M.Sc (Previous): Semester-I (2023-24)

Teaching Plans

1. Paper CH 101(T): Inorganic Chemistry
2. Paper CH 102(T): Organic Chemistry
3. Paper CH 103(T): Physical Chemistry
4. Paper CH 104(T): General Chemistry

DEPARTMENT OF CHEMISTRY
OSMANIA UNIVERSITY
(Effective from academic year 2023-2024 for Campus and Constituent colleges
[UNDER CBCS Scheme]
M.Sc CHEMISTRY SYLLABUS
SEMESTER –I

TEACHING PLANS

Paper I - Inorganic Chemsitry

Lesson Plan: IC-01: Symmetry of Molecules	
Lecture No	**Topic**
1	Introduction to symmetry, symmetry in nature, plants, leaves, flowers, animals, viruses, food, language, architecture, geometrical figures, polygons, pyramids, prisms and antiprisms, Molecular geometry, Concept of symmetry in molecules.
2	Symmetry operation, geometrical manipulation, equivalent and indistinguishable configurations, original and identical configurations of molecules. Operations- rotation, reflection and inversion. **Symmetry elements**: geometrical entity- point, line or plane in a molecule, five types of symmetry elements: Cn, σ, Sn, i and E.
3	Rotation operation, axis, direction of rotation, notation with arrows, order of rotational axis, equivalent or indistinguishable orientations, identical orientation, e.g. H_2O, NH_3, $[Ni(CN)_4]^{2-}$, etc., types of rotational axis- Principal rotational axis, simple or secondary or subsidiary axes, e.g. BF_3, C_6H_6, planar ethylene, allene, etc., Cn axis n = 1,2,3,-,- , Cα axis, $Cn^n = E$.
4	Reflection operation, bisecting plane, mirror images, e.g. H_2O, NH_3, etc., σ, $\sigma^2 = E$. Types of planes- a) vertical plane σv, e.g. H_2O, NH_3, BF_3, etc.; b) horizontal plane σh e.g. BF_3, C_6H_6, planar ethylene, etc. c) dihedral plane σd e.g. allene, regular tetrahedron, C_6H_6, etc., molecular plane, molecules with only plane of symmetry, e.g. HOD, C_6H_5OH, $POBrCl_2$ etc., molecules with no plane of symmetry, FClSO, PBrClFI etc.
5	Improper axis, rotational axis and perpendicular plane, order of improper axis, e.g. BF_3, eclipsed and staggered ethane, tetrahedron, etc., set of operations generated by S_n: molecules in which C_n axis is coincident with S_n axis, with same n order, with n = even order and n = odd order
6	Centre of symmetry, reflection operation through the center of gravity of molecule, direction, equivalent distance, equivalent atom, e.g. homo-diatomic molecules like H_2, O_2 etc, CO_2, C_2H_4 regular square planar and octahedral geometries, staggered ethane, chair form of cyclohexane, P_2F_4, etc., $i^2 = E$. **Identity element E**: doing nothing, rotation by 360°. Symmetry operations which give original orientation, identity operations C_n^n, S_n^n when n = even, S_n^{2n} when n = odd, i^n and σ^n, n = even.
7	Cartesian coordinates system and symmetry elements, coordinate axes, inversion centre at origin, proper and improper rotational axes of symmetry and Cartesian axes, principal rotational axis, z axis in the Cartesian system, x and y axes, correlation between the symmetry elements, presence of other symmetry elements, notation by lower order of C_n, S_n when n is of even and odd order.
8	Molecules as points, definition, symbols, notation of point groups, generators, order of the point group *n*, number of symmetry elements in a point group *h*,, classification of molecules into point groups, **Type I point group:** Non-axial groups, C_1- asymmetric compounds, no symmetry elements, C_S- only σ generator, C_i- molecules with only centre of symmetry,

	examples of non axial point groups.
9	**Type II**: Molecules with only one axis of rotation, axial point group- C_n- molecules with only rotational axis as symmetry element, S_n- molecules with improper axis with even order greater then two, C_{nv}- molecules with one proper axis and n number of vertical planes, $C_{\alpha v}$, C_{nh}- molecules with one proper axis, horizontal plane and inversion centre, examples of the axial point groups.
10	**Type III;** Dihedral point groups, molecules with one n fold axis and n number of two-fold axis, D_n- molecules with only one n fold axis and n number of two-fold axis as symmetry elements, D_{nh}- molecules C_n, nC_2's $\perp$ C_n, σh and nσv's, *i* when n is of even order, D_{nd}-molecules C_n, nC_2's $\perp$ Cn, σd's and *i* when n is of odd order, $D_{\alpha h}$. Examples of dihedral point groups
11	**Type IV**: Molecules with more than one rotational axis of higher order than two-fold, polyhedral molecules, platonic solids, tetrahedron, octahedron, cube, dodecahedron and icosahedrons, T_d- molecules with four C_3 rotational axis and no other higher order axis. Oh- molecules with three C_4 rotational axis, I and I_h- molecules with several five fold axes. Examples of the polyhedral point groups.
12	Spherical point group, K_h. Systematic procedure for symmetrical classification of molecules into point groups, flow chart with examples. Exercises with the models of various molecules.
13	**Descent in symmetry with substitution**, substitutions on AB_3- planar, AB_4- tetrahedral, square planar and square pyramidal, AB_5- square pyramidal and trigonal bipyramidal, AB6-octahedral geometries, benzene, borazole etc
14	**Exercises on molecular point groups** following the systematic procedure, working out point groups for common organic, inorganic and complex compounds.
15	**Symmetry and dipole moments**- molecules belonging to point groups C_n, C_S, C_{nv} possess permanent magnetic moment, **Symmetry criteria for optical activity**- dissymmetric and asymmetric molecules, molecules belonging to C_1, C_2, C_3, D_2 and D_3, diastereomers and mesomers

Lesson Plan: IC 02: Bonding in metal complexes-I	
Lecture No	**Topic**
1	Introduction to bonding in metal complexes, Theories of bonding- Werner's , Sidgwick's, Valence bond and Crystal field theory.
2	Salient features of Crystal field theory, Shapes of d orbitals.
3	d-orbital splitting patterns in Octahedral and Tetrahedral geometries.
4	Crystal field splitting in Tetragonal complexes -Jahn Teller theorem, z- in and z- out distortion, Consequences of Jahn Teller distortion.
5	Splitting of d orbitals in square planar and trigonal bipyramidal geometries.
6	Splitting of d orbitals in trigonal planar and trigonal bipyramidal geometries.
7	Splitting of d orbitals in Pentagonal bipyramidal and Linear geometries.
8	Factors influencing magnitude of Crystal field splitting- role of metal ion, Spectrochemical series and geometry of the complex.
9	Concept of strong and weak crystal fields, CFSE and calculation of CFSE in octahedral and tetrahedral geometries.

