SEMESTER-II
PAPER-I: GENERAL CHEMISTRY-II
(Effective from the admitted batch of 2023-2024)

Credits: 4		**Theory: 4 Hours**
Max Marks: 100	**External: 60**	**Internal: 40**

Course Outcomes (COs)/Course Specific Outcomes (CSOs):
Upon completion of the course the students will be able to:

CO 1: To know the concepts of classical and quantum mechanics of Wave equation.
CO 2: To solve the simple quantum mechanical problems such as simple harmonic oscillator, particle in a 1Dbox, rigid rotor, H atom etc.
CO 3: To solve wave equation of hydrogen atom and calculate energy and wave functions of perturbation theory.
CO 4: To calculate energy and wave functions of variation theory and its applications.
CO 5: To learn the Valence bond, LCAO approximation and the electronic transitions in the hydrogen molecule.

Course learning outcome (LOs):
Upon completion of the course the student will be able

LO 1: To learn the quantum mechanics methods for electron in the atom, ion and molecules.
LO 2: To acquire knowledge of molecular in one dimensional box, three-dimensional box and to solve wave equation problems.
LO 3: To acquire knowledge of molecular symmetry and group theory and to solve chemical problems.
LO 4: To develop the knowledge and learn the concept of tunneling, simple harmonic oscillator, rigid wave functions of electron in the atom.
LO 5: To derive the valence-hybridization-covalent bond-calculation of ionic and covalent bond contributions in hydrogen molecule.

Unit-I **[12 Hours]**

Wave equation – interpretation of wave function–properties of wave function–normalization and orthogonalization, operators–linear and non-linear commutators of operators.

Postulates of quantum mechanics, setting up of operators observables–Hermitian operator – Eigen values of Hermitian operator.

Unit-II **[12 Hours]**

Wave mechanics of simple systems with constant potential energy, particle in one dimensional box–factors influencing colour–the concept of tunneling.

Particle in a three-dimensional box, rigid rotor, wave mechanics of systems with variable potential energy-simple harmonic oscillator.

UNIT-III **[12 Hours]**

Hydrogen atom-solution of R(r), θ (θ) and Φ (ϕ) equations-probability density in orbitals-shapes of orbitals.

Perturbation theory- time independent perturbation (only first order perturbation is to be dealt with)–application to ground state energy of hydrogen and helium atom.

UNIT –IV **[12 Hours]**

Variation principle-applications to hydrogen and helium atoms-calculation of zero-point energy of harmonic oscillator-many electron atom- Comparison between Perturbation and variation theorems.
Hartee-Fock self-consistent field method and introductory concepts of Density functional theory (DFT).

UNIT-V **[12 Hours]**

Molecular orbital theory (MOT)–LCAO approximation, treatment of hydrogen molecule ion and hydrogen molecule by MOT-LCAO (fundamental concepts only), Valence bond theory approach, calculation of ionic and covalent bond contributions in hydrogen molecule by VBT, Hybridization, The electronic transitions in the hydrogen molecule.

Text Books:

1. Introductory Quantum Chemistry, A.K. Chandra, 4th Edition, Tata McGraw Hill, New Delhi (2006).

2. Quantum Chemistry and Spectroscopy, M.S. Pathania, Vishal Publishing Co., New Delhi (1981).

3. Quantum Chemistry, H. Eyring, J. Walter and G. Kimball, John Wiely & Sons, New York, (1944)

4. Fundamentals of Quantum Chemistry, R. Anantharaman, Macmillan Publishers India Ltd.,

New Delhi (2000)

5. Quantum Chemistry, Ira N. Levine, 7th Edition, Pearson, New Delhi, (2013)4. Group Theory and its Applications to Chemistry, K. V. Raman, Tata McGraw – Hill Publishing Company Ltd., New Delhi.

