**ANDHRA UNIVERSITY**
**SCHOOL OF CHEMISTRY**
**M.Sc. CHEMISTRY(PREVIOUS) SYLLABUSSEMESTER-I**
**PAPER-I: GENERAL CHEMISTRY-I**
**(Effective from the admitted batch of 2021-2022)**

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

Upon completion of the course the students will be able to,

**CO1:** Learn and understand the selection rules and criteria for molecules to exhibit rotational and IR spectroscopy.

**CO2:** Understand the Classical and quantum mechanical theories of Raman spectroscopy and basic concepts of electronic spectroscopy.

**CO3:** Learn spectroscopic methods based on magnetic resonance principles.

**CO4:** Learn basics of group theory and its application in chemistry.

**CO5:** Understand the basic concepts of FORTRAN programming and its applications.

**Learning Outcomes (LOs):**

Upon completion of the course the student will be able

- To apply the spectroscopic methods for structure elucidation of molecules.
- To acquire knowledge of molecular symmetry and group theory and to solve chemical problems.
- To write FORTRAN programs for simple chemical problems.

**COURSE CONTENT**

**UNIT – I** **[15 Hours]**

Rotational spectra of diatomic molecules-rigid rotor-selection rules-calculation of bond length-isotopic effect, second order stark effect and its applications, Infrared spectra of diatomic molecules-harmonic and anharmonic oscillators. Selection rules-overtones-combination bands calculation of force constant, anharmonicity constant and zero point energy. Fermi resonance, simultaneous vibration rotation spectra of diatomic molecules.

**UNIT-II** **[15 Hours]**

Raman effect-classical and quantum mechanical explanations-Rotational Raman and vibrational Raman spectra, Electronic spectra of diatomic molecules-Vibrational coarse structure-intensity of spectral lines-Franck Condon principle-applications, Rotational fine structure-band head and band shading, Charge transfer spectra.

**UNIT-III** **[15 Hours]**

Spin Resonance Spectroscopy: Principle and theory of NMR spectroscopy-Nature of spinning particle and its interaction with magnetic field. Chemical shift and its origin. Spin-Spin interaction-experimental methods. 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, metal complexes.

**UNIT-IV** **[15 Hours]**

Basic concepts of Symmetry and Group theory – Symmetry elements, symmetry operations and point groups – Schoenflies symbols – Classification of molecules into point groups – Axioms of Group theory – Group multiplication tables for $C_{2V}$ and $C_{3V}$ point groups – Similarity Transformation and classes – Representations – reducible and irreducible representations, Mulliken symbols, Orthogonality theorem and its implications, character table and its anatomy.

**UNIT-V** **[15 Hours]**

Basic components of Computers, higher and lower level languages, Microsoft Fortran: constants, variables and operators, arithmetic expressions, assignment and replacement statements, Input and Output statements – Format free and Format directed I/O statements – Iw, Fw.d, Ew.d and Gw.d format specifications, conditional and unconditional statements – 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. Solution of Quadratic equation – calculation of the roots of a quadratic equation.
3. Calculation of the pH and hydrogen ion concentration of an aqueous solution of a strong acid taking into account the auto ionization of water.
4. Calculation of the root of a polynomial using Gauss-Newton method – Application to Vander-Waal's equation.
5. Calculation of the rate constant of a first order reaction or calculation of molar extinction coefficient using Beer-Lambert's Law by Linear least-squares method.

## COURSE CONTENT

**UNIT-1** **[15 Hours]**

Structure & Bonding: Applications of VSEPR, Valence Bond and Molecular orbital theories in explaining the structures of simple molecules- role of p and d orbitals in pπ-dπ bonding, Bent's rule, Non-valence cohesive forces

Application of MO theory to square planar ($PtCl_4^{2-}$) and Octahedral complexes ($CoF_6^{3-}$, $Co(NH_3)_6^{3+}$).

