAM, MATHEMATICA and COMSOL.

TEXT BOOKS

1. Christian Hill, Python for Chemists, Cambridge University Press, 2024.
2. Jaan Kiusalaas, Numerical Methods in Engineering with Python, Cambridge University Press, 2005.
3. José J.C. Teixeira-Dias, Molecular Physical Chemistry-A Computer-based Approach using Mathematica® and Gaussian,, Springer, 2017.
4. J. B. Foresman and Æ Frisch, Exploring Chemistry with Electronic Structure Methods, 3rd ed., Gaussian, Inc.: Wallingford, CT, 2015.
5. Shafat Mubin and Jichin Li, Extending and Modifying LAMMPS, Packt Publishing, 2021.

6. Nguyen Tuan Hung, Ahmad R.T. Nugraha, Riichiro Saito, Quantum ESPRESSO Course for Solid-State Physics, CRC Press, 2022.
7. Michael Trott, The Mathematica GuideBook for Programming, Springer New York, NY, 2014.
8. Allen & Tildesley , Computer Simulation of Liquids, Oxford Chemistry Press, 2017
9. Frenkel & Smit , Understanding Molecular Simulation: From Algorithms to Application, Academic Press, 2002
10. "A Chemist's Guide to Density Functional Theory" by Wolfram Koch and Max C. Holthausen.
11. Density-Functional Theory of Atoms and Molecules" by Robert G. Parr and Weitao Yang.
12. Essentials of Computational Chemistry" by Christopher J. Cramer.

Paper Code CHE-621

Paper Type DSE

Paper Name INORGANIC CHEMISTRY SPECIAL -I

Credit = 4

Marks = 100

Learning Objectives:

- Gain fundamental knowledge of UV-Vis, EPR, NMR and IR spectroscopy, including electronic transitions, selection rules, solvent effects, and interpretation of functional group vibrations and Raman spectra.
- Apply spectroscopic techniques such as IR, Raman, and Mössbauer spectroscopy to investigate the structure and bonding in coordination and inorganic compounds involving key ligands and metal centres.
- Analyse inorganic and coordination compounds using magnetic resonance spectroscopy (ESR and NMR), with emphasis on metal-ligand bonding, magnetic properties, and structural elucidation through ^{31}P and ^{19}F NMR.
- Explore the principles and applications of X-ray crystallography, Electro and thermoanalytical methods for interpretation of inorganic compounds.

Course Learning Outcomes:

- Interpret UV-Vis and IR spectral data based on electronic and vibrational transitions, selection rules, solvent effects, and characteristic group frequencies, including the role of Raman spectra as a complementary technique.
- Interpret Electron Spin Resonance (ESR) and Nuclear Magnetic Resonance (NMR) data for coordination compounds to assess electronic structure, bonding, and molecular symmetry.
- Explain the principles and applications of X-ray crystallography, Electro and thermoanalytical methods in coordination chemistry and inorganic compounds.
- Fundamental understanding on the principle of Inorganic Photochemistry

Unit 1: *EPR Spectroscopy in inorganic chemistry:*

Principle, instrumentation, representation of EPR spectrum, line width, hyperfine splitting, magnetically equivalent and nonequivalent sets of nuclei, g-anisotropy, spectra of simple organic free radicals: Spectra of transition metal complexes, zero-field splitting, application: determination of oxidation state of metal ion in samples.

Unit 2: Spectral techniques in inorganic chemistry:

(a) ***IR and Raman spectroscopy:*** Structural studies of coordination compounds using IR and Raman spectroscopy. Dispersive and Fourier Transformed Raman, Resonance Raman and Surface Enhanced Raman Spectroscopy- Dispersive and Fourier Transformed.

(b) **UV-vis and Emission Spectroscopy:** Color and spectra of inorganic compounds, selection rules, fluorescence, phosphorescence, application. X-ray photoelectron spectroscopy (XPS), Auger Electron Spectroscopy (AES), ESCA, Atomic absorption and emission spectroscopy.

(c) **Mössbauer Spectroscopy:** Principles, isomer shift, quadrupole effect of magnetic field, applications of Mössbauer Spectroscopy involving iron and tin compounds.

(d) **Nuclear magnetic resonance spectroscopy:** Application of chemical shifts, signal intensities, and spin-spin coupling to structure determination of inorganic compounds carrying NMR active nuclei like ^1H , ^{15}N , ^{19}F , ^{13}C and ^{31}P etc. Effect of fast chemical reactions, coupling to quadrupolar nuclei, NMR of paramagnetic substances in solution, nuclear and electron relaxation time, the expectation value of, contact shift, pseudo contact shift, factoring contact and pseudo contact shift for transition metal ions.

Unit 3: X-ray Crystallography:

Principle and Instrumentation, Structure determination by single-crystal X-ray diffraction and Powdered XRD and size calculation.

Unit 4: Analytical techniques (Instrumentation and Applications)

(a) **Electroanalytical methods:-** Polarography (DC, AC, and pulse), cyclic voltammetry, coulometry and anode stripping voltammetry. .

(b) **Thermo-analytical Method:** Principles, instrumentation, and applications of thermoanalytical methods, viz. TGA, DTA, and DSC for inorganic compounds and complexes.

(c) **Imaging Techniques:** Electron microscopy (SEM, TEM)

(d) **Hifanated Techniques:** GC-IR, TG-IR Spectroscopy, GC-Mass Spectroscopy

Reference textbooks:

1. High Resolution NMR; E Beaker; Academic Press.
2. Fundamental of Molecular Spectroscopy; C N Banwell; Tata McGraw Hill.
3. Organic Spectroscopy; W Kemp; Educational Low-Price Book Scheme and Tata McMillan Press Ltd.
4. Ultraviolet and Visible Spectroscopy; C N Rao; Butterworth
5. Spectroscopy Identification of Organic Compounds; R.M. Silverstein, G C Bassler; John-Wiley and Sons Inc.
6. Spectroscopy of Organic Compounds; P S Kalsi; New Age International
7. Physical Methods in Chemistry; R S Dargo; Saunders College Publishers.
8. Spectroscopic Methods of Organic Chemistry; D H Williams, Tata-McGraw Hills
9. Instrumental Analysis; D A Skoog, F J Holler; S R Crouch; Brooks/Cole
10. Instrumental Methods of Analysis; H K Willard, L L Merrit, H A Dean; East West Edition
11. Thermal Methods of Analysis; W W Wendlant; Interscience
12. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry; R V Parish; Ellis Horwood

Paper Code CHE-622

Paper Type DSE

Paper Name INORGANIC CHEMISTRY SPECIAL -II

Credit = 4

Marks = 100

Learning Objectives:

- Understand the biological roles of essential and trace metals by studying metalloproteins and metal complexes involved in oxygen transport, electron transfer, and nitrogen fixation processes.
- Explore the stereochemical aspects of coordination compounds, focusing on optical activity, racemization mechanisms, and ligand stereospecificity in metal complexes.
- Examine the synthesis, structure, and bonding of boranes and metal carbonyl clusters, using electron counting rules and structural principles such as Wade's and isolobal analogies.
- Analyse the structural and electronic properties of solids, including metallic bonding, conductivity, band theory, and various types of crystal defects and non-stoichiometry.
- Understand and apply the principles of magnetochemistry, including the derivation of Russell-Saunders terms, spin-orbit coupling, and magnetic properties of transition metal ions with emphasis on orbital quenching and Hund's rules.
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Course Learning Outcomes (CLOs):

- Understand the biological roles of essential and trace metals, including the mechanisms of the Na^+/K^+ pump, oxygen transport in heme-proteins, and electron transport in metalloproteins such as cytochromes and iron-sulfur proteins.
- Explain the principles of crystal chemistry, including metallic bonding, band theory, electrical conductivity, and structural defects such as Schottky, Frenkel, and color centers.
- Analyse the mechanisms of racemization in coordination compounds, with emphasis on stereochemical changes, ligand stereospecificity, and structural rearrangements in Co(III), Fe(II), Ni(II), and Cr(III) complexes.

Unit-1: Bioinorganic Chemistry

Essential and trace metals, Na^+/K^+ pump, chlorophyll, photosystem I (PS I) and photosystem II (PS II) in cleavage of water, heme-proteins and oxygen uptake, structure and function of haemoglobin and myoglobin, hemerythrin and hemocyanin, structure and function of metalloprotein in electron transport process, cytochrome and iron-sulphur protein, biological nitrogen fixation, molybdenum nitrogenase. Bioenergetic principles and role of ATP and ADP. Biological membranes, mechanism of ion transport across membranes, Gibbs-Donnam Equilibrium, ionophores as metal ion carrier. Metal ions transport protein: ferritin, transferrin, ceruloplasmin.

Unit-2:Isomerization and Racemization in coordination chemistry

Optical activity and racemization of optically active compounds. Mechanism of intramolecular and intermolecular racemization reactions and molecular rearrangements involved in these mechanisms, ligand stereospecificity. Racemization of some optically active 2,2-bipyridine, phenanthroline, ethylenediamine and oxalate complexes with special reference to Co (III), Fe (II), Ni (II), and Cr (III) ions.

Unit-3: Crystal Chemistry

Structure of metals and alloys, metallic bond, free electron approximation, electrical conductivity of metal, insulators and semiconductors, electronic theory of solids, band theory, order-disorder transformation, atomic imperfection, Schottky and Frenkel defects, non-stoichiometric compounds, vacancy and its production by adding foreign atom, colour centres.

Unit-4: Magneto chemistry-II

Microstates and derivation of Russel-Saunders terms, p^2 , d^2 and $p-d$ configuration. Spin-orbit interaction, Lande interval rule, hole equivalency, Hund's third rule and energy of J levels. Magnetic properties of first transition series metal ions. Quenching of magnetic moment: orbital rotation and transformation model.

Reference textbooks:

1. Structural Inorganic Chemistry; A F Wells; Oxford University Press
2. Advanced Inorganic Chemistry; F A Cotton, G. Wilkinson; Wiley International
3. Lanthanides and Actinides Chemistry; F A Cotton; John-Wiley and Sons
4. Modern Aspects of Rare Earths and Their Complexes; V R Sastri, J R Perumereddi, V R Rao, G V S Rayudu, J C G Bunzli; Elsevier
5. Inorganic Chemistry: Principles of structure and Reactivity; J E Huheey, E A Keiter, R L Keiter; Pearson Education India
6. Inorganic Chemistry; F Shriver, P W Atkins; Oxford University Press
7. Inorganic Chemistry Part-I Principles, R L Dutta; The New Book Stall, Kolkata
8. Organometallic Chemistry; R C Mehrotra, A Singh; New Age International
9. Supramolecular Chemistry; J W Steed; Wiley
10. Supramolecular Chemistry-Fundamentals and Applications; Katsuhiko Ariga, Oyoki Kunitake; Springer

Paper Code CHE-623

Paper Type DSE

Paper Name INORGANIC CHEMISTRY SPECIAL LAB

Credit = 4

Marks = 100

Learning Objectives:

- Hands on experience on making various inorganic compounds by employing a variety of synthetic strategies and their characterization will be aimed.

Course Learning Outcomes:

- Students will learn to synthesize inorganic compounds, purify and characterize them.

Synthesis and Analysis

Synthesis of inorganic complexes/compounds and their characterization by various physicochemical methods, viz. IR, UV, Visible, NMR spectroscopy, magnetic susceptibility etc. Selection can be made from the following or any other from the existing literature.

- (i) Metal acetylacetonates
- (ii) *Cis* and *trans* isomers of $[\text{Co}(\text{en})_2\text{Cl}_2]\text{Cl}$
- (iii) Ion-exchange separation of oxidation states of vanadium.
- (iv) Preparation of Ferrocene.
- (v) Preparation of triphenyl phosphine Ph_3P , and its transition metal complexes.
- (vi) Determination of Cr(III) complexes. (vii) Tin(IV) iodide, Tin(IV) chloride, Tin(II) iodide.
- (viii) (*N,N*)-bis(salicylaldehyde)ethylenediamine Salen H_2 ; and its cobalt complex $[\text{Co}(\text{Salen})]$.
- (ix) Reaction of Cr(III) with multidentate ligands, a kinetics experiment.
 $[\text{Cr}(\text{H}_2\text{O})_6]\text{NO}_3 \cdot 3\text{H}_2\text{O}$; $[\text{Cr}(\text{H}_2\text{O})_4\text{Cl}_2]\text{Cl} \cdot 2\text{H}_2\text{O}$; $[\text{Cr}(\text{en})_3]\text{Cl}_3$; $\text{Cr}(\text{acac})_3$.
- (x) Vanadyl acetylacetonate.
- (xi) Mixed valence dinuclear complex of Manganese(III,IV).
- (x) Other new novel synthesis reported in literature from time to time.

Reference textbooks:

1. Vogel's Textbook of Quantitative Inorganic Analysis revised; J. Bassett, R.C. Denny, G.H. Jeffery, J. Mendham; ELBS/Longman
2. A Textbook of Macro and Semimicro Qualitative Inorganic Analysis; A.I Vogel; Orient Longman Ltd.

