



DEPARTMENT OF ORGANIC CHEMISTRY

**M.Sc. (PREVIOUS) CHEMISTRY SYLLABUS
SEMESTER-I**

**PAPER-I: GENERAL CHEMISTRY-I
(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: Learn and understand the selection rules and criteria for molecules to exhibit rotational and IR spectroscopy.
- CO 2: Understand the Classical and quantum mechanical theories of Raman spectroscopy and basic concepts of electronic spectroscopy.
- CO 3: Learn spectroscopic methods based on magnetic resonance principles.
- CO 4: Learn basics of group theory and its application in chemistry.
- CO 5: Understand the basic concepts of FORTRAN programming and its applications.

Course learning outcome (LOs):

Upon completion of the course the student will be able

- LO 1: To apply the spectroscopic methods for structure elucidation of molecules.
- LO 2: To apply the spectroscopic methods for structure elucidation of molecules.
- LO 3: To acquire knowledge of molecular symmetry and group theory and to solve chemical problems.
- LO 4: To determine the group multiplication tables for C_{2v} and C_{3v} point groups.
- LO 5: To write FORTRAN programs for simple chemical problems

UNIT – I

[12 Hours]

Rotational spectra of diatomic molecules-rigid rotor-selection rules-application of rotational spectra-calculation of bond length- isotopic effect, stark effect-selection rules and its applications.

Infrared spectra of diatomic molecules-harmonic and anharmonic oscillators, Applications of IR-Fundamental-overtone-calculation of force constant, combination bands and difference bands in IR spectroscopy, Fermi resonance.

UNIT-II

[12 Hours]

Raman effect-classical and quantum mechanical explanations, rotational Raman and vibrational Raman spectra- intensity of stoke and anti-stokes in Raman.

Electronic spectra of diatomic molecules, vibrational coarse structure-intensity of spectral lines, Rotational fine structure-vibrational and rotational Raman spectra, Franck Condon principle-applications of band head and band shading.

UNIT-III

[12 Hours]



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Spin Resonance Spectroscopy: Principle and theory of NMR spectroscopy- Chemical shift and its origin. Spin-Spin interaction. Application of NMR to structural elucidation-Structure of ethanol, dimethylformamide, styrene and acetophenone.

Principle and theory of ESR, g-factor, hyperfine interactions-applications of ESR studies to the structure of free radicals.

UNIT-IV

[12 Hours]

Basic concepts of Symmetry and Group theory – Symmetry elements, symmetry operations and point groups – Axioms of Group theory, Anatomy of character table, Mulliken and Classification of molecules into point groups.

Similarity Transformation and classes – Representations of reducible and irreducible representations, Group multiplication tables for C_{2v} and C_{3v} point groups Orthogonality theorem and its implications.

UNIT-V [12 Hours]

Microsoft Fortran: constants, variables and operators, arithmetic expressions, assignment and replacement statements, Input and Output statements-format specifications, conditional and unconditional statements for arithmetic IF, Logical IF, Block IF and Go To statements, Do statement – syntax and rules.

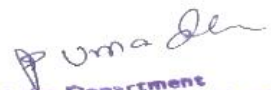
Application of Chemical Problems:

Flowcharts and Programs for

1. Statistical Analysis calculation of arithmetic mean, mean deviation, variance and standard deviation of replicate measurements.
2. Calculation of the pH and hydrogen ion concentration of an aqueous solution of a strong acid considering the auto ionization of water.
3. Calculation of the rate constant of a first order reaction.
4. Calculation of molar extinction coefficient using Beer-Lambert's Law by Linear least-squares method.

Text Books:

1. Symmetry and Spectroscopy of Molecules, K Veera Reddy, New Age International Publishers.
2. Physical Chemistry by Peter Atkins and Julio de Paula, Oxford University Press.
3. Chemical Applications of Group Theory, F. A. Cotton Wiley Eastern Limited New Delhi.
4. Group Theory and its Applications to Chemistry, K. V. Raman, Tata McGraw – Hill Publishing Company Ltd., New Delhi.
5. Computer programming in Fortran-IV by V. Rajaraman, Prentice-Hall of India Pvt. Ltd., New Delhi.
6. Molecular Spectroscopy, - Gordon M. barrow
7. Fundamentals of Molecular Spectroscopy – Banwell.