10	Application of CFSE in determination of structures of normal and inverse spinels
11	Magnetic properties of metal complexes- Types of magnetic behaviour- para, dia, ferro and anti ferromagnetic substances.
12	Magnetic susceptibility, Calculation of magnetic moment from magnetic susceptibility
13	Spin only formula,Calculation of spin only magnetic moment of transition metal complexes. Quenching of orbital angular momentum .
14	Determination of magnetic moment by Guoy balance method
15	Application of magnetic moment in the determination of oxidation state, bond type and stereochemistry. High spin-low spin crossover.

Lesson Plan: IC 03: Coordination Equilibria	
Lecture No	**Topic**
1	Solvation of metal ions- Metal complex formation in solution-Binary metal complexes
2	Stability constants (types and relationships between them)
3	Step wise and over all stability constant. Kinetic stability and thermodynamic stability
4	Factors influencing the stability constants- Metal ion effects – effect of charge on metal ion, size of metal ion, charge/size ration, ionic potential,
5	crystal field effect, and Jahn-Teller effect
6	Pearson theory of hard and soft acids and bases (HSAB)- class A and Class B metals
7	Effect of factors - electronegativity and softness on stability constant and symbiosis
8	Factors influencing the stability constants- Ligand effects – Basic nature of ligand, effect of substituent on ligand, steric effect,
9	Chelate effect – definition of chelation – effect of size of chelate ring and number of chelate ring formed.
10	Macrocyclic effect and cryptate effect – examples like crown ethers, cryptands, Macrocycles with pendent groups
11	Formation of macrocycles – size selectivity and concept of hole size match and its limitations
12	Methods used for the determination of Stability constants (Basic Principles only): pH metric method
13	Spectrophotometric method – mole ratio and jobs method
14	Polarographic methods – Polarography, diffusion current and stability constant relation
15	Ternary Metal Complexes – definition – Formation of ternary metal complexes – Step-wise and simultaneous equilibria with simple examples

SEMESTER-I Paper I– CH (OC) 102T: Organic Chemistry

UNIT I: Stereo Chemistry 15 Hrs

Lecture 1.	Brief review of concept of Stereo Chemistry
Lecture 2.	Molecular representations: Wedge, Fischer, Newman and Saw-horse formular, their description and interconversions
Lecture 3.	Molecular Symmetry & Chirality: Symmetry operations and symmetry elements (Cn and Sn) Criteria for Chirality. Desymmetrization
Lecture 4.	Axial, planar and helical chirality: Axially chiral allenes and spiranes
Lecture 5.	Axial, planar and helical chirality: alkylidene cycloalkanes, chral biaryls, atropisomerism
Lecture 6.	Buttressing effect, planar chiral ansa compounds and trans cycloalkenes(upto cyclodecene and their methyl analogues)
Lecture 7.	Helically chiral compounds and their configurational nomenclature
Lecture 8.	Relative and absolute configuration. Determination of configuration by chemical correlation methods
Lecture 9.	Racemisation and resolution techniques: Racemisation, mechanism Via carbocation, carbanions and free radical
Lecture 10.	Resolution by direct crystallization
Lecture 11.	Diastereoisomer salt formation chiral chromatography
Lecture 12.	Asymmetric transformation.
Lecture 13.	Determination of configuration in E. Z-isomers
Lecture 14.	Spectral and Chemical methods of configuration determination of EZ isomers
Lecture 15.	Determination of configuration in aldoximes and ketoximes

UNIT II: Reaction Mechanism-I 15 Hrs

Lecture 1.	Brief review of concept of Reaction mechanism
Lecture 2.	Reaction mechanism Introduction
Lecture 3.	Stereo selective addition to carbon carbon double bond, anti-addition: Bromination
Lecture 4.	Stereo selective addition to carbon carbon double bond, anti-addition: epoxidation
Lecture 5.	By ring opening in addition OsO_4

Lecture 6.	By ring opening in addition $KMnO_4$
Lecture 7.	Elimination reactions Elimination reactions E2, El, E1CB mechanism
Lecture 8.	Orientation and stereo selectivity in E2 eliminations. Pyrolytic syn elimination
Lecture 9.	Orientation and stereo selectivity in E2 eliminations. α-climation, elimination Vs substitution
Lecture 10.	Determination of reaction mechanism: Energy profile diagramme of addition and elimination reactions
Lecture 11.	Determination of reaction mechanism: Transition state and product isolation
Lecture 12.	Use of isotopes and isotope effects
Lecture 13.	Use of Cross over experiment
Lecture 14.	Use of crossover experiments
Lecture 15.	Use of IR and NMR in the investigation of reaction mechanism

UNIT III: Confermational analysis (acyclic systems) 15 Hrs

Lecture 1.	Brief review of concept of Conformational analysis
Lecture 2.	Introduction of Conformational analysis
Lecture 3.	The concept of dynamic stereochemistry: Conformational diastereomers
Lecture 4.	The concept of dynamic stereochemistry: Conformational enantiomers
Lecture 5.	Conformational nomenclature Conventional method and limitations
Lecture 6.	Explanation of Klyne Prelog terminology
Lecture 7.	Study of conformation in ethanes and butane
Lecture 8.	Study of conformation in dihalobutane and halohydrin
Lecture 9.	Study of conformation in butane-2, 3-diol, amino alcohols
Lecture 10.	Study of conformation in ethylene glycol and 1,1,2,2-tetrahalobutanes
Lecture 11.	Conformations of unsaturated acyclic compounds: Propylene, 1-butene, Acetaldehyde, propionaldehyde and Butanone
Lecture 12.	Physical methods for conformational Analysis: Use of dipole moment, UV, IR and NMR. spectral methods in conformationalanalysis

Lecture 13.	Conformational affects on the stability and reactivity of acyclic diastereoisomers: Steric and stereoelectronic factors-examples
Lecture 14.	Explanation of Winstein-Holness equation
Lecture 15.	Explanation of The Curtin-Hammett principle

Paper-III (CH103T): PHYSICAL CHEMISTRY

PC-01: Thermodynamics (15 h)

Lecture-1: **Introduction -** Briefly introduce the scope of the lesson, explain the importance of thermodynamics in understanding chemical and physical processes, rewrap of I & II laws of thermodynamics.