Paper Code CHE-631
Paper Type DSE
Paper Name ORGANIC CHEMISTRY SPECIAL-I
Credit = 4
Marks = 100

COURSE OBJECTIVES (COs):

CO1. Explore the use of specific reagents and catalysts in organic synthesis, including organometallic reagents (like Gilman's reagent, LDA, Pd complexes), coupling reactions (Suzuki, Heck, etc.), and phase transfer catalysts for designing synthetic pathways and functional group interconversions.

CO2. Understand the scope and mechanisms of reduction reactions including catalytic hydrogenation (heterogeneous and homogeneous), dissolving metal reductions, and reductions using hydrazine derivatives for various functional group transformations. Gain detailed knowledge of metal hydride reductions, exploring the stereochemistry, mechanisms, and synthetic applications of reagents such as LiAlH_4 , NaBH_4 , 9-BBN, and hydroboration techniques.

CO3. Analyse oxidation reactions using chromium, manganese, peracids, and other oxidants to understand their selectivity, mechanisms, and utility in transforming alcohols, alkenes, and carbon-hydrogen bonds.

CO4. Explore the concepts and molecular interactions in supramolecular chemistry, including host-guest chemistry, macrocyclic and pre-organized systems, and the design and function of molecular devices.

Unit 1: Reagents in Organic Synthesis

Use of the following reagents in organic synthesis and functional group transformations, Gilman's reagent, lithium dimethyl cuprate, lithium di-isopropylamide (LDA), dicyclohexylcarbodiimide (DCC), trimethyl-silyl iodide, thallium nitrate, DDQ, phase transfer catalysis, crown ethers, Merrifield resin, Baker yeast. Application of Pd(0) and Pd(II) complexes in organic synthesis: Stille, Suzuki, Sonogoshira coupling, Heck and Negishi coupling. Organocatalyst and application in organic synthesis: L-Proline, 4-Dimethylaminopyridine, Ureas & Thioureas.

Unit 2: Reduction

Catalytic hydrogenation: Scope and mechanisms for heterogeneous catalytic hydrogenation of olefins and other functional groups, reduction selectivity, catalytic poisoning and desulfurization, homogeneous catalytic hydrogenation with Wilkinson's catalyst, olefinic double bond isomerization. Dissolving metal reductions: Scope and basic mechanisms; liquid ammonia reduction with alkali metal: Birch reduction; Clemmenson reduction, acyloin condensation and related reactions.

Metal hydrides and related reductions: Scope, stereochemistry and mechanisms of metal hydride reductions, lithium aluminum hydride, sodium borohydride. Alkoxy metal hydrides, Meerwein-Ponndorf-Verley reduction, hydroboration and synthetic utility of alkyl boranes, 9-BBN reduction, tri- n-butyltin hydride. Reduction with hydrazine and derivatives: Wolf-Kishner reductions, reduction with tosylhydrazine, diimide, semicarbazide, use of hydrazine with other reducing agents.

Unit 3: Oxidation Reaction

- a) Oxidation with chromium and manganese compounds, mechanisms and stereochemistry for oxidation of alcohol and aldehydes with Cr (VI) and Mn (VII) oxidants, oxidation of C=C double bonds and carbon-hydrogen bonds, use of pyridinium chlorochromate (PCC).
- b) Oxidation with peracides and peroxides: Peracid epoxidation of C=C double bonds, use of metal/alkyl hydroperoxides, Sharpless asymmetric epoxidation, Baeyer-Villiger oxidation.
- c) Other methods of oxidation: Prevost-Woodward hydroxylation of alkene, oxidative cleavage of C-C single and double bonds, use of osmium tetroxide, periodate, lead tetraacetate, mercuric acetate, selenium dioxide and singlet molecular oxygen for various organic oxidations

Unit.4 Organic Supramolecules

Concepts in supramolecular chemistry, bonding in supramolecular chemistry, Host-guest chemistry, Chelate and macrocyclic effect, Self-Assembly, Thermodynamic and kinetic selectivity, supramolecular interactions, Cation, Anion, and Neutral molecule binding, Crown ether, cryptand, podand and lariat ether, Catenanes, rotaxanes, spherand, and calixarene, Cyclodextrins, Molecular devices, Applications of supramolecular chemistry.

COURSE LEARNING OUTCOMES (CLOs):

After successful completion of this course, students will be able to:

CLO1. Apply the use of specialized reagents (e.g., Gilman's, LDA, DCC, DDQ, Pd-catalyzed coupling agents) and Organocatalyst for organic synthesis and functional group interconversions, with a focus on modern synthetic methodologies..

CLO2. Demonstrate comprehensive understanding of catalytic and dissolving metal reduction mechanisms, including Birch and Clemmensen reductions, and apply this knowledge to functional group transformations. Analyze and apply the stereochemistry, scope, and mechanisms of metal hydride reductions (e.g., LAH, NaBH₄, hydroboration) and nitrogen-based reductions (e.g., Wolff-Kishner, diimide).

CLO3. Evaluate various oxidation methods (Cr, Mn compounds, peroxides, peracids, osmium, selenium, etc.) and predict outcomes in oxidation of alcohols, alkenes, and C-C bonds.

CLO4. Explain the principles and applications of supramolecular chemistry including host-guest interactions, macrocyclic effects, and molecular devices

Text Books:

1. Modern Synthetic Reactions; H O House; W A Benzamin; New York and Menlo Park, California
2. Advanced Organic Chemistry: Synthetic and Reactions; J March; McGraw Hill
3. Supramolecular Chemistry, J. W. Steed and J. L. Atwood; Wiley Reprinted (2002)
4. Supramolecular Chemistry: Concepts and Perspectives; [Jean-Marie Lehn](#), John-Wiley
5. Name Reactions and Reagents in Organic Synthesis; Mundy, P Bradford, G Ellerd, Michael, Favaloro, G Frank; New York, Wiley Interscience
6. Organic Chemistry; J. Clayden, N. Greeves, S. Warren; Oxford

Paper Code CHE-632

Paper Type DSE

Paper Name ORGANIC CHEMISTRY SPECIAL-II

Credit = 4

Marks = 100

COURSE OBJECTIVES (COs):

- CO1. Develop an advanced understanding of modern spectroscopic techniques, including UV-Visible, IR, NMR (^1H , ^{13}C , and multidimensional NMR), and Mass Spectrometry, and their applications in molecular structure determination.
- CO2. Equip students with the ability to integrate and interpret spectroscopic data for the comprehensive structural elucidation of simple and complex organic molecules, including natural products, pharmaceuticals, and biomolecules.
- CO3. Cultivate strategic thinking in organic synthesis through retrosynthetic analysis, synthetic planning, functional group interconversions, and carbon-carbon bond-forming methodologies for the design of efficient synthetic routes.
- CO4. Introduce modern concepts of medicinal chemistry and computer-aided drug design, enabling students to understand molecular recognition, structure-activity relationships, molecular modeling, and rational drug discovery processes.