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SEMESTER-I

PAPER-II: INORGANIC CHEMISTRY-I

(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 on applications of VSEPR, Molecular orbital theories in explaining the structures of simple molecules.
- CO 2: Understand the concept of MO theory to square planar (PtCl_4^{2-}) and Octahedral complexes (CoF_6^{3-} , $\text{Co}(\text{NH}_3)_6^{3+}$). Walsh diagram for H_2O molecule.
- CO 3: Apply the knowledge and understanding of understand the Orgel and Tanabe-Sugano diagrams for $d^1 - d^9$ octahedral and tetrahedral transition metal complexes of 3d series stonily prepared metal complexes.
- CO 4: To understand the concept of Term symbols and Electronic spectra and Magnetic properties of complexes.
- CO 5: Develop interest in the areas of magnetic properties of transition and inner transition metal complexes – spin and orbital moments – quenching of orbital momentum by crystal fields in complexes.

Course learning outcome (LOs):

At the end of the course, the learners should be able to:

- LO 1: Explain idea of structure and bonding theories of inorganic compounds.
- LO 2: Interpret Walsh diagram for other liner and bent molecules
- LO 3: Introduce electron counting rules for higher boranes.
- LO 4: Analyze the preparation and structures of heteropoly acids.
- LO 5: Understanding structure and bonding in coordination compounds.
- LO 6: Explain selections rules, Tanabe-Sugano diagrams. Orgel diagrams.
- LO 7: Experimentally identify the covalence in metal complexes.
- LO 8: To calculate the magnetic susceptibility of metal complexes.
- LO 9: To understand and analyse structure-property correlation of coordination compounds
- LO 10: design new coordination compounds based on a fundamental understanding of their electronic properties

UNIT-1

[12 Hours]

Structure & Bonding: VSEPR theory and applications (PCl_5 , SF_6 , IF_7 , ClF_3 and SF_4) Molecular orbital theories in explaining the structures of simple molecules C_2 , N_2 , O_2 , F_2 , CO and NO .

Bent's rule, Non-valence cohesive forces, Walsh diagrams for linear (BeH_2) and bent (H_2O) molecules.



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UNIT-II

[12 Hours]

Inorganic cage and ring compounds: preparation, structure and reactions of boranes (special reference to B₁₂ icosahedra), carboranes, metallocarboranes, Boron-Nitrogen (B₃N₃H₆, B₃N₃H₁₂) Phosphorus-Nitrogen (N₃P₃Cl₆) and Sulphur-Nitrogen (S₄N₄, (SN)_x) cyclic compounds. Electron counting rules in boranes – Wades rules (Polyhedral skeletal electron pair theory).

UNIT-III

[12 Hours]

Coordination compounds: Crystal field theory - crystal field splitting patterns in octahedral, tetrahedral, tetragonal, square planar, square pyramidal and trigonal bipyramidal geometries. Calculation of crystal field stabilization energies. Factors affecting crystal field splitting energies – Spectrochemical series, Jahn – Teller theorem (static and dynamic Jahn-Teller theorem), Molecular Orbital Theory of bonding for Octahedral, tetrahedral and square planar complexes. π -bonding and MOT-Effect of π - donor and π -acceptor ligands on Δ_o . Application of MO theory to square planar (PtCl₄²⁻) and octahedral complexes (CoF₆³⁻, (Co(NH₃)₆)³⁺).

UNIT- IV

[12 Hours]

Electronic spectra of transition metal complexes: Term symbol-Energy Levels: Configurations, Terms, States and Microstates, calculation of Microstates for p² and d² Configuration, Russell- Saunders Coupling Schemes, derivation of terms for various configurations p² and d² configuration, spectroscopic Ground state, Hole Formalism, Energy ordering of terms (Hund's Rules). Selection rules: Laporte orbital selection rule, spin selection rules. Splitting of energy levels and spectroscopic states: Orgel diagrams of d¹ to d⁹ metal complexes. Interpretation of electronic spectra of aquo complexes of Ti(III), V(III), Cr(III), Fe(II), Co(II), Ni(II) and Cu(II).

UNIT- V

[12 Hours]

Tanabe- Sugano diagrams for d¹ –d⁹ octahedral and tetrahedral transition metal complexes of 3d series. Calculation of Dq, Racah Parameter (B), nephelauxetic effect and nephelauxetic parameter (β), Charge transfer (L→M and M→L) spectra of metal complexes.

Magnetic properties of metal Complexes: Types of magnetic behavior, Temperature independent paramagnetism. spin and orbital moments – quenching of orbital momentum by crystal fields in complexes. Orbital contribution to magnetic moment (Oh and Td Complexes)

Text books:

1. Advanced Inorganic Chemistry by F.A. Cotton and G. Wilkinson, IV Edition, John Wiley and Sons, New York, 1980.
2. Inorganic Chemistry by J.E. Huheey, III Edition, Harper International Edition, 1983.
3. Theoretical Inorganic Chemistry, II Edition by M.C. Day and J. Selbin, Affiliated East-West press Pvt. Ltd., New Delhi.
4. Inorganic Chemistry by Shriver and Atkins, Oxford University Press (1999).