Lecture-2: Third Law of Thermodynamics - Define the third law of thermodynamics, explain the concept of absolute entropy, discuss evaluation of absolute entropies from heat capacity data for solids, liquids, and gases and introduce standard entropies and their significance.

Lecture-3: **Gibbs Equations and Non-equilibrium Systems –** Deduce Gibbs equations for non-equilibrium systems, explain material and phase equilibrium

Lecture-4: **Clausius-Clapeyron equation –** Derivation, applications, limitations and numerical problems.

Lecture-5: **Chemical Potential -** Define chemical potential and its importance, explain the chemical potential of ideal gases, variation of chemical potential with T and P.

Lecture-6: **Ideal-gas reaction equilibrium -** Derive the equilibrium constant for ideal-gas reactions, discuss temperature dependence of equilibrium constant using the van’t Hoff equation, numerical problems.

Lecture-7: **Solutions and Partial Molar Properties -** Explain partial molar properties and their significance.

Lecture-8: **Gibbs-Duhem equation** - derive the Gibbs-Duhem equation and explain its significance.

Lecture-9: **Ideal Solutions -** Define ideal solutions and their thermodynamic properties, discuss mixing quantities and vapour pressure (Raoult’s law).

Lecture-10: Ideally dilute solutions - Explain the properties of ideally dilute solutions and Henry’s law, derive Henry’s law equation from Gibbs-Duhem equation.

Lecture-11: **Non-ideal Systems -** Discuss non-ideal solutions, Introduce the concept of fugacity and fugacity coefficient, explain the determination of fugacity, derivation of expression.

Lecture-12: **Activities and activity coefficients –** Explain the concept of activity and activity coefficients, explain standard-state conventions for non-ideal solutions, numerical problems.

Lecture-13: **Multicomponent Phase Equilibrium -** Discuss the various colligative properties viz., vapour pressure lowering, freezing point depression, and boiling point elevation in multicomponent systems.

Lecture-14: **Derivation of relationships** - Derive expressions for relative lowering of vapour pressure, depression in freezing point/elevation in boiling point with molar mass of a non-volatile solute.

Lecture-15: **Numericals & Summary** – Solve numerical problems on colligative properties and summarize the topic, give questions & problems for assignment submission.

PC-02: **Electrochemistry (15 h)**

Lecture-1: **Introduction** - Introduce the topic of electrochemical cells, outline the key points to be covered in the lesson.

Lecture-2: **Nernst Equation**-Derive the Nernst equation, solve example problems to illustrate the application of the Nernst equation.

Lecture-3: **Chemical and Concentration Cells**-Explain chemical cells and concentration cells (with and without transference), discuss practical examples and applications,

Lecture-4: **Derivation of expressions** - derive expression for EMF of chemical/concentration cells with and without transference.

Lecture-5: L**iquid Junction Potential** - Define liquid junction potential (LJP), derive the expression for LJP, discuss methods for determination and elimination of LJP.

Lecture-6: **Types of Electrodes** - Describe various types of electrodes: Gas electrodes, Metal-metal ion electrodes. Reference electrodes, Indicator electrodes, Ion-selective electrodes, Metal-insoluble salt-anion electrodes, Redox electrodes – explain the working with examples.

Lecture-7: **Applications of EMF Measurements** -Explain the applications of EMF measurements: Solubility product, equilibrium constant measurements, determination of pH using glass electrode -numerical problems

Lecture-8: **Applications of EMF Measurements** - Potentiometric titrations – acid-base, redox, precipitation, complexometric titrations.

Lecture-9: **Decomposition potential** - Discuss decomposition potential and its significance.

Lecture-10: **Electrode polarization and over potential** - Explain electrode polarization, its causes, and elimination, Concentration Over-potential- define concentration over-potential, discuss its significance and applications.

Lecture-11: **Activity and Activity Coefficients** - Introduce the concept of activity and activity coefficients in electrolytic solutions, explain the mean ionic activity coefficient, numerical problems.

Lecture-12: **Debye-Huckel Theory** - Summarize the Debye-Huckel theory of electrolytic solutions, discuss the Debye-Huckel limiting law and its applications (derivation not required), limitations of the theory and numerical problems.

Lecture-13: **Extended Debye-Huckel Law and Electrolytic Conductance** - Discuss the extended Debye-Huckel's law, Explain the theory of electrolytic conductance.

Lecture-14: **Debye-Huckel-Onsager equation** - Derive the Debye-Huckel-Onsager equation and discuss its validity and limitations.

Lecture-15: **Summary and Q&A** - Summarize the key points covered, clarifications, give questions and problems for submission of assignment.

PC-03: **Quantum Chemistry-I (15 h)**

Lecture-1: **Introduction**-Revision of Planck's equation and emergence of quantum mechanics.

Lecture-2: **Schrodinger wave equation**-Wave mechanics and derivation of time-independent Schrodinger wave equation.

Lecture-3: **Operators**- Operator algebra. Commutation of operators, linear operators, problems.

Lecture-4: **Complex functions** -Hermitian operators. Operators ∇ and ∇^2.

Lecture-5: **Eigenfunctions and eigenvalues** – numerical problems, Degeneracy. Linear combination of eigenfunctions of an operator.

Lecture-6: **Well behaved functions**-characteristics and examples, Normalized and orthogonal functions-examples & numericals

Lecture-7: **Postulates of quantum mechanics**-detailed explanation of postulates, Physical interpretation of wave function. Observables and Operators. Measurability of operators. Average values of observables.

Lecture-8: **The time dependent Schrodinger equation**-Separation of variables and the time-independent Schrodinger equation from the time dependent equation.