Unit 1 *Designing Organic Synthesis:*

Synthons and synthetic equivalents, Definitions, Guidelines, Functional group interconversions, Use of acetylenes and aliphatic nitro compounds in organic synthesis; one group C-X and two group C-X (1,1 & 1,2 and 1,3) disconnections, Two-group C-C disconnections – Diels-Alder reaction, 1,3- and 1,5-difunctional compounds (Michael addition and Robinson annulation), Order of events in organic synthesis, Chemoselectivity, Reversal of polarity (umpolung-(epoxide, Haloketones and esters, 1,3 dithiane, cyanide, Nitro, alkynes)), Cyclisation reactions, Amine synthesis. Synthesis of Salbutamol, Paracetamol, Benzocaine, (+)-Disparlure and Jasmone.

Unit 2 *Medicinal Chemistry I:*

Drug design and synthesis, Molecular and quantum mechanics; Drawing chemical structures, equations, and diagrams; 3D structures; Molecular modelling and Energy Minimization; Molecular properties, Conformational analysis, Docking Procedures, De novo design, Molecular Recognition, Receptor Based Molecular Modeling, QSAR studies, Antineoplastic agents, cardiovascular drugs, Local anti-infective drugs, Antimalarial, Antibiotics, Anticholinergic and CNS-active drugs. retrosynthetic analysis and full synthesis of some selected organic molecules used as drugs, Aspirin, Propranolol, L-Dopa.

Unit 3 *Medicinal Chemistry II:*

Advancements in Targeted Drug Delivery and Encapsulation Technologies: Importance of Targeted Drug Delivery, Efficacy, Safety and Toxicity Issues. Molecular basis of targeted drug delivery. Drug Release and Uptake Phenomenon. Drug Encapsulation Technologies. Different Carriers for Drug Encapsulation-nanomaterials dendrimers, organogels, multiple emulsions and nanoemulsions..

Unit 4 Biomolecules-III

Enzymes: Enzymes: Basic concepts of enzyme, General mechanisms of enzyme regulation, sigmoidal and allosteric enzymes, Hill and Scatchard plots, positive and negative co-operativity with suitable examples (like aspartate transcarbamoylase & phosphofructokinase); Applied Enzymology: Applications of enzymology; structure and function of enzymes; Enzyme engineering with suitable examples. Metal activated enzymes and metalloenzymes.

Heterocyclic compounds in biological system: Heterocyclic Amino Acids and Related Substances, Enzyme Co-Factors and Co-Enzymes- ATP, NADP, NADH; Heterocyclic Vitamins; Niacin (Vitamin B3) Pyridoxine (Vitamin B6), Riboflavin (Vitamin B2), Thiamin,

co-enzyme A. Lipoic acid, pyridoxal phosphate, tetrahydrofolic acid, flavin co-enzyme, heme co-enzyme, biotin and vitamin B12

COURSE LEARNING OUTCOMES (CLOs):

After successful completion of this course, students will be able to:

CLO1. Analyse the structure, stereochemistry, and biosynthesis of natural alkaloids, steroids and terpenoids; artificial hormones, including cholesterol, testosterone, and stilboestrol.

CLO2. Understand enzyme mechanisms and drug interactions; explain enzyme action, factors affecting activity, enzyme specificity, and inhibition types, and correlate enzyme interactions with drug-receptor binding and structure-activity relationships and importance of heterocyclic compounds in biomolecules such as coenzymes and vitamins.

CLO3. Analyse structural features and biosynthetic pathways of plant pigments such as flavones, flavanols, isoflavones, and anthocyanidins, including their synthesis and functional significance and Classify and evaluate different types of carotenoids, understand their stereochemistry, and explain the structure and synthesis of β -carotene, lycopene, and vitamin A.

CLO4. Understand and explain the roles of co-enzymes and enzymes in the biosynthesis of natural products, with specific emphasis on coenzyme A, lipoic acid, thiamine, biotin, and vitamin B12.

CLO5. Understand other bioactive compounds such as pyrethroids, insect pheromones,

Text Books:

1. Natural Products Chemistry, Vol. I and II; K Nakanishi; Academic Press
2. Natural Products: Chemistry and Biological Significance; J Mann, R S Davidson, J B Hobbs, D.V. Banthorpe, J B Harborne
3. Biochemistry; A I Lehninger; Kalyani Publishers
4. Outlines of Biochemistry; E S Cohn, R K Stumpf; Wiley Eastern
5. Organic Chemistry Vol.2: Stereochemistry and the Chemistry of Natural Products; I L Finar; Educational Low-priced Book Scheme, Pearson Education Limited.
6. Heterocyclic Chemistry Synthesis, Reactions and Mechanism, R K Bansal; Wiley-Eastern, New Age International

Paper Code CHE-633

Paper Type DSE

Paper Name ORGANIC CHEMISTRY SPECIAL LAB

Credit = 4

Marks = 100

Experiments:

1. Analysis of spectra of UV-Vis, FTIR, NMR and Mass of simple organic compounds prepared by:
 - (i) Synthesis of Benzimidazole.
 - (ii) Synthesis of Anthranilic Acid.
 - (iii) Synthesis of Sulphanilamide.
 - (iv) Synthesis of benzoic acid from benzyl alcohol
2. Identification of an organic compound of complex nature, separation of an organic mixture containing two simple compounds and their identification (complete systematic identification with preparation of derivatives is required)
3. Simple Isolation and characterization of natural products from plant extracts.
4. Other experiments suggested from time to time.

Paper Code CHE-641

Paper Type DSE

**Paper Name PHYSICAL CHEMISTRY SPECIAL – I
ELECTROCHEMISTRY AND CHEMICAL DYNAMICS**

Credit = 4

Marks = 100

UNIT 1 Ions in Solutions:

Ion-solvent interactions: Born Model, Ion-ion interactions: Debye-Huckel (ion-cloud) model Bjerrum's concept of ion association, probability of finding oppositely charged ions near each other, the fraction of ion-pairs, the ion-association constant K_A of Bjerrum, Fuoss approach ion-pair formation, from ion-pairs to triple ions to clusters of ions (elementary idea only). Ion-transport in solution: Drift velocity, relation between the current density and drift velocity. Einstein relation between the absolute mobility and diffusion current, Stokes-Einstein relation and Nerst-Einstein equation and their validity and limitations.