Walsh diagrams for linear ($BeH_2$) and bent ($H_2O$) molecules

**UNIT-II** **[15 Hours]**

Inorganic cage and ring compounds – preparation, structure and reactions of boranes, carboranes, metallocarboranes, boron–nitrogen ($H_3B_3N_3H_3$), phosphorus–nitrogen ($N_3P_3Cl_6$) and sulphur-nitrogen ($S_4N_4$, $(SN)_x$) cyclic compounds. Structure and bonding in higher boranes with (special reference to B12 icosahedra). Electron counting rules in boranes – Wades rules (Polyhedral skeletal electron pair theory).

Polyacids: Introduction to polyacids- Types of polyacids- Isopolyacdis, Isopoly molybdates, Isopolytungstates, Isopolyvanadates, Structures of Polyacids $]Mo_7O_{24}]^{6-}$ $(V_{10}O_{28})^{6-}$ and $W4O_{16}]^{8-}$, Heteropolyacids- properties of heteropolyacids and salts, structures of heteropolyacids and theories , Mialalicopause and Roscnneium theories , Pauling's theory and keggin's theory, applications of polyacids.

**UNIT-III** **[15 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) and its consequences, nephelauxetic effect, applications and limitations of CFT; ligand field theory

Experimental evidences for covalence in complexes. 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 Δo. Experimental evidence for π - bonding in complexes

**UNIT- IV** **[15 Hours]**

Electronic spectra of transition metal complexes:

Term symbol-Free Ion terms and Energy Levels: Configurations, Terms, States and Microstates, calculation of Microstates for $P^2$ and $d^2$ Configuration, Russell- Saunders Coupling Schemes, J-J Coupling scheme, derivation of terms for various configurations $P^2$ and $d^2$ 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 $d^1$ to $d^9$ metal complexes. Interpretation of electronic spectra of aquo Complexes of Ti(III), V(III), Cr(III), Mn(II), Fe(II), Fe(III), Co(II), Ni(II) and Cu(II). Calculation of interelectronic and spectral parameters for $d^8$ metal complexes.

**UNIT- V** **[15 Hours]**

Tanabe- Sugano diagrams for $d^1$ –$d^9$ octahedral and tetrahedral transition metal complexes of 3d series. Calculation of Dq, Racah Parameter (B) 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. Magnetic properties of transition and inner transition metal complexes – spin and orbital moments – quenching of orbital momentum by crystal fields in complexes. Magnetic susceptibility and its

**UNIT- V** **[12 Hours]**

Tanabe- Sugano diagrams for $d^1$ –$d^9$ octahedral and tetrahedral transition metal complexes of 3d series. Calculation of Dq, Racah Parameter (B) 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. Magnetic properties of transition and inner transition metal complexes – spin and orbital moments – quenching of orbital momentum by crystal fields in complexes. Magnetic susceptibility and its determination by Gouy's method, and Faraday's method. orbital contribution to magnetic moment ( $O_h$ and $T_d$ 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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**UNIT - I**

**Aliphatic Nucleophilic Substitutions**: The SN2, SN1, SNi and SET mechanisms. Substitution reactions of ambident nucleophiles, anchimeric assistance, the neighbouring group mechanism: neighbouring group participation by O, N, S, halogens, aryl groups, alkyl and cycloalkyl groups in nucleophilic substitution reactions. Sigma, Pi bond participation in acylic and bicyclic systems (Non- classic carbocations). Nucleophilic Substitution at allylic, trigonal and Vinylic carbons. Effect of substrate, attacking nucleophile, leaving group and reaction medium.

**UNIT-II**

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

**UNIT-III**

**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, racemisation 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, effect of conformations on reactivity.