Lecture-9: **Theorems of quantum mechanics**-Real nature of the eigen values of a Hermitian operator, orthogonal nature of the eigen values of a Hermitian operator-significance of orthogonality

Lecture-10: Expansion of a function in terms of eigenvalues-Eigen functions of commuting operators-significance.

Lecture-11: Uncertainty Principle-Simultaneous measurement of properties and the uncertainty principle, numerical problems.

Lecture-12: Particle in a box - Particle in a box- one dimensional. Derivation of expression for energy of a particle in a 1-D box, Application to the spectra of conjugated molecules. numerical problems.

Lecture-13: Particle in a 3-D box- Particle in 3- dimensional box, expression for energy derivation, degeneracy of energy states.

Lecture-14: Plots of ψ and ψ^2 -discussion, Calculations using wave functions of the particle in a box.

Lecture-15: Measurability of energy-position and momentum, average values and probabilities, summary of the topic, allotting questions & problems for assignment submission.

Semester I Paper-IV: CH 104 (Analytical Techniques and Spectroscopy – I)

Lesson plans

Lesson Plan: ASP-01: Techniques of Chromatography and UV Visible Spectroscopy	
Lecture number	**Topic**
1	Introduction and principles of chromatography, classification of chromatographic techniques, differential migration rates
2	Partition ratio, retention time, relation between partition ratio and retention time
3	capacity factor, selectivity factor. Efficiency of separation – resolution, diffusion
4	plate theory and rate theory
5	Gas chromatography, principle, instrumentation, working of the components
6	Detectors used in GC, working of the detectors- TCD, FID, ECD
7	Derivatization techniques in GC, Programmed temperature gas chromatography.
8	Application of GC in the analysis of hydrocarbons in a mixture, Principle of HPLC
9	HPLC: instrumentation, of HPLC, the working of the components with examples, application of HPLC in the analysis of paracetamol tablets.
10	Detectors used in HPLC: UV detectors, Photodiode array detector, fluorescence detector

11	UV Visible Spectroscopy: Principle, selection rules, types of electronic spectra
12	Woodward-Fieser rules for conjugated dienes, trienes and polyenes
13	Woodward-Fieser rules for unsaturated carbonyl compounds
14	Benzene, mono substituted derivative (Ph-R) and substituted benzene derivatives (R-C_6H_4-COR′).
15	Exercises of calculation of λ_{max} using Woodward-Fieser rules.

Lesson Plan: ASP 02: NMR spectroscopy-I	
Lecture number	**Topic**
1	Magnetic properties of nuclei, principles of NMR spectroscopy, theory of resonance, relaxation, Larmour frequency, nuclear spin quantum number examples of NMR active and inactive nuclei, standard substances
2	Instrumentation: CW and pulsed FT instrumentation, diagrams and working of the components, recording of the spectra
3	Equivalent and non-equivalent protons, basic examples with increasing types of equivalent protons, information from NMR spectra
4	Chemical shifts, TMS- uses and advantages, calculation of chemical shifts- variation in applied magnetic field, factors affecting the chemical shifts, shielding and deshielding effects, upfield and downfield shifts with examples
5	Factors affecting the chemical shifts –anisotropy in ring current, discussion in ethylene, acetylene, benzene, anulenes, acids, carbonyls, cyclohaxane etc., effect of electronegativity with examples
6	Signal integration, calculation of number of protons with signal integral value
7	Spin-spin coupling, vicinal, germinal and long range coupling constants, factors affecting coupling constants
8	Chemically and magnetically equivalent protons, examples. Discussion with examples of homotopic, enantiotopic and diastereotopic protons
9	Applications of ^{1}H NMR spectroscopy: Reaction mechanisms (cyclic bromonium ion, electrophilic and nucleophilic substitutions, carbocations and carbanions)
10	NMR spectra of E, Z isomers with examples, conformation of cyclohexane and decalins
11	Study of keto-enol Tautomerism using NMR, hydrogen bonding: intermolecular and intra-molecular hydrgen bonding, proton exchange processes (alcohols, amines and

	carboxylic acids)
12	Study of C-N rotation in dimethyl formamide by NMR. Magnetic resonance imaging (MRI), theory, applications
13	^{1}H-NMR of organic molecules: ethyl acetate, 2-butanone, mesitylene and paracetamol
14	Interpretation of NMR spectrum of asprin, ethylbenzoate, benzyl acetate, 2-chloro propionic acid
15	^{1}H-NMR of metal complexes $[HNi(OPEt_3)_4]^+$, $[HRh(CN)_5]$ (Rh I= ½), discussion of M-H upfield to TMS, H-Rh coupling. Revision of the topic

Lesson Plan: ASP 03: Vibrational Spectroscopy	
Lecture number	**Topic**
1	Interaction of Electromagnetic Radiation with Matter Basics of electromagnetic radiation
2	Absorption, emission, and scattering processes, Factors affecting the width and intensity of spectral lines
3	IR Spectroscopy: Principle, Vibrational energy levels of diatomic molecules
4	Selection rules for vibrational transitions (brief overview) Calculation of force constant from vibrational frequency
5	Anharmonic oscillator and Morse potential energy diagram
6	Types of transitions: Fundamental bands, overtones, and hot bands, Fermi resonance and its implications
7	Vibration-Rotation Spectra: Vibration-rotation spectroscopy in diatomic molecules P, Q, R branches
8	Vibration-rotation spectra of polyatomic molecules: Linear, symmetric top, and asymmetric top molecules
9	Principles of FTIR (Fourier Transform Infrared Spectroscopy)
10	Vibrations of Polyatomic Molecules: Normal modes of vibration, Concept of group frequencies
11	Characteristics of vibrational frequencies in functional groups, Stereochemical effects: Carbonyl group
12	Application of IR spectroscopy in the study of cis-trans isomerism, hydrogen bonding and

	Isotopic effects on group frequencies
13	Raman Spectroscopy: Classical and quantum theories of Raman effect, Stokes and anti-Stokes lines
14	Complementary nature of IR and Raman spectra Pure rotational, vibrational, and vibration-rotation Raman spectra, Selection rules and depolarization factors
15	Instrumentation and applications of Raman spectroscopy.