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SEMESTER-II
PAPER-II: INORGANIC CHEMISTRY-II
(Effective from the admitted batch of 2023-2024)

Credits: 4		**Theory: 4 Hours**
Max Marks: 100	**External: 60**	**Internal: 40**

Course Outcomes (COs)/Course Specific Outcomes (CSOs):

CO 1: Understanding of metal-metal bonds in metal clusters.
CO 2: To know the isolobal relationships, electron rules and isoelectronic relationships in organometallic Compounds.
CO 3: To explain metal ligand equilibrium, spectrophotometric and pH metric methods in order to understand the stability of metal complexes.
CO 4: Understanding of various reaction mechanisms in coordination chemistry.
CO 5: Develop interest chemistry of Natural products the synthesis of terpenes, alkaloids and flavonoids.

Course learning outcome (LOs):

Upon completion of the course the students should be able to:
LO 1: The basic concepts of structure and bonding of metal clusters.
LO 2: Acquire knowledge on ligands and fluxional molecules, different organic ligands and metal complexes.
LO 3: Methods to determine stability of metal complexes.
LO 4: Different types of reaction mechanisms of metal complexes.
LO 5: Structure, synthesis, and reactivity of various natural products like terpenes, alkaloids and flavonoids.

UNIT-I **[12 Hours]**

Metal cluster compounds – definition, classification – evidences for existence of M-M bonds - conditions favorable for formation of M-M bonds.
Preparation, structure and bonding of the following metal cluster compounds.
$[Re_2Cl_8]^{2-}$, $[Mo_2Cl_8]^{4-}$, $Re_2(RCOO)_4X_2$, $Mo_2(RCOO)_4(H_2O)_2$, $Cu_2(RCOO)_4(H_2O)_2$, $[Mo_2Cl_9]^{3-}$, $[W_2Cl_9]^{3-}$, Re_3Cl_9, $[Re_3Cl_{12}]^{3-}$, $[Mo_6Cl_8]^{4+}$ and $[Nb_6X_{12}]^{2+}$.
Polyatomic clusters – Zintle ions, Chevrel phases.

UNIT-II **[12 Hours]**

Organometallic compounds - 16 and 18 electron rules.
Isoelectronic relationship - Synthesis, structure, bonding and reactions of carbon monoxide, dinitrogen, nitric oxide complexes and metallocene with special reference to ferrocene.
Isolobal relationship – H, Cl, CH_3, $Mn(CO)_5$; S, CH_2, $Fe(CO)_4$; P, CH, $Co(CO)_3$.

UNIT-III **[12 Hours]**

Metal Ligand equilibria in solution:
Step wise and overall formation constants and their interaction. Trends in stepwise constants (statistical effect and statistical ratio).
Factors affecting the stability of metal complexes, stability correlations - Irwing -William's series, Pearson's theory of hard and soft acids and bases (HSAB), application of HSAB. chelate effect and its thermodynamic origin.

UNIT-IV **[12 Hours]**

Determination of stability constants of complexes by spectrophotometric method ((Job's method) and pH –metric method (Bjerrum's).

Reactivity of metal complexes – inert and labile complexes. Explanation of lability on the basis of valence bond and crystal field theories.

UNIT- V **[12 Hours]**

Reaction Mechanisms of Metal Complexes:

Kinetics and mechanisms of substitution reactions A, D, I_d and I_a. kinetics of substitutions reactions in octahedral complexes: acid hydrolysis of Co(III) complexes, factors affecting acid hydrolysis, base hydrolysis of Co(III) complexes, Conjugate base mechanism.

Substitution reactions in square planar complexes: Trans-effect, Theories of Trans effect.

Electron transfer reactions: concept of complementary and non-complementary reactions with examples, inner sphere and outer sphere mechanisms, Marcus theory.

Text books:

1. Advanced Inorganic Chemistry by F.A. Cotton and R.G. Wilkinson, IV Edition, John, John Wiley and Sons, New York, 1980.