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PAPER: INORGANIC CHEMISTRY LABORATORY-I
(Effective from the admitted batch of 2023-2024)

1. Synthesis of Inorganic Metal Complexes: Synthesis of 3d transition metal complexes of tetrahedral, square planar and octahedral geometries.

- (i) Preparation of Tetraammine Copper (II) sulphate monohydrate
- (ii) Potassium tris-oxalatoferrate (III) trihydrate
- (iii) Tris-thiourea copper(I) sulphate

2. Systematic Semi micro Qualitative Analysis of Inorganic six radical mixtures

In systematic Semi micro qualitative inorganic analysis, inorganic mixture contains three cations and three anions. The analysis involves identification and confirmation of cations and anions containing one less familiar cation (Tungsten, Molybdenum, Zirconium, Thorium, Titanium, Uranium, Cerium, Vanadium, Lithium, Berkelium Etc... and one interfering anion

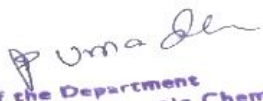
Anions: CO_3^{2-} , S^{2-} , SO_3^{2-} , Cl^- , Br^- , I^- , NO_3^- , SO_4^{2-} , CH_3COO^- , $\text{C}_2\text{O}_4^{2-}$, $\text{C}_4\text{H}_4\text{O}_6^{2-}$, PO_4^{3-} , CrO_4^{2-} , AsO_4^{3-} , F^- , BO_3^{3-}

Cations: Ammonium (NH_4^+), 1st group: Hg, Ag, Pb, Tl, W; 2nd group: Hg, Pb, Bi, Cu, Cd, As, Sb, Sn, Mo; 3rd group: Fe, Al, Cr, Ce, Th, Ti, Zr, V, U, Be
4th group: Zn, Mn, Co, Ni. 5th group: Ca, Ba, Sr. 6th group: Mg, K, Li

Note: A minimum of 4 inorganic mixtures must be analysed in this Semester

REFERENCE BOOKS:

1. Practical Inorganic Chemistry, G. Marr and B. W. Rockett.
2. Practical Inorganic Chemistry by G.Pass H.Sutchiffe, 2nd edn John Wiley & Sons.
3. Experimental Inorganic/Physical Chemistry, M. A. Malati, Horwood Publishing, Chichester, UK (1999)


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Paper- III: ORGANIC CHEMISTRY-I Semester-I
(Effective from 2023-2024 admitted batch)

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 aromaticity, anti-aromaticity, non-benzenoid compounds and reactive intermediates.
- CO 2: Acquire the knowledge of nucleophilic substitution reactions at aliphatic, allylic, trigonal and Vinylic carbons and neighboring group participation. Also develop knowledge on Aromatic nucleophilic substitution reactions.
- CO 3: Acquire the knowledge of Electrophilic substitution reactions at aliphatic and Aromatic centers.
- CO 4: Acquire the Knowledge of Stereochemistry of conformations and configurations. Know the utility of stereochemistry in synthesis.
- CO 5: Develop interest chemistry of heterocyclic compounds in Structure, reactivity and synthesis of various sizes.

Course learning outcome (LOs):

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

- LO 1: Basic aspects of aromaticity and mechanism in organic chemistry
- LO 2: Different nucleophilic substitution reactions and their importance in organic synthesis
- LO 3: Different electrophilic substitution reactions and their importance in organic synthesis
- LO 4: To determine the stereochemistry of different organic molecules and various possible conformations of organic compounds
- LO 5: Structure, synthesis, and reactivity of various heterocyclic compounds.
- LO 6: Explain aliphatic nucleophilic, electrophilic substitution reactions, stereochemistry and conformational analysis and chemistry of heterocyclic compounds

UNIT-I: Aromaticity

[12 Hours]

A) Aromaticity: Concept of Aromaticity, Aromaticity of five membered, six membered and fused systems - non-benzenoid aromatic compounds: cyclopropenylcation, cyclobutadienyldication, cyclopentadienyl anion - tropyliumcation and cyclooctatetraenyl di anion -annulenes. Homo aromaticity, Anti aromaticity and Pseudo aromaticity.

Reactive Intermediates and Name Reactions

B) Reactive Intermediates: Generation, structure, stability and reactivity of Reactive intermediates: carbanion, carbocation, free radicals, carbenes and nitrenes.