M.Sc (Previous): Semester-II (2023-24)

Lecture handouts

1. Paper CH 201(T): Inorganic Chemistry
2. Paper CH 202(T): Organic Chemistry
3. Paper CH 203(T): Physical Chemistry
4. Paper CH 204(T): General Chemistry

M.Sc CHEMISTRY SYLLABUS
SEMESTER –II

Paper: I Inorganic Chemistry

Lesson Plan:IC-04: Reaction mechanisms of transition metal complexes	
Lecture No	**Topic**
1	Ligand substitution reactions- Energy profile of a reaction- Endothermic reactions-Exothermic reactions- Transition state or Activated Complex – Reaction energy-Electrophilic agent-Nucleophilic agent
2	Classification of reaction mechanism- Types of substitution reactions (SE, SN, SN^1, SN^2). Langford and Grey classification – A mechanism, D-Mechanism, Ia, Id, and Intimate mechanism.
3	Substitution reactions in octahedral complexes- Nucleophilic substitution reactions-Electrophilic substitution reactions-SN^1 mechanism-SN^{II} mechanism
4	Ligand substitution reactions in octahedral complexes: Aquation or Acid hydrolysis reactions, Factors effecting Acid Hydrolysis-charge on the substrate- effect of leaving group- effect of inert ligand- steric hindrance – chelate effect
5	Base Hydrolysis, Conjugate Base (SN^1CB) Mechanism, and Evidences in favor of SN^1CB Mechanism.
6	Substitution reactions with out Breaking Metal-Ligand bond. Anation reaction
7	Ligand Substitution reactions in Square-Planar complexes: Mechanism of Substitution in Square-Planar complexes- Trans-effect, Trans-influence, and Trans-effect series.
8	Theories of Trans-effect - Grienberg’s Polarization theory and Π - bonding theory
9	Applications of Trans-effect in synthesis of Pt (II) complexes
10	Electron Transfer Reactions (or Oxidation-Reduction Reactions or Redox reactions) in Coordination compounds
11	Mechanism of One-electron Transfer Reactions – classification-Introduction of Inner Sphere Mechanism and Outer Sphere Mechanism
12	Atom (or group) Transfer or Ligand bridge mechanism or Inner Sphere Mechanism
13	Direct electron Transfer or Outer Sphere Mechanism. – Self exchange reaction and cross exchange reaction.
14	Factors affecting direct electron transfer reactions
15	Cross reactions and Marcus-Hush theory

Lesson Plan:IC-05: Bonding in Metal complexes -II	
Lecture No	**Topic**
1.	Free ion Terms and Energy levels: Energy levels in an atom- n, l, m, mS.Configuration of the free ion, energy state of the atom, terms, inter electronic repulsion perturbations and spin-orbit coupling perturbations, microstates.
2.	Microstates: formulae for calculating number of microstates, general equation, equations for equivalent electrons, inequivalent electrons, calculation of microstates for p^n and d^n configurations.

3.	Orbital angular momentum of the electron, and resultant orbital angularmomentum, notation of terms χ, vector coupling of orbital angular momenta, p-p configuration, p-d configuration and d-d configuration.
4.	Spin angular momentum of the electron m_S, and resultant spin angular momentum Σm_S = S, two electron configurations- p^2 and d^2 cases, threeelectron configurations- p^3 and d^3 cases. Spin orbit coupling- theory, types- phenomenon of L-S (Russell- Saunders) coupling scheme, j-j coupling scheme
5.	Russell- Saunders or L-S coupling scheme: Spin orbit coupling constantJ, vector coupling of orbital and spin angular moments for p^2 configurations and p-d configurations, representation of term symbols, spin multiplicities, j-j coupling scheme.
6.	Derivation of Terms using the allowed values of m_l and m_S values for single electron p^1 and d^1 configurations, calculation of M_L, M_S and single electron wave functions for all microstates, summary of microstates table, assignment of Terms.
7.	Derivation of Terms for the allowed microstates for p^2 configuration, calculation of M_L, M_S and single electron wave functions for all microstates, summary of microstates table, assignment of Terms.
8.	Derivation of Terms for the allowed microstates for d^2 configuration, calculation of M_L, M_S and single electron wave functions for all microstates, summary of microstates table, assignment of Terms.
9.	Concept of Hole formalism: Hole formulation, spin factoring, holes equivalent to number of unpaired electrons in half filled andcompletely filled shells, Hole equivalents.
10.	Energy ordering of Terms- Hund's rules. Determination of ground states for d^1 to d^9 configurations.
11.	Spin orbit coupling parametres- Condon Shortley parameters and Racah parameters.
12.	Inter electron repulsion parameters: Racah parameters- A, B and C, Condon-Shortley parameters- F_0, F_2 and F_4. Relation between the two parameters, Energies of the terms of d^2 configuration, Racah parametervalues for some metal ions.
13.	Effect of weak crystal field on S,P , D and F terms. Splitting of D and F terms in weak Octahedral and tetrahedral crystal fields
14.	**Ligand field diagrams in Weak crystal fields- Orgel diagram for** d^1, d^4, d^6 and d^9 configurations, Assignment of Electronic transitions in these complexes.
15.	**Orgel diagram for** d^2, d^3, d^7 and d^8 configurations, d^5 configuration, Assignment of Electronic transitions in these complexes.