2. Inorganic Chemistry by J.E. Huheey, III edition, Harper International Edition, 1983.

3. Organometallic Chemistry-A unified approach by A. Singh and R.C. Mehrotra, Wiley Eastern Ltd.

4. Inorganic Chemistry by Shriver and Atkins, Oxford University Press (1999)

5. Theoretical Inorganic Chemistry, II Edition by M.C. Day and J. Selbin, Affiliated East-West press Pvt. Ltd., New Delhi.

6. Mechanisims of Inorganic reactions in solution by D. Benson, McGraw Hill, London, 1968.

7. Inorganic chemistry by K.F. Purcell and J.C. Kotz, W.B. Saunders company, New York, 1977.

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M.Sc. (PREVIOUS) CHEMISTRY SYLLABUS
SEMESTER-II
PAPER: INORGANIC CHEMISTRY LABORATORY-II
(Effective from the admitted batch of 2023-2024)

Quantitative analysis:

1. Volumetric methods of Analysis:

i) Determination of Ferric iron by photochemical reduction
ii). Determination of Nickel by EDTA
iii) Determination of Calcium and Magnesium in a mixture by EDTA
iv) Determination of Copper (II) in presence of iron (III)

2. Gravimetric methods of Analysis:

i) Determination of Zinc as Zinc pyrophosphate
ii). Determination of Nickel from a mixture of Copper and Nickel.

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SEMESTER-II
PAPER-III: ORGANIC CHEMISTRY-II
(Effective from the admitted batch of 2023-2024)

Credits: 4		**Theory: 4 Hours**
Max Marks: 100	**External: 60**	**Internal: 40**

Course Outcomes (COs)/Course Specific Outcomes (CSOs):

CO 1: Acquire the knowledge of addition to carbon-carbon multiple bonds by electrophiles, nucleophiles and free radicals
CO 2: Acquire the knowledge of addition to carbon-Hetero atom multiple bonds through reductions of carbonyl group.
CO 3: Acquire the knowledge of molecular rearrangement to electron deficient carbon, to electron deficient Nitrogen and on electron deficient oxygen
CO 4: Acquire the Knowledge of different kinds of spectroscopic techniques like NMR, IR, UV and mass.
CO 5: Develop interest chemistry of Natural products the synthesis of terpenes, alkaloids and flavonoids.

Course learning outcome (LOs):

Upon completion of the course the students should be able to:

LO 1: Analyze and solve to add nucleophiles, electrophiles and free radicals to carbon-carbon multiple bonds
LO 2: Analyze and solve to add nucleophiles, electrophiles and free radicals to carbon-hetero atom multiple bonds
LO 3: Know different molecular rearrangements on electron deficient carbon, nitrogen and oxygens
LO 4: Have a basic knowledge on different spectroscopic techniques
LO 5: Structure, synthesis, and reactivity of various natural products like terpenes, alkaloids and flavonoids.
LO 6: Explain addition reactions, molecular rearrangements, spectroscopic techniques and natural products

UNIT-I: Addition Reactions: **[12 Hours]**

(a) **Addition to carbon-carbon multiple bonds**- Addition reactions involving electrophiles, nucleophiles and free radicals, cyclic mechanisms. Stereochemistry and reactivity. Hydrogenation of double and triple bonds, Michael reaction, Prins reaction.
(b) **Addition to carbon-hetero atom multiple bonds**: Addition of Grignard reagents, Mannich reaction, Reformatsky reaction, Tollen's reaction.

UNIT-II: Elimination Reactions: **[12 Hours]**

Mechanisms of E2, El, and E1CB, factors-effects of substrate, attacking base, leaving group and medium. Stereochemistry of eliminations in acyclic and cyclic systems. Saytzeff elimination, Hoffman elimination and pyrolytic elimination.

UNIT-III: Molecular Rearrangements **[12 Hours]**

Molecular Rearrangements:

Types of molecular rearrangements, migratory aptitude.