UNIT 2 Electrochemistry and Interfacial Processes

Processes at electrodes: double layer at interface, different models of double layers, rate of charge transfer, over potential, aspects of current-voltage relation, Butler-Volmer equation, Tafel plot, i - v curves, deviation from equilibrium. Electrolytic conductance, transport number and its determination, Kohlrausch's law and application to determine solubility; degree of dissociation; Activity and activity coefficient, Debye-Huckel limiting law, Electrochemical processes: Dissolution and deposition at electrodes-current affecting potential of a cell, power generation and storage process fuel cells-power shortage. Corrosion: Thermodynamics of corrosion, kinetics of corrosion, and inhibition of corrosion.

UNIT 3 Chemical Dynamics I:

Collision theory, steady state approximation, cross sections, cross molecular beam, potential energy surfaces, Collinear collision of an atom with a diatomic molecule, saddle points and their characterization, reaction pathways, contour diagrams (for simple cases). Effect of translation and vibration. Transition state theory and derivation of rate expression using partition functions. Probing the transition state. Lindemann's Mechanism, Hinshelwood Treatment, Rice-Ramsperger-Kessel-Marcus (RRKM) theory. Applications of transition state theory to reactions in solutions, oscillatory reactions.

UNIT 4 Chemical Kinetics II:

Review of elementary principles: rate of reaction and rate laws, order and molecularity of reaction, integrated rate equation (zero, first, second order), Half-life and Arrhenius equation, activation energy and temperature dependence; unimolecular reactions: Decomposition of O_3 and N_2O_5 , thermal decomposition of ethane. Chain reactions (H_2-Br_2), Branched chain reactions (H_2-O_2), Explosions, Oscillatory reactions (B-Z reaction). enzyme catalyzed, salt effects Experimental techniques for fast reactions (Temperature Jump method, Flash photolysis and Stopped-flow method).

Paper Code CHE-642

Paper Type DSE

Paper Name PHYSICAL CHEMISTRY SPECIAL – II

STATISTICAL MECHANICS, NON-EQUILIBRIUM THERMODYNAMICS AND
SOLID STATE CHEMISTRY

Credit = 4

Marks = 100

UNIT 1 *Statistical Thermodynamics-I:*

Basic postulates of statistical thermodynamics, Relationship between entropy and thermodynamic probability, Different types of ensembles. Sterling's approximation, Derivation of Maxwell Boltzmann distribution equation for energy. Evaluation of Boltzmann Constant, Applications of Maxwell-Boltzmann distribution law. Maximization under certain constraints and Lagrange's method of undetermined multipliers. Quantum statistics of identical particles, Bose-Einstein and Fermi-Dirac distribution laws. Comparison of Maxwell-Bose (M-B), Bose-Einstein (B-E) and Fermi-Dirac (F-D) distribution laws. Derivation of black body radiation equation (Planck's equation) from B-E statistics. Bose-Einstein condensation, thermodynamic properties of ideal Bose-Einstein gas, Fermi level and Fermi energy, electrons in metals, electronic heat capacity.

UNIT 2 *Statistical Thermodynamics-II:*

Partition functions and their physical significance, translational partition function, rotational partition function, vibrational partition function, electronic partition function, entropy of monoatomic molecules. Seckur-Tetrode equation, chemical equilibrium for ideal gases and expression for equilibrium constant in terms of partition function, application to some chemical equilibrium.

UNIT 3 *Non-equilibrium Thermodynamics:*

Entropy production, entropy production in chemical reactions, entropy production and entropy flow in open systems. Onsager's theory, validity of Onsager's equation and its verification. The principle of microscopic reversibility and Onsager reciprocal relations, electro kinetics phenomena, diffusion, electric conduction, couple reactions.

UNIT 4 *Solid State Chemistry:*

Phase changes, Role of phase boundaries in solid state reactions, Reaction rate processes in solids, Defining heterogeneous nucleation processes, Tarnishing reactions, Fick's law of diffusion, Diffusion mechanism, Analysis of diffusion reactions, Diffusion in silicates, Diffusion mechanisms when a cation changes valence. Crystals and crystal defects, solid solutions, metals, semiconductors, semi-insulators and insulators. Band theory of solids and band structure. Superconductors, Bardeen-Cooper-Schrieffer (BCS) theory, Messner effect. Nanotechnology, Moor's law, zero-, one-, and two-dimensional nanostructures.

Paper Code CHE-643

Paper Type DSE

Paper Name PHYSICAL CHEMISTRY SPECIAL LAB

Credit = 4

Marks = 100

1. Determination of the equivalent conductivity of a strong electrolyte (NaCl or KCl) in different composition of water-ethanol/dioxane mixture and hence verification of the applicability of Debye-Huckel-Onsager equation (**Instrument (s) or Technique (s) to be used: Conductometer, Conductometric titration**)
2. Determination of surface excess concentration and critical micelle concentration (CMC) of a given surfactant using tensiometer (**Instrument (s) or Technique (s) to be used: Tensiometer**)
3. Construction of a ternary phase diagram for a three-component system-water, acetic acid, and benzene/toluene/chlorobenzene/CCl₄/cyclohexane/ethylenediamine; and study the effect of at least two different concentrations of NaCl/KCl for the same composition (**Instrument (s) or Technique (s) to be used: Acid-base titration**)
4. Compare the strengths of hydrochloric acid and sulphuric acid by studying the rate of hydrolysis of methyl acetate.
5. Study the saponification of ethyl acetate with sodium hydroxide volumetrically.
6. Determination of acid-base dissociation constant of a given weak acid in water and in presence of an organic solvent (**Instrument (s) or Technique (s) to be used: pH meter, Acid-base titration**)
7. To find the strength of HCl and acetic acid in a mixture of both by titrating it against NaOH solution (**Instrument (s) or Technique (s) to be used: pH meter, Acid-base titration**)
8. Determination of acid and basic dissociation constant (pK_a and pK_b) of an amino acid, and hence the isoelectric point of the acid with the help of pH meter (**Instrument (s) or Technique (s) to be used: pH meter, Acid-base titration**)
9. To study and evaluate the oscillatory strength of the electronic spectra of diiodine (I₂) in various solvents using a UV-Visible spectrophotometer (**Instrument (s) or Technique (s) to be used: UV-Visible spectrophotometer**)

*(Suitable experiments can be added from time to time if required)

COURSE LEARNING OUTCOMES (CLOs):

After successful completion of this course, students will be able to:

- CLO1. Apply conductometric techniques to determine equivalent conductivity in mixed solvents and verify the Debye-Hückel-Onsager equation.
- CLO2. Analyse electronic transitions and ligand field effects in transition metal complexes using UV-Visible spectroscopy.
- CLO3. Evaluate complex formation equilibria and stoichiometry through spectrophotometric techniques such as Job's method.
- CLO4. Synthesize and characterize metal and semiconductor nanoparticles using green chemistry and spectrophotometric methods.