Lesson Plan: IC-06: Metal Clusters and Ligational Aspects of Diatomic molecules	
Lecture No	**Topic**
1	**Metal Clusters:** Definition, Factors favouring metal-metal bonding.
2	**Metal Carbonyl Clusters:** Introduction, structure of CO, Bonding modes of CO: Different types of bonding modes of CO: terminal mode with examples and bridging mode with examples. No. of electrons donated by CO in both modes, Reasons for the formation of bridging carbonyl complexes by only early transition metals.
3	18 Valence electron rule and its application: Definition, explanation of the rule with many examples (mononuclear and dinuclear metal carbonyl complexes). Its application in predicting the stability of the complexes.
4	Classification of carbonyl clusters. Low nuclearity carbonyl clusters: M_3 and M_4 clusters, structural patterns in $M_3(CO)_{12}$ (M=Fe, Ru, Os) and $M_4(CO)_{12}$ (M=Co, Rh, Ir) clusters. High nuclearity carbonyl clusters: M_5, M_6, M_7, M_8 and M_{10} clusters.
5	Polyhedral skeletal electron pair theory and Total electron count theory. Capping rule.
6	Structural features of Polyhedral High nuclearity carbonyl cluster – closo, Nido, Arachino, formula involved n = N, N' = n –1, N" = n-2 - skeletal – Non skeletal electrons
7	Structural patterns in $[Ni_5(CO)_{12}]^{2-}$, $[Os_6(CO)_{18}]^{2-}$, $[Os_7(CO)_{21}]$, $[Os_8(CO)_{22}]^{2-}$ and $[Os_{10}C(CO)_{24}]^{2-}$.
8	Capping rule – electron count number of Skeletal electrons - -number of Skeletal electrons – number of vertices – prediction of Cluster structure – Correlation with the Wades rule
9	Metal carbonyl scrambling, stereo chemical non-rigidity in $[Rh_4(CO)_{12}]$ and $[Fe_2(Cp)_2(CO)_4]$.
10	**Boranes and Carboranes**: Wade's rules, STYX rule
11	**Metal Nitrosyls**: Introduction, structure of NO, electronic configuration, NO as a ligand. Bonding modes of NO – terminal mode – linear & bent, bond angle , hybridization, no. of electrons donated; bridging mode , with examples.
12	Structural aspects of [IrCl(PPh3)2(CO)(NO)]+ : binding mode of NO as a ligand, bond length, bond angle , hybridization, no. of electrons donated. [RuCl(PPh3)2(NO)2]: binding mode of NO as a ligand (different binding modes in one complex) , bond length, bond angle , hybridization, no. of electrons donated by 2 NO's. Stereo chemical control of valence in [Co(diars)2(NO)]2+ and Co(diars)2(NO)(SCN)]+.
13	Metal Halide Clusters: Major structural types in Dinuclear metal – metal systems – Edge sharing Bioctahedra - face sharing Bioctahedra
14	Metal Halide Clusters - -Tetragonal prismatic – Trigonal Antiprismatic Structures with examples
15	Structure and bonding in $[Re_2Cl_8]^{2-}$ and octahedral halides of $[Mo_6(Cl)_8]^{4+}$ and $[Nb_6(Cl)_{12}]^{2+}$.

SEMESTER-II ; PAPER –CH202T

UNIT I: REACTION MECHANISM-II and MOLECULAR REARRANGEMENTS 15 Hrs

Lecture 1.	Criteria for determining the participation of neighbouring group.
Lecture 2.	Evidences as Enhanced reaction rates, retention of configuration, isotopic labeling
Lecture 3.	Cyclic intermediates as evidence and Neighbouring group participation involving Halogens
Lecture 4.	Neighbouring group participation involving Halogens, Oxygen, Sulphur
Lecture 5.	Neighbouring group participation involving Nitrogen, Aryl, Cycloalkyl groups.
Lecture 6.	Neighbouring group participation involving σ and π- bonds
Lecture 7.	Nonclassical carbocation and their importance in chemical reactions
Lecture 8.	Generation, detection, structure, stability and reactions of , carbenes and of nitrenes
Lecture 9.	Definition and classification. Molecular rearrangements involving electron deficient carbon: Allylic and Wolf rearrangement.
Lecture 10.	Definition and classification. Molecular rearrangements involving electron deficient Nitrogen: Hofmann, Lossen
Lecture 11.	Definition and classification. Molecular rearrangements involving electron deficient Nitrogen Curtius, Schmidt and Beckmann rearrangements
Lecture 12.	Definition and classification. Molecular rearrangements involving electron deficient Oxygen: Baeyer-Villiger
Lecture 13.	Definition and classification. Molecular rearrangements involving Base catalysed rearrangements: Benzilic acid Favourski
Lecture 14.	Definition and classification. Molecular rearrangements involving electron deficient Base catalysed rearrangements Transannular , Sommlett-Hauser.
Lecture 15.	Definition and classification. Molecular rearrangements involving Base catalysed rearrangements: Smiles rearrangement

UNIT II: PERICYCLIC REACTIONS-I 15 Hrs

Lecture 1.	Introduction to pericyclic reactions Classification: Electrocyclic, cycloadditions, sigmatropic, ene, and chelotropic reactions
Lecture 2.	Electrocyclic Reactions Con rotation and dis rotation Electrocyclic closure and opening in 4n and 4n+2 systems

Lecture 3.	Cycloaddition Reactions Suprafacial and antarafacial additions in 4n and 4n+2 cycloadditions
Lecture 4.	Sigmatropic Reactions [i, j] Suprafacial and antarafacial shifts Cope and Claisen rearrangement reactions
Lecture 5.	Aromatic Transition States (ATS)/Perturbation Molecular Orbitals (PMO) approach Concept of Huckel-Mobius aromatic and antiaromatic transition states
Lecture 6.	Framing Woodward-Hofmann selection rules for pericyclic reactions by ATS approach Solving problems based on ATS approach
Lecture 7.	Molecular orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene Molecular orbitals of allyl cation, allyl radical, pentadienyl cation, pentadienyl radical
Lecture 8.	Concept of Frontier Molecular Orbital (FMO) approach Solving problems based on FMO approach
Lecture 9.	Conservation of orbital symmetry Correlation diagrams for electrocyclic and cycloadditions & cycloreversions
Lecture 10.	Solving practice problems on electrocyclic reactions Application of ATS, FMO, and correlation diagrams approaches
Lecture 11.	Solving practice problems on cycloaddition reactions Application of ATS, FMO, and correlation diagrams approaches
Lecture 12.	Solving practice problems on sigmatropic reactions Application of ATS, FMO, and correlation diagrams approaches
Lecture 13.	Detailed on pericyclic reactions in organic synthesis
Lecture 14.	Review and Problem-Solving Session
Lecture 15.	Summary and Final Review :Summary of all topics covered

UNIT III: PHOTOCHEMISTRY

15 Hrs

Lecture 1.	Introduction to photochemistry and a comparative study with thermal chemistry.
Lecture 2.	Photochemistry of olefins and discussion on cis-trans isomerisation
Lecture 3.	Definition and discussion on photo stationary state, its importance.
Lecture 4.	Sensitized isomerization
Lecture 5.	Singlet and triplet excited states in dimerisations.
Lecture 6.	Photodimerisation of non-conjugated dienes
Lecture 7.	Photodimerisation of conjugated dienes involving singlet and triplet state.
Lecture 8.	Photocycloaddition of alkenes to unsaturated carbonyl compounds.

