Dhanamanjuri University

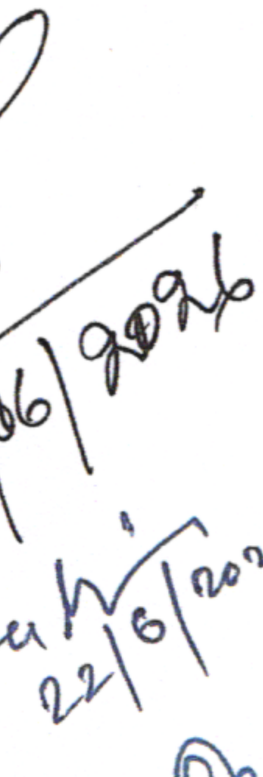
Master of Science in Chemistry

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

DHANAMANJURI
UNIVERSITY

Dhanamanjuri University

Master of Science in Chemistry

COURSE STRUCTURE OF

1-YR PG PROGRAMME
(TWO-SEMESTERS PG PROGRAMME)

2026

Department of Chemistry
School of Mathematical and Physical Sciences
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COURSE STRUCTURE OF 1-YR PG PROGRAMME

(TWO-SEMESTERS PG PROGRAMME)
TOTAL MARKS=1050
TOTAL CREDITS=42

SEMESTER-I

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	PHYSICALCHEMISTRY 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 first 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-II

Paper Code	Paper Type	Paper Title	Internal Assess. Marks	End-Sem. Marks	Total Marks	No. of Credits
CHE-613	DSC	CHEMICAL INTERACTIONS AND BINDING	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	PHYCICAL 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
VAC-001	VAC/AEC			50	50	2
Total					500	22

*A second 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 CHE-624
Set 2: Organic Chemistry Special CHE-634
Set 3: Physical Chemistry Special CHE-644
The student has to continue in the same specialization as in Semester-I

(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 22.

***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-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, (C2v, C3v, C4v), 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 σand π bonding, analysis of symmetry allowed combination of atomic 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 Molecular Spectroscopy-II

^{1}H 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; A_2, AB, AX, AMX, ABX, and ABC spin systems; D_2O exchange; shift reagents; effect of chiral centers; applications of ^{19}F and ^{31}P NMR; structure elucidation of organic compounds using ^{1}H NMR spectroscopy. Explain with appropriate examples.

^{13}C NMR Spectroscopy
Introduction to ^{13}C NMR spectroscopy; correlation charts for ^{13}C chemical shifts; proton-coupled and proton-decoupled ^{13}C spectra; carbon–deuterium coupling; Nuclear Overhauser Effect (NOE); structural applications of ^{13}C 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 $^{1}H^{35}Cl$, 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:*
Hatree-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) Chemsketch (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 PhysicalChemistry-A Computer-based Approach usingMathematica® 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 ^{1}H, ^{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, ionosphores 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 $[Co(en)_2Cl_2]Cl$
(iii) Ion-exchange separation of oxidation states of vanadium.
(iv) Preparation of Ferrocene.
(v) Preparation of triphenyl phosphene Ph3P, 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(salicyldehyde)ethylenediamine Salen H2; and its cobalt complex [Co(Salen)].
(ix) Reaction of Cr(III) with multidentate ligands, a kinetics experiment.
$[Cr(H_2O)_6]NO_3.3H_2O$; $[Cr(H_2O)_4Cl_2]Cl.2H_2O$; $[Cr(en)_3]Cl_3$; $Cr(acac)_3$.
(x) Vanadyl acetylacetonate.
(xi) Mixed valence dinuclear complex of Mangenese(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, thalium 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-Pondorf-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-Villinger oxidation.

c) Other methods of oxidation: Prevost-Woodward hydroxylation of alkene, oxidative cleavage of C-C single and double bonds, use of osmium tetraoxide, 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, $NaBH_4$, 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 (^{1}H, ^{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, Anticholenergic 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 terpenoidsl 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. Banthrope, 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 KA 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 DynamicsI:***
Collision theory, steady state approximation, cross selections, 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 4Chemical 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, activationenergy 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 catalyste, 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-Schieffer (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 (pKa and pKb) 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-II

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, hail-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 lase radiation, Ruby lase, 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 asmall 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 2Surface-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 andtreatment, Basic concepts of photo-induced electron transfer (PET) and Marcus theory,fluorescence, phosphorescence chemiluminscence and photosensitization, quantum yield,radiative transfer: short range and long-range energy transfers, Kinetics of photochemicalprocesses, 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

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]