**UNIT-IV**

**Chemistry of heterocyclic compounds :** Structure, reactivity and synthesis of reduced three membered Heterocycles: (a) Oxirane: Sharpless method, Shi epoxidation, Jacobsen epoxidation, etc, (b) Aziridine; four membered Heterocycles: (a) Oxetane (b) Azetine; five membered Heterocycles: (a) Pyrrole: Paal Knorr, Hantzsch Methods, etc, (b) Thiophene: Paal Knorr, Hinsberg method, etc. (c) Furan: Paal Knorr, Fiest-Benary, Industrial Method, etc.; (d) Pyrazole, Imidazole, Oxazole, Thiazole; Six membered Heterocycles: (a) Pyridine, Pyridazine, pyrimidine and Pyrazine; Aromatic heterocyclics: a) Indole: Fischer indole synthesis, Bischler synthesis, Madelung synthesis, Domino and cascade methods of indole synthesis, (b) Quinoline and Isoquinoline, (c) Coumarins and Chromones.

**UNIT-V**

**Chemistry of Natural Products**

**A) Terpenoids: -** Occurrence, Isolation, isoprene rule, structure elucidation and synthesis of α- Terpineol and α- pinene

**B) Steroids:-** Nomenclature of steroids, structure elucidation and synthesis and stereochemistry of cholesterol and progesterone

**C) Lipids:-** Classification, chemistry, properties and function-free fatty acids, triglycerides, phospholipids, glycolipids & waxes conjugated lipids- lipoproteins

**Reference Books**


1. Advanced Organic Chemistry: Reactions Mechani;sms 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.

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**UNIT-I** **[12 Hours]**

Basic concepts of second law of Thermodynamics-Entropy- Entropy changes accompanying different processes-Entropy changes in an ideal gas, entropy changes in the mixing of ideal gases, entropy as a function of V and T and entropy as a function of P and T- Entropy change in isolated systems-Clausius inequality-Helmholtz and Gibbs energy -Maxwell relations - Criteria for spontaneity-variation of Gibbs energy with temperature and pressure for solids, liquids and gases-Concept of fugacity-determination of fugacity coefficient of gases- Thermodynamics of phase transitions- Concept of chemical potential-Location of phase boundaries- (Clausius-Clapeyron equation for Liquid- Vapour, Solid -Liquid and Solid- Vapour boundaries)-Ehrenfest classification of phases.

**UNIT-II** **[12 Hours]**

Thermodynamics of mixtures -partial molar quantities - experimental methods of determination of partial molar quantities -Gibbs-Duhem equation and Duhem-Margules equation-Thermodynamics of mixing of liquids ($\Delta H_{mix}$, $\Delta G_{mix}$ and $\Delta S_{mix}$) - Thermodynamics of ideal solutions - Raoult's law - Thermodynamics of colligative properties of dilute solutions - concept of activity and activity coefficient- Experimentaldetermination of activity coefficient - Thermodynamic concept of equilibrium, variation of equilibrium with temperature (Van't Hoff equation) and pressure - Nernst heat theorem, Third law of thermodynamics- exceptions to third law of thermodynamics.

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

Surface tension- Capillary action- Adsorption-Adsorption isotherms-Freundlich adsorption isotherm, Langmuir adsorption isotherm-limitations - BET adsorption isotherm-estimation of Surface area.Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization-phase separation and mass action models.

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

Chemical Kinetics: Theories of reaction rates- Collision theory-Limitations, Transition state theory.Lindeman's theory of unimolecular reactions -Limitations. Diffusion controlled reactions. Effect of ionic strength on rates of reactions- Primary and secondary salt effects.

Effect of dielectric constant on reactions - kinetic isotope effect -Primary and secondary isotopic effects -Effect of substituent -Linear free energy relationships-Hamett equation -limitations- Taft equation. Kinetics of consecutive reactions, parallel reactions, opposing reactions (Uni molecular steps only, no derivation).

**UNIT-V** **[12 Hours]**

Specific and general acid-base catalysis. Skrabal diagrams. Steady state approximation- Enzyme catalysis- Michaelis -Menten mechanism. Derivation of Kinetic equation and Kinetic parameters. Lock and Key hypothesis-pH dependence of enzyme catalyzed reactions.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