Rearrangements to electron deficient carbon: Pinacol-pinacolone, Wagner-Meerwein and Benzil-Benzilic acid,
Rearrangements to electron deficient nitrogen: Beckmann, Hofmann, Curtius, Schmidt and Lossen rearrangements.
Rearrangements to electron deficient oxygen: Baeyer-Villiger, Dakin rearrangements.
Other rearrangements: Neber rearrangement and Favorskii rearrangements.

UNIT - IV: Spectroscopy **[12 Hours]**

A) **UV Spectroscopy**: Various electronic transitions, selection rules, effect of solvent on electronic transitions, the absorption laws, chromophores, auxochromes, bathochromic and hypso chromic shifts, hyperchromic and hypochromic effects,
B) **Infrared Spectroscopy**: Basic principles: types of molecular vibrations, fingerprint region and identification of functional groups.
C)**Nuclear Magnetic Resonance Spectroscopy (^{1}H-NMR)**: nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shifts, factors affecting the chemical shift.
D) **Mass Spectroscopy**: Basic Principles, instrumentation, isotope abundance, the molecular ion, metastable ions, base peak, fragment ions, even-electron rule and nitrogen rule. simple cleavage – retro Diels Alder reaction and Mclafferty rearrangement -

UNIT-V

Chemistry of Natural Products: **[12 Hours]**

study of the following compounds involving their isolation - structure elucidation - synthesis and biogenesis
A) Terpenoids: - Occurrence, Isolation, isoprene rule, structure elucidation and synthesis ofα- Terpineol and α- pinene
B) ALKALOIDS: Occurrence, Isolation, classification based on nitrogen heterocyclic ring and synthesis of quinine and nicotine
C) Natural plant pigments; anthocyanins, Flavonoids and isoflavonoids: Cyanidin, Quercetin, and Genistein.

Text books:

1. Organic Chemistry Vol. I (Sixth Edn.) and Vol. II (Fifth Ed.,) by IL finar ELBS.
2. Organic Chemistry (fifth Edn.,) by Morrison and Boyd, PHI, India.
3. Organic Chemistry (fifth edition) by Francis A. Carey Tata McGraw Hill publishing Company Limited, New Delhi.
4. Reaction Mechanism in Organic Chemistry by Mukherjee Sirigh, N Terniitarr, Indiar
5. A guidebook to mechanism in Organic Chemistry by Peter Sykes, ELBS.
6. Advanced organic chemistry by Jerry March (4th Edition) Wiley Eastern. .
7. Stereochemistry of carbon compounds by E. Eliel, John Wiley & Sons, Inc.
8. Stereochemistry of Organic compounds by D. Nasipuri.
9. Chemistry of Natural products by R.S. Kalsi Kalyani Publ.

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M.Sc. (PREVIOUS) CHEMISTRY

PAPER: ORGANIC CHEMISTRY LABORATORY-II
(Effective from the admitted batch of 2023-2024)

Identification of the unknown organic compounds:
Systematic identification of organic compounds – preliminary tests, detection of extra elements, solubility, common functional group tests (determination of functional group/s in a single compound, if present), preparation of two rational derivatives
The given organic compound must be identified by comparing the melting point /Boiling point of the compound and melting points of its derivatives with the literature.

List of suggested compounds:
Glucose, fructose, benzaldehyde, p-anisaldehyde, p-chloro benzaldehyde, acetophenone, phenol, cresols, naphthols, esters, p-chloro benzoic acid, aniline, p-tolune, p-anisidine, p-chloroaniline, diphenyl amine, N, N-dimethylaniline, benzamide, naphthalene and anthracene.

TEXT BOOKS
1. A Textbook of Practical Organic Chemistry by A. I. Vogel, ELBS and Longman group.
2. Practical Organic Chemistry by Mann and Saunders, ELBS and Longman group.