Text Books:

1. Experimental Physical Chemistry; F A Bettelheim
2. Experimental Physical Chemistry; G P Matthews
3. Experimental Physical Chemistry; F Daniels
4. Experimental Physical Chemistry; A Halpern and G McBane
5. Experimental Physical Chemistry; D P Shoemaker, C W Garland, and J W Nibler
6. Physical Chemistry Practical; S K Maity, N K Ghosh
7. Advanced Practical Physical Chemistry; J B Yadav
8. Practical Physical Chemistry; B Viswanathan, P S Raghavan

SEMESTER-IV

Paper Code CHE-613

Paper Type DSC

Paper Name CHEMICAL INTERACTIONS AND BINDING

Credit = 4

Marks = 100

Unit.1 Interaction of Electromagnetic Radiation with Matter

Time dependent Schrodinger equation, interaction of electromagnetic radiation with matter, solution of the total wave function, rate of change of a system from one stationary state to another stationary state, transition moment integral, Einstein's coefficients, correlation of Einstein's coefficient with experimental data, oscillator strength and its physical significances.

Unit 2 Chemical bonding:

Born-Oppenheimer approximation. Variational treatment of hydrogen molecule ion. Valence bond and MO (LCAO) treatment of hydrogen molecule. Comparison of the MO and VB treatments and their equivalence limit. Configuration Interaction. Symmetry-adapted linear combinations (SALC), Extension of MO theory to other systems- Homonuclear and heteronuclear diatomics, polyatomics, Walsh diagrams for dihydrides, linear and bent triatomics.

Unit 3 Molecular Interactions:

Attraction between molecules. Various types of weak Van der Waals' interaction and dispersion forces. Bond and molecular dipole moments. Molecular and bond polarizability. Dipole-dipole, Ion-dipole, Dipole-quadrupole, Pi-pi and Cation-pi interactions. Inter and intramolecular hydrogen bonds. Clausius-Mossotti equation.

Unit 4 Molecular Structure

Molecular orbitals and electronic configuration of homonuclear diatomic molecules, and bonds; Non-crossing rule and correlation diagram (both homonuclear and heteronuclear diatomic). Elementary treatment of polyatomic molecules, concept of hybridization, mathematical treatment and shapes of polyatomic molecules, Bond length, bond angles, bond order and bond energies.

Paper Code CHE-614

Paper Type DSC

Paper Name PHYSICAL METHODS IN CHEMISTRY

Credit = 4

Marks = 100

CO1. Develop a comprehensive understanding of thermal analytical techniques (TGA, DTA, DSC), including their principles, instrumentation, and applications in analyzing inorganic, organic, polymeric, and industrial materials.

CO2. Introduce and explain electrochemical methods such as polarography and cyclic voltammetry, covering theoretical concepts like current-potential relationships, diffusion current, Ilkovic equation, and the interpretation of kinetic and adsorption waves.

CO3. Provide foundational knowledge of mass spectrometry, including its operating principles, ionization techniques, instrumentation (e.g., double focusing spectrometers), and applications in determining molecular structures.

Unit 1 Mass Spectrometry:

Principles of mass spectrometer, outline on instrumentation, simple types of ions produced, double focusing spectrometers, molecular ions produced

Unit.2 Electrochemical Methods

Classification of electroanalytical methods, Polarography, Cyclic voltammetry: Instrumentation, theory of current-potential curve, diffusion current and evaluation of diffusion coefficient, dropping mercury electrode, Ilkovic equation, half-wave potentials and their significance, interpretation of catalysis, kinetic and adsorption wave, polarography maxima minima suppressors, applications of polarographic technique. basic principle of pH metric, potentiometric and conductometric titrations. Techniques used for the determination of equivalence points. determination of pKa values..

Unit 3 Raman and Laser Spectroscopy: Absorption and emission of light, Einstein's prediction of probability of induced or simulated emission. Lasing materials, Population inversion, Optical cavity, properties of laser radiation, Ruby laser, He-Ne laser, Ar⁺ laser, Nd-YAG laser, Dye laser, applications of lasers in chemical science. Raman effect, classical and quantum theory of Raman effect, Rotational Raman spectra, Vibrational Raman spectra, Polarization of Raman scattered light, Resonance Raman scattering, applications of Raman spectroscopy.

Unit 4 Scattering and Diffraction Diffraction Methods.

Atomic scattering factors. Scattering by a small crystal. Direct and reciprocal lattice. Miller indices. Bragg's law and Laue's equations. Electron diffraction: Scattering intensity versus scattering angle, Wierl equation, measurement technique, Neutron diffraction: Scattering of neutrons by solids and liquids, magnetic scattering, measurement techniques.

Essential Readings

1. Moore, E. & Smart, L. Solid State Chemistry: An Introduction 2nd Ed., Chapman & Hall (1996).
2. Rhodes, G. Crystallography Made Crystal Clear: A Guide for Users of Macromolecular Models 3rd Ed., Elsevier (2006).
3. Massa, W. Crystal Structure Determination 2nd Ed., Springer (2004).
4. Warren, B. E. X-Ray Diffraction 1st Ed., Dover Publications (1990).
5. Sands, D. E. Introduction to Crystallography Reprint, Dover Publications (1994).

Paper Code CHE-624

Paper Type DSE

Paper Name INORGANIC CHEMISTRY SPECIAL-III

Credit = 4

Marks = 100

Learning Objectives:

- Explain mechanisms and dynamics of inorganic substitution reactions, particularly in coordination complexes.
- Explore photochemical processes in inorganic systems, comprehend fundamental photochemical laws, reaction pathways, quantum yield, and applications of photochemistry in synthesis and catalysis of metal complexes.
- Develop the ability to identify and classify molecular symmetry using symmetry elements and operations, understand symmetry point groups, and relate symmetry to chemical properties and reactivity in coordination compounds.

Course Learning Outcomes (CLOs):

- Explain mechanisms in coordination complexes, interpret their kinetics, and analyze the reactivity of inorganic complexes
- Interpret electronic configurations and magnetic properties of transition metal ions using microstate analysis, Russell-Saunders terms, spin-orbit coupling, and magnetic moment quenching models.
- Analyse and classify molecules based on symmetry elements, operations, and point groups, including applications in coordination compounds with varying coordination numbers.
- Explain the principles and mechanisms of inorganic photochemical reactions, including energy transfer, quantum yield, photoinduced substitution/redox processes, and actinometry.