Lecture 9.	Regiochemistry issues in such reactions
Lecture 10.	Electrocyclisations and sigmatropic reactions under photochemical conditions.
Lecture 11.	Di-π-methane reactions and its regioselectivity
Lecture 12.	Excites states of aromatic compounds
Lecture 13.	Photoisomerisation of benzene and its analogues
Lecture 14.	Lecture 14: photochemistry of coarbonyl compounds with Norrish type-I&II reactions
Lecture 15.	Paterno-Buchi and Barton reactions

Paper-III (CH203T): PHYSICAL CHEMISTRY

PC-04: Chemical Kinetics and Photochemistry (15 h)

Lecture-1: Introduction, Collision theory - Failures of collision theory; Steric factor – problems based on collision theory.

Lecture-2: Transition state theory - reaction coordinate, activated complex and the transition state, Thermodynamic formulation of transition state theory, Erying equation.

Lecture-3: **Activation parameters, Hammond's postulates** - Activation parameters and their significance; Examples & problems based on transition state theory, Hammond's postulates and their significance.

Lecture-4: Unimolecular reactions – Derivation of rate law based on Lindamann's theory – limitations, problems.

Lecture-5: Complex reactions - opposing reactions & parallel reactions (all first order) with examples, Consecutive reactions (I order) with examples.

Lecture-6: Chain reactions – general characteristics; steady-state treatment; example – H_2 – Br_2 reaction, derivation of rate law.

Lecture-7: Effect of structure on reactivity – linear free energy relationships; Hammett and Taft equations – substituent (σ and σ*) and reaction constants (ρ and ρ*) with examples.

Lecture-8: Deviations from Hammett correlations – change of mechanism, resonance interaction with examples.

Lecture-9: Taft four parameter equation – significance of the Taft four parameter equation, problems on Hammett & Taft equations

Lecture-10: The Franck-Condon Principle – statement, significance.

Lecture-11: Electronically Excited Molecules - Singlet and triplet states, Radiative lifetimes: Theoretical treatment of excited state lifetimes, comparison with measured lifetimes, and their impact on quantum yield.

Lecture-12: Quantum Yield - Definition and significance, Derivation of fluorescence and phosphorescence quantum yields.

Lecture-13: Photophysical Processes - Photophysical kinetics of unimolecular reactions, Calculation of rate constants for various photophysical processes with example problems.

Lecture-14: Photosensitization and Quenching - Explanation of photosensitization. Quenching mechanisms and derivation of the Stern-Volmer equation/

Lecture-15: Introduction to Fast Reactions-Principle of flash photolysis as a technique to study fast photophysical and photochemical reactions.

PC-05: Quantum Chemistry-II (15 h)

Lecture-1: Introduction to coordinate systems-Cartesian (x, y, z), Polar (r, θ), and Spherical Polar (r, θ, φ), interconversion between cartesian, polar and spherical polar coordinates.

Lecture-2: Schrödinger Equation for the Hydrogen Atom-Introduction to the Schrödinger equation for hydrogen atom, Separation into three equations: radial, angular (θ), and azimuthal (φ).

Lecture-3: Hydrogen-like wave functions- general form and solutions.**Lecture-4: Radial functions –** explain the radial distribution plots, significance

Lecture-5: Angular functions – explanation, Quantum numbers n, l and m and their importance.

Lecture-6: Hydrogen like orbitals and their representation

Lecture-7: Various representation of plots - Polar plots, contour pots and boundary diagrams.

Lecture-8: Many electron systems- Introduction to approximate methods.

Lecture-9: The variation method-variation theorem and its proof.

Lecture-10: Trial variation function and variation integral-Examples of variational calculations. Particle in a box. Construction of trial function by the method of linear combinations.

Lecture-11: Variation parameters-Secular equations and secular determinant.

Lecture-12: Bonding in molecules- Molecular orbital theory-basic ideas, Construction of MOs by LCAO, H_2^+ ion.

Lecture-13: The variation integral for H_2^+ ion-Detailed calculation of wave functions and energies for the bonding and antibonding MOs.

Lecture-14: Bonding and anti-bonding Mos- Physical picture of bonding and antibonding wave functions, energy diagram.

Lecture-15: Comparison of MO and VB models -The MO wave function and the energy of H_2 molecule MO by LCAO method and Valence bond method, summary of the topic, giving assignment questions & problems.

PC-06: Solid State Chemistry (15 h)

Lecture-1: Introduction, Electronic Properties of Solids - Differentiate between metals, insulators, and semiconductors based on their electronic structure, ntroducei band theory and Fermi level, explain K space and Brillouin Zones, and their relevance to band structure.

Lecture-2: Band Structure - Compare the band structure of metals, insulators, and semiconductors, discuss the roles of electrons, holes, and excitons in these materials, analyze the temperature dependence of conductivity in extrinsic semiconductors.

Lecture-3: Photo Conductivity and Photovoltaic Effect - Explain photo conductivity and the photovoltaic effect in p-n junctions, working principle of p-n junction in diode as rectifier, applications.

Lecture-4: Superconductivity - Occurrence and key characteristics of superconductivity, classification of superconductors based on critical temperature and magnetic behaviour, with examples.

Lecture-5: Magnetic behaviour - Describe the Meissner effect and how magnetic fields destroy superconductivity, type-I & II superconductors based on magnetic behaviour, examples.

Lecture-6: High-Temperature Superconductors-Structure of defect perovskites and high Tc superconductivity in cuprates.

Lecture-7: Theories of Superconductivity – Microscopic BCS theory, salient features

Lecture-8: 123 superconductor - Phase diagram and crystal structure of Y-Ba-Cu-O system, particularly $YBa_2Cu_3O_{7-x}$, methods for preparing 1-2-3 materials and the origin of high T_c superconductivity.

Lecture-9: Nanomaterials - Introduction to nanoparticles and the concept of reduced dimensionality in solids, classification of nanomaterials based on dimensionality – 0D, 1D, 2D with examples.

Lecture-10: Preparation methods-briefing on top-down and bottom-up approaches

Lecture-11: Description of preparation methods - sol-gel, chemical vapor deposition, and thermolysis with examples.

