ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
M.Sc CHEMISTRY(PREVIOUS)SYLLABUS
SEMESTER-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 **[12 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 **[12 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 **[12 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 **[12 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[12 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.

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.

ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
M.Sc CHEMISTRY (PREVIOUS) SYLLABUS
SEMESTER-I
PAPER-II: INORGANIC CHEMISTRY-I
(Effective from the admitted batch of 2021-2022)

CourseObjectives:Tomakethestudents

CO 1:Acquiretheknowledgeon applications of VSEPR, Valence Bond and Molecular orbital theories in explaining thestructures of simple molecules **and** role of p and d orbitals in pi bonding.

CO 2:Understandthe concept of MO theory to square planar ($PtCl_4^{2-}$) and Octahedral complexes (CoF_6^{3-}, $Co(NH_3)_6^{3+}$). And Walsh diagram for H_2O molecule

CO 3:Apply theknowledgeandunderstandingofUnderstand the Orgel and Tanabe-Sugano diagrams for d^1 –d^9 octahedral and tetrahedral transition metal complexes of 3d series stonewly prepared metal complexex

CO 4: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.

CO5: To understand the concept of Term symbols and Electronic spectra and Magnetic properties of complexes

LearningOutcomes: Attheendofthecourse,thelearnersshouldbeableto:

LO 1:Explainidea of structure and bonding theories of inorganic compounds

LO 2:InterpretWalsh diagram for other liner and bent molecules

LO 3:Introduce electron counting rules for higher boranes

LO 4:Analyse 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

LO7: Experimentally Identify the covalency in metal complexes.

LO8:To calculate the magnetic susceptibility of metal complexes

LO9: understand and analyse structure-property correlation of coordination compounds

LO10:design new coordination compounds based on a fundamental understanding of their electronic properties

COURSE CONTENT

UNIT-1 **[12 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 **[12 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 **[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) 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 **[12 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 **[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)

ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
M.Sc CHEMISTRY (PREVIOUS) SYLLABUS
SEMESTER-I
PAPER-III: ORGANICCHEMISTRY-I
(Effective from the admitted batch of 2021-2022)

CourseObjectives:Tomakethestudents

CO 1:Acquiretheknowledgeofaliphaticnucleophilic,aliphaticelectrophilic,stereochemistry and conformational analysis, chemistry of heterocyclic compoundsandchemistryofnaturalproducts

CO 2:Understandaliphaticnucleophilic, aliphaticelectrophilic, stereochemistry andconformational analysis, chemistry of heterocycliccompounds and chemistry ofnaturalproducts

CO3:Applytheknowledgeandunderstandingofaliphaticnucleophilic,aliphaticelectrophilic,stereochemistryandconformationalanalysis,chemistryofheterocycliccompoundsandchemistryofnaturalproductstonewsituations

CO 4:Develop interest in the areas of aliphatic nucleophilic, aliphatic electrophilic,stereochemistry and conformational analysis, chemistry of heterocyclic compoundsandchemistryofnaturalproducts

LearningOutcomes: Attheendofthecourse,thelearnersshouldbeableto:

LO 1:Explainaliphaticnucleophilic,aliphatic electrophilic,stereochemistryandconformational analysis, chemistry of heterocycliccompounds and chemistry ofnaturalproducts

LO 2:Interpretaliphaticnucleophilic,aliphatic electrophilic,stereochemlstryandconformational analysis, chemistry of heterocycliccompounds and chemistry ofnaturalproducts

LO 3:Comparealiphaticnucleophilic, aliphaticelectrophilic,stereochemistryandconformational analysis, chemistry of heterocycliccompounds and chemistry ofnaturalproducts

LO 4:Analysealiphaticnucleophilic,aliphaticelectrophilic,stereochemistryandconformational analysis, chemistry of heterocycliccompounds and chemistry ofnaturalproducts

LO 5:SolvealiphaticnucleophillG,aliphaticelectrophilic,stereochemistryandconformational analysis, chemistry of heterocycliccompounds and chemistry ofnaturalproducts

LO6: Identify aliphatic nucleophilic,aliphaticelectrophilic, stereochemistry andconformationalanalysis,chemistryofheterocycliccompoundsand chemistryofnaturalproducts

LO7: Apply aliphaticnucleophilic,aliphaticelectrophilic, stereochemistry andconformationalanalysis,chemistryofheterocycliccompoundsand chemistryofnaturalproducts

COURSE CONTENT

UNIT–I [12 Hours]

Aliphatic Nucleophilic Substitutions: The SN2, SN1, SNi and SET mechanisms.Substitutionreactionsofambidentnucleophiles,anchimericassistance,theneighbouring group mechanism: neighbouring group participation by 0,N, S,halogens, aryl groups, alkyl and cycloalkyl groups in nucleophilic substitutionreactions. Sigma, Pi bond participation in acylic and bicyclic systems (Non-classiccarbocations).NucleophilicSubstiłutional allylic,ŁrigonalandVinyliccarbons.Effectofsubstrate,attackingnucleophile,leavinggroupandreactionmedium.