Unit-1: Reaction Mechanisms in Inorganic Chemistry/Inorganic Reaction Mechanisms

Mechanisms of substitution reactions of tetrahedral, square planar, trigonal bipyramidal, square pyramidal, and octahedral complexes. Potential energy diagrams, transition states and intermediates, isotope effects, Berry's pseudo rotation mechanism, factors affecting the reactivity of square planar complexes, Swain-Scott equation, Trans effect and its application to the synthesis of complexes. Molecular rearrangement processes: electron-transfer reactions (outer- and inner-sphere), HOMO and LUMO of the oxidant and reductant, chemical activation. Precursor complex formation and rearrangement, nature of bridge ligands, fission of successor complexes, Two-electron transfers, Synthesis of coordination compounds using electron transfer reactions, mixed valence complexes, and internal electron transfer.

Unit-2: Chemistry of Inorganic Rings, Cages and Metal Cluster Compounds

Neutral higher borane (B_4H_{10} , $B_{10}H_{14}$): Preparation, structure, and reactions. Borane anion, closo-carborane ($B_{10}C_2H_{12}$): metalloboranes and metallocarborane, low nuclear carbonyl cluster (LNCC) and high nuclear carbonyl cluster (HNCC), skeleton electron counting, Wade-Mingos-Lamther rule, application of isoelectronic and isolobal relationship, capping rule. Metal atom

cluster compound, metal-metal multiple bonds involving transition metal complexes, major structural types, synthesis, structure, bonding, and magnetic properties of octachlorodirhenate(Re_2Cl_8) compounds, one-dimensional solid, non-carbonyl (higher oxidation state extended array, quadruple bond)

Unit 3: Supra molecular Chemistry

Concepts in supramolecular chemistry, bonding in supramolecular chemistry, Host-guest chemistry, Chelate and macrocyclic effect, Pre-organization, Thermodynamic and kinetic selectivity, supramolecular interactions, Cation, Anion, and Neutral molecule binding, Crown ether, cryptand, podand, and lariat ether, Catenanes, rotaxanes, spherand, and calixarene, Molecular devices, Applications of supramolecular chemistry.

Unit 4: Inorganic materials and Inorganic Solids:

Introduction to the solid state, metallic bond, Band theory (Zone model, Brillouin Zones, Limitations of the Zone model). Superconductors, with special emphasis on the synthesis and structure of high-temperature superconductors. Solid State Lasers (Ruby, YAG, and tunable lasers): Inorganic phosphor materials; Synthesis and advantages of optical fibers over conducting fibers. Diffusion in solids, catalysis, and Zone refining of metals.

Silicates and aluminosilicates: Classifications, structure, properties, and applications of naturally occurring silicates and aluminosilicates. Syntheses of pillared clays and zeolites. Characterization of clays, pillared clays, and zeolites from measurement of surface area, surface activity, pore size, distribution, and interlayer spacing. Application of clays, pillared clays, and zeolites with emphasis on catalysis.

Unit 5: Organometallic chemistry-II

Preparation, reactions, structure, and bonding of transition metal complexes of olefins, dienes, dienyl, trienes, and arene complexes. Bonding in metal complexes of phosphines and arsine. Medicinal and environmental aspects of organometallic compounds. Metal-carbon multiple bonds. Fluxional organometallic compounds including π -allyl complexes and their characterization. Metallocycles, unsaturated nitrogen ligands including dinitrogen complexes.

Reference textbooks:

1. West, A.R. Solid State Chemistry & its Applications, John Wiley & Sons (1987).
2. West, A.R. Basic Solid State Chemistry, 2nd Edition, John Wiley & Sons (2000).
3. Smart, L.E. & Moore, E.A. Solid State Chemistry - An Introduction, 3rd Edition, CRC Press (2005).
4. Rodgers, G.E. Descriptive Inorganic, Coordination & Solid-State Chemistry, 3rd Edition, Brooks/Cole, Cengage learning (2002).

Paper Code CHE-634
Paper Type DSE
Paper Name ORGANIC CHEMISTRY SPECIAL -III
Credit = 4
Marks = 100

COURSE OBJECTIVES (COs):

CO1. Understand the structural and stereochemical aspects of Alkaloids, steroids and Terpenoids; and their biological relevance through the study of biosynthesis, and chemical properties, natural and synthetic hormones.

CO2. To study the mechanisms of enzyme action and enzyme inhibition, highlighting their significance in biochemical reactions and drug-receptor interactions and heterocyclic compounds and their roles in biological systems, including the chemistry of vitamins, enzyme cofactors, and heterocyclic amino acids.

CO3. Gain insights into by exploring their classification, stereochemistry, synthesis, and functional roles of carotenoids compounds like β -carotene, lycopene, and Vitamin A and synthesis, and biosynthetic pathways of plant pigments such as flavonoids and anthocyanins, and other bioactive compounds-pyrethroids and insect hormones.

Unit 1: Biomolecules-IV

Alkaloids: Morphine, papaverine, quinine, reserpine,

Steroids: Occurrence, nomenclature, basic structure, Diel's hydrocarbon, Stereochemistry and Absolute configuration of steroids, structure and synthesis of cholesterol, androsterone, testosterone, progesterone, Artificial hormones: Stilboestrol and Hexoestrol.

Terpenoids: General biosynthetic studies of Terpenoids; trans-chrysanthemic acid, cyclopentane monoterpene lactones, biosynthetic and synthetic studies of loganin. Synthesis of cis-juvenile hormone, santonic acid and, synthesis of abietic acid,

Unit 2: Bioactive compounds-I

Occurrence; synthesis and basic concepts in the biosynthesis of common plants products: Polyphenols, flavones, flavanols, isoflavones and anthocyanide.

Carotenoids: Introduction, classification and stereochemistry of carotenes, structural analysis and synthesis of β - carotene, Lycopene, Xanthophylls and Carotenoid acids; Capsorubin and Bixin.

Unit 3: Bioactive compounds-II

Pyrethroids: Introduction; structure elucidation and synthesis of pyrethroids, namely pyrethrins, cinerins and jasmoline; Synthetic pyrethroids: Structure-activity relationships; synthesis of various synthetic pyrethroids.

Insect pheromones: Semiochemicals, pheromones, primers and releasers, different classes of pheromones, synthesis of different pheromones; advantages of pheromones over conventional pesticides.