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SEMESTER-II
PAPER-IV: PHYSICAL CHEMISTRY-II
(Effective from the admitted batch of 2023-2024)

Credits: 4		**Theory: 4 Hours**
Max Marks: 100	**External: 60**	**Internal: 40**

Course Outcomes (COs)/Course Specific Outcomes (CSOs):

CO 1: To know the various types of crystal structures of solids, determine the Bragg's equation, Band theory and Basic concept of superconductivity.
CO 2: Understanding of magnetic resonance spectroscopies and its applications in free radicals systems.
CO 3: To know various polymerizations and its determination through various methods.
CO 4: To know the importance of photochemistry and its applications in organic and inorganic chemistry.
CO 5: Understanding of various electrochemical cells and concentration cells with and without transference.

Course learning outcome (LOs):
Upon completion of the course the students should be able to:
LO 1: To learn the various types of crystal structures of solids, Miller indices.
LO 2: Determination of structures of molecules using NMR and ESR.
LO 3: Different types of polymerization reactions useful in polymer industry.
LO 4: Basic concepts of photochemistry and how reactions will be affected in presence of light.
LO 5: Calculations of solubility product and EMF of a cell.

UNIT-I **[12 Hours]**
Crystal structure of solids: Structures and types of solids, symmetry elements in crystals, Fundamental of lattices, unit cell, Bravais lattices, radius ratios; Miller indices. Structure determination by X-ray diffraction (Bragg's equation). Magnetic properties of solids- classification of magnetic materials, Magnetic susceptibility and its measurement.
Electric properties-Band theory, the band structure of metals, insulators, and semiconductors. The temperature dependence of conductivity of extrinsic semiconductors. Basic concept of superconductivity.

UNIT-II: **[12Hours]**
Classification of polymers - Free radical, ionic and Zeigler - Natta Polymerization - kinetics of free radical polymerization - Techniques of polymerization - Glass transition temperature - Factors influencing the glass transition temperature.
Number average and Weight average Molecular weights - molecular weights determination by Osmometry and Viscometry methods.

UNIT-III: **[12 Hours]**

Electrochemistry I: Ionic mobilities and conductivities - Debye-Huckel theory of strong electrolytes, Debye-Huckel onsagar equation-limitations- mean activity coefficient-Verification of Debye-Huckel limiting law.
Electro chemical cell- Galvanic and electrolytic cell. Nernst equation- Concentration cell with and without transference- effect of complexation on redox potential- ferricyanide/ferrocyanide couple, Fuel Cells.

UNIT-IV: **[12 Hours]**
Electrochemistry II: The electrode-electrolyte interface. The electrical double layer. Gouy-Chapman diffuse-charge model and Stern model. Electrodics: Charge transfer reactions at the electrode-electrolyte interface.
Derivation of Butler-Volmer equation, Tafel equation, over voltage and its types, Corrosion and its types, Polarography-Half wave potential and Ilkovic equation.

UNIT-V: **[12 Hours]**
Photochemistry: Electronic transitions in molecules, Franck-Condon principle. Electronically excited molecules- singlet and triplet states, Quantum yield and its determination by Actinometry. Quenching effect- Stern Volmer equation.
Photochemical equilibrium and delayed fluorescence- E-type and P-type. Photochemical primary processes, types of photochemical reactions- photodissociation, addition and isomerization reactions with examples.

Text Books:
1. Physical Chemistry by Peter Atkins and Julio de Paula, Oxford University Press.
2. Physical Chemistry by G.W. Castellon, Narosha Publishing House
3. Physical chemistry by K.L. Kapoor.
4. Principles of photochemistry, Rohitgee Mukhargee.

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SEMESTER-II
PAPER: PHYSICAL CHEMISTRY LABORATORY-II
(Effective from the admitted batch of 2023-2024)

1. Potentiometric titration of Iron (II) using potassium dichromate.
2. Potentiometric titration of strong acid with a strong base using quinhydrone electrode.
3. Determination of kinetics of Ester hydrolysis.
4. Determination of Equilibrium constant of Potassium Iodide-Iodine system.
5. Determination of Critical solution temperature of phenol-water system.
6. Determination of effect of electrolyte (NaCl) on the miscibility temperature of Phenol-water system.

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