UNIT-II

[12 Hours]

A) Aliphatic Nucleophilic Substitutions: The SN_1 , SN_2 , SN_i and SET mechanisms. Substitution reactions of ambident nucleophiles, anchimeric assistance, the neighboring group mechanism: neighboring group participation



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by O, N, S, halogens, aryl groups, alkyl and cycloalkyl groups in nucleophilic substitution reactions. Sigma, Pi bond participation in acyclic and bicyclic systems (non-classic carbocations). Nucleophilic Substitution at allylic, trigonal and Vinylic carbons. Effect of substrate, attacking nucleophile, leaving group and reaction medium.

B) Aromatic Nucleophilic Substitutions: The S_NAr , S_N1 , and benzyne Aryne mechanisms. Reactivity: Effect of substrate, leaving group and attacking nucleophile.

UNIT-III

[12 Hours]

A) Aliphatic Electrophilic Substitutions: $SE1$ $SE2$ and SEi mechanisms. Reactivity- effects of substrate, leaving group and solvent. Reactions- hydrogen exchange, migration of double bonds, halogenation of aldehydes, ketones, carboxylic acids, acyl halides, sulphoxides and sulphones.

B) Aromatic electrophilic substitutions: Alkylation, acylation, nitration, sulfonation, halogenation.

UNIT-IV

[12 Hours]

Stereochemistry and Conformational Analysis: Optical Isomerism: optical activity, molecular dissymmetry and chirality - elements of symmetry. Fisher's projection D,L. and R,S. configurations - relative and absolute configurations optical isomerism due to asymmetric carbon atoms - optical isomerism in biphenyls, allenes and spirans- optical isomerism of nitrogenous compounds, racemization and resolution.

Geometrical isomerism: E, Z -configurations, properties of geometrical isomers. Conformational analysis: Conformations of acyclic molecules -alkanes and substituted alkanes- compounds having intramolecular hydrogen bonding. Conformations of cyclohexane, mono and disubstituted cyclohexanes and decalins.

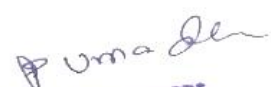
UNIT-V

[12 Hours]

Chemistry of Heterocyclic Compounds: Structure, reactivity and synthesis of five membered Heterocycles: (a) Pyrrole: Paal Knorr, Hantzsch Methods, etc, (b) Thiophene: Paal Knorr, Hinsberg method, etc. (c) Furan: PaalKnorr, Fiest-Benary, Industrial Method, etc.; (d) Pyrazole, (e) Imidazole, (f) Oxazole, (g) Thiazole; Six membered Heterocycles: (a) Pyridine, (b)Pyridazine,(c) pyrimidine and (d) Pyrazine; Aromatic heterocyclics: a) Indole: Fischer indole synthesis, and Bischler synthesis(b) Quinoline and Isoquinoline.

Reference Books

1. Advanced Organic Chemistry: Reactions Mechanisms and Structure by Jerry March, Mc.Graw Hill and Kogakush.
2. Organic Chemistry Vol. I (Sixth Ed.) and Vol. II (Fifth Ed.) by I L Finar ELBS.
3. Organic Chemistry (fifth Ed.,) by Morrison and Boyd, PHI, India.
4. Organic Chemistry (fifth edition) by Francis A. Carey Tata McGraw Hill publishing Company Limited, New Delhi.
5. Stereochemistry of Organic compounds by Ernest L. Eliel, Samuel H. Wilen
6. Chemistry of natural products by S. V. Bhat, B. A. Nagasampangi and M. Sivakumar Narosa Publishing House, 6th reprint 2010


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Synthesis of Organic compounds:

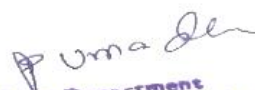
Synthesis, purification and characterization of about ten organic compounds involving one or two stages.

List of some suggested compounds

1. β -Naphthyl methyl ether from β -Naphthol
2. m-dinitrobenzene from Nitrobenzene
3. Azo dye from primary amine
4. Aromatic acid from ester
5. Benzanilide from aniline
6. p-nitroaniline from Acetanilide
7. p-Bromo acetanilide from aniline
8. Phthalimide from phthalic acid
9. 1,2,3-Tribromo benzene from aniline
10. Benzanilide from Benzophenone

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-I

PAPER-IV: PHYSICAL CHEMISTRY-I

(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: Explain the basic concepts of Thermodynamics and its applications.
- CO 2: Understand the concepts of thermodynamics of solutions.
- CO 3: To understand the principle of micellization.
- CO 4: Understand the various kinetic theories, measurements of reaction rates.
- CO 5: Learn experimental techniques for measuring the kinetics of fast reactions and homogenous catalyzed reactions.