UNIT-II **[12 Hours]**

Aliphatic ElectrophilicSubstitutions: SEI SE2 and SEi mechanisms. Reactivity-effects of substrate, leaving group and solvent. Reactions- hydrogen exchange,migration of doublebonds, halogenation of aldehydes, ketones, carboxylic acids, acylhalides,sulphoxidesandsulphones.

UNIT-III **[12 Hours]**

Stereochemistry and Conformational Analysis: Optical Isomerism:FtiCal activity,moleculardissymmetryand chirality- elements of symmetry.Fisher'sprojectionD,L. and R,S. configurations - relative and absolute configurations optical isomerismdue to asymmetric carbon atoms - optical isomerism in biphenyls, allenes andspirans-opticalisomerismofnitrogenouscompounds,racemisationandresolution.

Geometricalisomerism:E,Z-configurations,propertiesofgeometricalisomers.Conformationalanalysis:Conformationsofacyclicmolecules-alkanesandsubstitutedalkanes-compoundshavingintramolecularhydrogenbonding.Conformations of cyclohexane, mono and disubstituted cyclohexanes and decalins,effectofconformationsonreactivity.

UNIT—IV **[12 Hours]**

Chemistry of Heterocyclic Compounds :Structure, reactivity and synthesis of threemembered Heterocycles: (a) Oxirane: Sharpless method, Shi epoxidation, Jacobsenepoxidation, etc, (b) Aziridine; four membered Heterocycles: (a) Oxetane (b) Azetine;five memberedHeterocycles:(a) Pyrrole: Paa1 Knorr, Hantzsch Methods,etc, (b)Thiophene: Paa1 Knorr, Hinsberg method, etc. (c) Furan: Paa1 Knorr, Fiest-Benary,IndustrialMethod, etc.; (d) Pyrazole,(e) Imidazole,(f) Oxazole, (g) Thiazole; Sixmembered Heterocycles: (a) Pyridine, (b)Pyridazine,(c) pyrimidine and (d) Pyrazine;Aromatic heterocyclics: a) Indole: Fischer indole synthesis, Bischler synthesis, andMadelungsynthesis(b)QuinolineandIsoquinoline,(c)CoumarinsandChromones.

UNIT—V **[12 Hours]**

ChemistryofNaturalProducts:

A) Terpenoids:-Occurrence,Isolation,isoprenerule,structureelucidationandsynthesisofn-Terpineolandn-pinene

B) Steroids:-
Nomenclatureofsteroids,structureelucidation,synthesisandstereochemistryofcholesterolandprogesterone

C) Lipids:-Classification,propertiesandfunction-
freefattyacids,triglycerides,phospholipids,glycolipids&waxesconjugatedlipids-lipoproteins

ReferenceBooks

1. AdvancedOrganicChemistry:ReactionsMechanismsandStructurebyJerryMarch, Mc.GrawHillandKogakush.

2. OrganicChemistryVol.I(Sixth Ed.)andVol.II(FifthEd.)byILFinarELBS.

3. OrganicChemistry(fifthEd.,)byMorrison andBoyd,PHI,India.

4. OrganicChemistry(fifthedition)byFrancisA.CareyTataMcGrawHillpublishing CompanyLimited,NewDelhi.

5. StereochemistryofOrganiccompoundsbyErnestL.E1ie1,SamuelH.Wilen

6. Chemistry of natural products by S. V. Bhat, B. A. Nagasampangi and M.Sivakumar NarosaPublishingHouse,6threprint2010

ANDHRA UNIVERSITY

SCHOOL OF CHEMISTRY

M.Sc CHEMISTRY (PREVIOUS) SYLLABUS SEMESTER-I

PAPER-IV: PHYSICALCHEMISTRY-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: Explain the basic concepts of Thermodynamics and its applications

CO2: Understand the concepts of thermodynamics of solutions.

CO3: To understand the principle of micellisation.

CO4: Understand the various kinetic theories, measurements of reaction rates.

CO5: Learn experimental techniques for measuring the kinetics of fast reactions and homogenous catalyzed reactions.

Learning Outcomes (LOs):

Upon completion of the course the student will be able to understand

- To apply the concepts of thermodynamics to various problems in chemistry.
- To predict various reaction mechanisms.
- To apply the concept of micellization to various chemical reactions.

COURSE CONTENT

UNIT-I **[12Hours]**

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 **[12Hours]**

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 (ΔH_{mix}, ΔG_{mix} and ΔS_{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 onreactions - 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

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