Lecture-12: Characterization of Nanoparticles-Experimental methods: Powder X-ray Diffraction – analysis, crystallite size measurement

Lecture-13: Methods for Morphological characterization-SEM, TEM, and AFM description of working principle, examples.

Lecture-14: Optical Properties - Discuss the optical properties of nanoparticles and their various applications.

Lecture-15: Applications & Summary - Various applications of nanomaterials, Josephson tunnelling effect, SQUIDs, summarize the topic, allotting questions & problems for assignment submission.

Semester II Paper-IV: CH 204 (Analytical Techniques and Spectroscopy – II)

Lesson Plan: ASP-04: Electro and thermal Analytical Techniques	
Lecture number	Topic
1	Introduction to electro-analytical techniques - Types and Classification of Electro analytical Methods
2	D.C Polarography: Instrumentation - Dropping mercury electrode (diagram and explanation of each component)
3	Working of polarograph and interpretation of polarogram
4	Types of current involved in polarography – Residual current, Migration, Limiting current,
5	Two electrode assembly -Working electrode, reference electrode. Three electrode assemble – WE, RE and Auxiliary electrode
6	Ilkovic equation and its significance – consequence of Ilkovic equation
7	Applications of polarography in qualitative and quantitative analysis – mixture analysis, application to inorganic (metal ion) and organic compounds analysis
8	Determination of stability constant – derivation
9	Brief account of (i) A.C. polarography (ii) Square-wave polarography (iii) Pulse polarography (iv) Differential pulse polarography – principle, model plots, and advantages

	over DC polarography
10	Amperometric titrations: Principle, Instrumentation. Types and applications of amperometric titrations. Determination of SO_4^{2-}, metal ions viz., Mg^{2+}, Zn^{2+}, Cu^{2+} and other substances like Pb^{2+}, organic compounds
11	Cyclic Voltammetry: Principle, instrumentation, Applications. Cyclic voltammetric study of insecticide parathion
12	HOMO-LUMO Calculations of Ferrocene Using Cyclic Voltammetry
13	Thermal techniques-Introduction, types of thermo analytical methods – TGA, DTA, DSC, TT, TMA, DMA, etc.
14	Thermogravimetry principle and applications of thermogravimetry – instrumentation and working
15	Differential thermal analysis- principle and applications of DTA. Differential scanning calorimetry. DSC: Principle, and application of DSC

Lesson Plan: ASP- 05: NMR-II and ESR Spectroscopy	
Lecture number	**Topic**
1	First order and non-first order spectra, features of the NMR spectra in both the orders, examples
2	Spin notations, Pople notations examples and spectral representations of AX, AX_2, AX_3, A_2X_3, AMX and AB, ABC spin notations
3	Simplification of complex spectra: increased field strength examples, deuterium exchange in molecules with heteroatoms, Lanthanide shift reagents Eu(II) complexes
4	Simplification of complex spectra: double resonance techniques. Discrimination of enantiomers by use of chiral NMR solvents (CSAs)
5	Chiral lanthanide shift reagents and Mosher’s acid Mosher’s method, determination of absolute and relative configurations
6	Nuclear Overhauser Enhancement (NOE) examples and application of NOE, Homoatomic and heteroatomic NOE, experiment
7	Study of fluxional molecules using NMR: bullvalene-Valence Tautomerism and Cope rearrangement, $[\eta^1\text{-}C_5H_5M]$- 1,3 shift of metal ion, $[\eta^5\text{-}(C_5H_5)_2Ti\eta^1\text{-}(C_5H_5)_2]$ at varied

	temperatures-ring whizzing, and [η^4-$C_8H_8Ru(CO)_3$]- metal hopping
8	^{19}F NMR spectroscopy: ^{19}F chemical shifts and coupling constants, standard reference, applications of ^{19}F NMR involving coupling with ^{19}F, ^{1}H and ^{31}P: 1,2-dichloro-1,1-difluoro ethane, BrF_5, SF_4
9	Applications of ^{19}F NMR: PF_5, ClF_3, IF_5, CF_3CH_2OH. ^{31}P NMR spectroscopy: ^{31}P chemical shifts and coupling constants, standard reference, applications of ^{31}P NMR involving coupling with ^{31}P, ^{19}F, ^{1}H and ^{13}C: ATP
10	Applications of ^{31}P NMR: Ph_3PSe, P_4S_3, H_3PO_4, H_3PO_3, H_3PO_2, HPF_2
11	Applications of ^{31}P NMR: PF_6^-, PH_3, $[Rh(PPh_3)_3Cl]$ (Rh: I= ½).
12	Introduction to solid state NMR: problems in recording solid state NMR, Magic angle spinning (MAS), applications of solid state NMR
13	Electron Spin Resonance Spectroscopy: Introduction, principle, theory, selection rules, energy of transition, ESR spectrum, Instrumentation of ESR
14	Interpretation of Lande's factor 'g'. Hyperfine and super hyperfine Coupling. Simple example H_2
15	Study of free radicals using ESR spectroscopy, methyl radical, phenyl radical. Revision

Lesson Plan: ASP - 06: Mass spectrometry	
Lecture number	**Topic**
1	Introduction to mass spectrometry, Origin of mass spectrum, principle and theory
2	Principle of EI mass spectrometer, components and working
3	Types of fragments: Odd electron and even electron containing neutral and charged species (even electron rule), examples
4	Nitrogen rule, isotopic peaks
5	Determination of molecular formula, metastable ion peaks –significance and uses
6	Principle and applications of High resolution mass spectrometry
7	Salient features of fragmentation pattern of organic compounds: β-cleavage and Mclafferty rearrangement with examples
8	Retro Diels – Alder fragmentation and ortho effect with examples

9	Ionization techniques: Principle of Electron Ionization
10	Principle and theory of Chemical ionization technique
11	Principle and theory of Secondary Ion Mass Spectrometry (SIMS)
12	Principle and theory of Electrospray ionization (ESI) and
13	Principle and theory of Matrix Assisted Laser Desorption Ionization (MALDI)
14	Introduction, principle and applications of Gas Chromatography-Mass Spectrometry (GC-MS)
15	Introduction, principle and applications of Liquid chromatography-Mass Spectrometry (LC-MS)