Course learning outcome (LOs):

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

- LO 1: To apply the concepts of thermodynamics to various problems in chemistry.
- LO 2: To predict various thermodynamics of mixing of liquids (ΔH_{mix} , ΔG_{mix} and ΔS_{mix}) of ideal gases.
- LO 3: Adsorption-Adsorption isotherms- Freundlich adsorption isotherm, Langmuir adsorption isotherm-limitations
- LO 4: To determine the stereochemistry of different organic molecules and various possible conformations of organic compounds
- LO 5: To understanding the effect of dielectric constant on reactions - Effect of substituent-linear free energy relationships-Hamett equation
- LO 6: To apply the concept of micellization to various chemical reactions. Explain specific and general acid-base catalysis. Steady state approximation- Enzyme catalysis.

UNIT-I

[12 Hours]

Basic concepts of second law of Thermodynamics: Entropy Concept-Entropy changes accompanying different processes, Entropy changes in an ideal gas, Entropy changes in irreversible and reversible processes, Entropy change mixing in ideal gasses, Entropy as a function of V and T and entropy as a function of P and T- Entropy change in isolated systems.

Thermodynamic potentials-Helmholtz free energy function and Gibbs free energy function, derivation of Gibbs- Helmholtz equations, Maxwell relations, Variation of Gibbs energy with temperature and pressure for liquids and gases.

UNIT-II

[12 Hours]

Thermodynamics of mixtures: Partial molar quantities, Gibbs-Duhem equation-chemical potential, Gibbs-Duhem-Margules equation, Thermodynamics of mixing of liquids (ΔH_{mix} , ΔG_{mix} and ΔS_{mix}) - Thermodynamics of ideal solutions - Raoult's law.

Thermodynamics of colligative properties of dilute solutions-lowering of vapour pressure, boiling point of elevation, osmotic pressure and freezing point of



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depression, Thermodynamic concept of equilibrium-Van't Hoff equation, Third law of thermodynamics-application of third law of thermodynamics.

UNIT-III

[12 Hours]

Adsorption and Surface Chemistry: Adsorption and its types-Adsorption isotherms-adsorption of gases on the surface of solid or liquid (Freundlich adsorption isotherm, Langmuir adsorption isotherm-limitations), BET adsorption isotherm.

Surface active agents: Types and classification of surface-active agents, micellization-micells and their structures, critical micellar concentration (CMC), factors affecting the CMC of surfactants.

UNIT-IV

[12 Hours]

Chemical Kinetics of theories of reaction rates: Collision Theory-Limitations, Transition state theory (Absolute reaction rate theory), Lindeman's theory of unimolecular reactions, Effect of ionic strength on rates of reactions-primary and secondary salt effects.

Effect of substituent-linear free energy relationships-Hamett equation - limitations, Taft equation, Kinetics of consecutive reactions, Kinetics of parallel reactions (side reactions-Uni molecular steps only, no derivation).

UNIT-V

[12 Hours]

Empirical rate laws for zero order, 1st order and 2nd order, Specific and general acid-base catalysis, Steady state approximation-Enzyme catalysis-Michaelis-Menten mechanism,

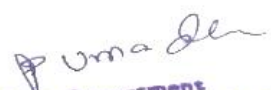
Fast reactions- different methods of studying fast reactions- flow methods, relaxation methods- temperature jump and pressure jump methods.

Text Books:

1. Physical Chemistry by Peter Atkins and Julio de Paula, Oxford University Press.
2. Chemical Kinetics by K. J. Laidler, McGraw Hill Pub.
3. Physical chemistry by K.L. Kapoor

Reference Books:

1. Thermodynamics for Chemists, Samuel Glasstone
2. Physical chemistry by Puri, Sharma and Pathania
3. Micelles, Theoretical and applied aspects, V. Moroi, Plenum publisher


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Conductometry and Potentiometry

1. Conductometric titration of strong acid (HCl) vs strong base (NaOH).
2. Conductometric titration of weak acid (CH₃COOH) vs strong base NaOH).
3. Conductometric titration of mixture of acids (HCl + CH₃COOH) vs strong base (NaOH).
4. Determination of Cell constant of conductivity cell.
5. Determination of dissociation constant of weak acid by conductometric Method.
6. Potentiometric titration of Iron (II) using potassium permanganate.

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