Hormones: General study of hormones including classification, mechanism of action of water soluble and fat-soluble hormones, secondary messengers, negative feedback mechanism; Antifertility agents.

Unit 4 Organic Spectroscopy

Structural Elucidation of Organic Compounds: Application of UV-Vis, MS, IR and NMR spectroscopic techniques for solving structure of organic molecules. Such as Paracetamol, Benzocaine, Aspirin, Propranolol,

Essential Readings

1. Mathiowitz, E. (Ed.) – Encyclopaedia of Controlled Delivery (1999).
2. Joseph R. Robinson & Vincent H. L. Lee – Controlled Drug Delivery – Fundamentals and Applications.

COURSE LEARNING OUTCOMES (CLOs):

Upon successful completion of this course, students will be able to:

- CLO1. Critically analyze and interpret UV–Visible, IR, NMR, and Mass Spectral data to identify molecular structures, functional groups, stereochemical features, and conformational characteristics of organic compounds.
- CLO2. Integrate information from multiple spectroscopic techniques to solve complex structural elucidation problems involving natural products, heterocyclic compounds, pharmaceuticals, and biomolecules.
- CLO3. Design and evaluate synthetic pathways for target organic molecules using retrosynthetic strategies, synthons, synthetic equivalents, chemoselectivity, regioselectivity, and modern carbon–carbon bond-forming reactions.
- CLO4. Apply principles of medicinal chemistry, molecular modeling, docking studies, and QSAR analysis to investigate drug–target interactions and support the rational design and optimization of therapeutic agents.

TEXT BOOKS:

1. Carruthers, W. Modern Methods of Organic Synthesis Cambridge University Press (1996).
2. Carey, F.A. & Sundberg, R. J. Advanced Organic Chemistry, Parts A & B, Plenum: U.S. (2004).
3. Kemp, W. Organic Spectroscopy 3rd Ed., W. H. Freeman & Co. (1991).
4. Silverstein, R. M., Bassler, G. C. & Morrill, T. C. Spectroscopic Identification of Organic Compounds John Wiley & Sons (1981).
5. Pavia, D. L.; Lampmann, G. M.; Kriz, G. S.; Vyvyan, J. R. Introduction to Spectroscopy Cengage Learning (2014).
6. March, J. Advanced Organic Chemistry John Wiley & Sons (1992).
7. Organic Structures from spectra; L. D. Field, S. Sternhell and J R Kalman, John Wiley & Sons Ltd., 2007

Paper Code CHE-644

Paper Type DSE

**Paper Name PHYSICAL CHEMISTRY SPECIAL-III
SURFACE, MACROMOLECULAR AND PHOTOCHEMISTRY**

Credit = 4

Marks = 100

UNIT 1 Surface Chemistry:

Adsorption by solids, types of adsorption, adsorption isotherms, Freundlich, Langmuir and Temkin adsorption isotherm, multilayer adsorption and derivation of BET equation, surface area and catalytic activity of surfaces, adsorption from solution and Gibbs adsorption isotherm, techniques for investigating surfaces: LEED, PES, STM, EXAFS and SEXAFS.

UNIT 2 Surface-Active Agents :

Surface active agents, surfactants, classification of surfactants, surfactants in solution, micelle formation by surfactants in aqueous and mixed aqueous systems, factors affecting critical micelle concentration (CMC) of surfactants, thermodynamics of micellizations. General experimental techniques employed in surfactant studies like tensiometry, conductometry, viscometry, and spectrophotometry. Mixed surfactant systems, molecular interactions and synergism in mixed surfactant systems and their importance.

Unit.3 Macromolecular Chemistry:

Number average and weight average molecular weights. Theory and instrumentation of determination of molar mass by viscometer, light scattering and ultracentrifugation. General idea about kinetics and mechanism of polymerization reactions. Stereochemistry and average end to end distance of polymers.

UNIT 4 Molecular Photochemistry:

Electronically excited states, Jablonskii diagram, radiative and non-radiative transitions, Foster resonance energy transfer (FRET) and Dexter energy transfer (DET) mechanism and treatment, Basic concepts of photo-induced electron transfer (PET) and Marcus theory, fluorescence, phosphorescence chemiluminescence and photosensitization, quantum yield, radiative transfer: short range and long-range energy transfers, Kinetics of photochemical processes, Static and dynamic quenching, Stern-Volmer analysis.

Paper Code CHE-R01
Paper Type DSC
Paper Name RESEARCH METHODOLOGY
Credit = 2
Marks = 50

Course Objectives:

- CO1. To develop fundamental knowledge of research methodology, scientific writing and ethical practices in academic research.
- CO2. To train students in thesis and manuscript preparation, including data presentation, referencing, and plagiarism-free writing.
- CO3. To equip students with quantitative analysis skills and computer applications relevant for research, data, analysis, and scientific communications.

Course Learning Outcomes:

By the end of the course, the students will be able to:

- CLO1. Develop research skills by conducting literature surveys, preparing abstract, manuscripts, and review articles with appropriate use of units, abbreviations, and scientific symbols.
- CLO2. Acquire competence in academic writing and ethics through thesis preparation, proper referencing, understanding plagiarism, and adhering to copyright guidelines.
- CLO3. Apply analytical and computational tools by performing errors analysis, qualitative data interpretations, and using software applications such as MS Office, Origin, ChemDraw, and computational chemistry package (Hartee-Fock, DFT, Gaussian, ORCA).

Unit 1. General Research Methodology

Literature survey, Abstract preparation, Manuscript preparation-short communication, articles and reviews, Units, Abbreviations and symbols.

Unit 2. Thesis writing

Acknowledgement, Introduction, Materials and methods, Results and discussion, References, Copyright, Academic misconduct/Plagiarism.

Unit 3. Quantitative Analysis

Error Analysis, Standard deviations, Least squares techniques.

Unit 4 Use of new softwares and AI in Chemistry

Paper Code CHE-R02
Paper Type RESEARCH
Paper Name RESEARCH-PROJECT WORK/DISSERTATION
Credit = 6
Marks = 150

Course Objectives:

CO1. To enable students to independently design, execute, and analyse a research problem by applying theoretical knowledge and experimental/analytical skills, thereby fostering critical thinking and scientific writing abilities.

CO2. To enhance skills in scientific communication through preparation of project reports, presentations, and defence of research outcomes.

Course Learning Outcomes:

By the end of the course, the students will be able to:

CLO1. Independently design, execute, and present a research project by applying scientific methods, data analysis, and critical thinking skills.

*[The Topic of the Project Work/Dissertation/ should be decided by the supervisor concerned]