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.

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:Understand the 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 **[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

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)

MODEL QUESTION PAPER

ANDHRA UNIVERSITY SCHOOL OF CHEMISTRY

M.Sc. Chemistry (Previous)Paper- II: GENERAL CHEMISTRY-ISemester-I

(Effective from 2021-2022 admitted batch)

Time: 3 hours **Answer ALL questionsMax. Marks**: 80 **(5x16=80 Marks)**

1. (a) (i)What kind of molecules exhibit microwave spectra.
   (ii) Discuss isotope effect in microwave spectra.

(or)

(b) (i)Derive an expression for energy or harmonic oscillator and discuss the selection rules.
   (ii) Describe the origin of PQR structure of Vibrational-Rotational spectra.

2. (a)(i) Discuss the classical and quantum mechanical theories of Raman spectra.
   (ii) Explain rotational fine structure in electronic spectroscopy?

(or)

(b) (i)State and explain Franck Condon principle.
   (ii) Write a short note on charge transfer spectra.

3 (a) (i)Explain the terms spin active nuclei, resonance, larmor precession and chemical shifts in NMR.
   (ii) Explain hyperfine interactions in ESR spectroscopy taking examples.

(or)

(b) (i)What are the factors affecting g value in ESR spectroscopy.
   (ii) Explain spin-spin interactions in NMR spectroscopy?

4 (a) (i)State and explain the axioms of group theory.
   (ii) State the great Orthogonality theorem and discuss its implications.

(or)

(b) (i)Give the points groups for NH_3, XeF_4, eclipsed C_2H_6, Cis C_2H_4, $B_3N_3H_6$ and allene.
   (ii) Describe the anatomy of character table.

5 (a) (i)Write a flowchart and FORTRAN program for calculation of rate constant of a first order reaction.
   (ii) Give the syntax and rules of DO statement.

(or)

(b) (i)Write a flowchart and FORTRAN program for calculation of pH and hydrogen ion concentration of an aqueous solution of a strong acid taking into account the auto ionization of water.
   (ii) Write a brief note on format directed Input/output statements.

MODEL QUESTION PAPER

ANDHRA UNIVERSITY SCHOOL OF CHEMISTRY

M.Sc. Chemistry (Previous) Paper- II: INORGANIC CHEMISTRY-ISemester-I

(Effective from 2021-2022 admitted batch)

Time: 3 hours **Answer ALL questions** **Max. Marks**: 80 **(5x16=80 Marks)**

1. (a) (i)Predict the geometries of ClF_3, XeF_4 and SF_4 molecules using VSEPR theory.
(ii)What is LCAO method? Predict bond order and bond lengths in O_2^+ and O_2^- ions based on MO energy level diagram

OR

(b) (i)Draw the MO energy level diagram for $[Co(NH_3)_6]^{3+}$ and discuss its magnetic properties.
(ii) Draw the Walsh diagram for H_2O molecule and predict its structure.

2. (a) (i)Discuss the preparation of, structure of, and bonding in $N_3P_3Cl_6$.
(II) Discuss the structure and properties of borazole.

OR

(b) (i)Explain Mialalicopause and Roscnneium theories, Pauling's theory and keggin's theory of polyacids.
(ii) Explain the method of counting skeletal electrons in cluster compounds

3. (a) (i)Draw and explain the crystal field splitting of 'd ' orbitals in square planar and trigonal bipyramidalgeometries.
(ii) Discuss the factors affecting crystal field splitting energies.

OR

(b) (i) what are static and dynamic Jahn-Teller theorem and discuss its consequences
(ii) Write a note on nephelauxetic effect

4. (a) (i)How do Tanabe – Sugano diagrams differ from Orgel diagrams? Draw Tanabe – Sugano diagram for $[V(H_2O)_6]^{3+}$
(ii) Draw the Orgel diagram for $[TiCl_4]^-$ ion and explain the electronic transitions.

OR

(b) (i)Write an account on Russell – Saunders coupling.
(ii) Derive the term symbols for Ni^{2+} and identify the ground state term symbol

5. (a) (i)Discuss different types of paramagnetic behaviourof transition metal complexes
(ii) Calculate the spin only magnetic moments of the $[MnCl_6]^{3-}$ and $[Fe(CN)_6]^3$

OR

(b) (i)Describe the Magnetic properties of inner transition metal complexes
(ii) Determination of magnetic susceptibility a determination by Gouy's and Faraday's methods

School of Chemistry
Andhra University
M.Sc.(Previous) Chemistry Syllabus for II Semester
Paper I: General chemistry
(w.e.f. 2021-2022 admitted batch)

Unit I **[15 Hours]**

Wave equation – interpretation of wave function – properties of wave function – normalization and orthogonalisation, 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 **[15 Hours]**

Wave mechanics of simple systems with constant potential energy, particle in one dimensional box – factors influencing colour – transition – dipole integral, symmetry arguments in deriving the selection rules-the concept of tunneling – particle in a three dimensional box, Rigid rotor, wave mechanics of systems with variable potential energy-simple harmonic oscillator-solution of wave equation-selection rules.

UNIT-III **[15 Hours]**

Hydrogen atom-solution of R(r), $\theta(\theta)$ and $\Phi(\phi)$ 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 **[15 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 **[15 Hours]**

Valence bond approach-directed valence-hybridization-covalent bond-calculation of ionic and covalent bond contributions in hydrogen molecule. Molecular orbital theory – LCAO approximation – hydrogen molecule ion – hydrogen molecule (fundamental concepts only) – The electronic transitions in the hydrogen molecule.

ANDHRA UNIVERSITY
SCHOOL OF CHEMISTRY
M.ScCHEMISTRY (PREVIOUS) SYLLABUSSEMESTER-II
PAPER-II: INORGANICCHEMISTRY-II

(Effective from the admitted batch of 2021-2022)

CourseObjectives:Tomakethestudents

CO1:To give a basic and updated knowledge for the students on metal clusters,
Organometallic chemistry of transition metals
CO 2:To discuss the preparation and structures of and functional aspects of metal clusters
CO 3: Design new coordination compounds based on a fundamental understanding of their electronic properties
CO4: To discuss basics principles of reaction mechanism in metal complexes
CO5: To understand the concept of Term symbols and Electronic spectra and Magnetic properties of complexes
LearningOutcomes: Attheendofthecourse,thelearnersshouldbeable to:

LO 1:Explain the idea of metal clusters
LO 2:Interpret the bonding nature in metal clusters
LO 3:understand the basics of inorganic and coordination chemistry
LO 4:verify the 18 electron rules in various metal clusters
LO 5:determine the stability constants of metal complexes
LO6: Explain the kinetics of substitution reaction, conjugate bas mechanism and trans effect
LO 7: design new coordination compounds based on a fundamental understanding of their Reaction mechanism

COURSE CONTENT

UNIT-I **[15 Hours]**

Metal cluster compounds - definition – 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.
$Re_2Cl_8^{2-}$, $Mo_2Cl_8^{4-}$, $Re_2(RCOO)_4X_2$, $Mo_2(RCOO)_4(H_2O)_2$, $Cr_2(RCOO)_4(H_2O)_2$, $Cu_2(RCOO)_4(H_2O)_2$, $Cr_2Cl_9^{3-}$, $Mo_2Cl_9^{3-}$, $W_2Cl_9^{3-}$, Re_3Cl_9, $Re_3Cl_{12}^{3-}$, $Mo_6Cl_8^{4+}$, $Nb_6X_{12}^{2+}$ and $Ta_6X_{12}^{2+}$.
Polyatomic clusters – Zintle ions, Chevrel phases.

UNIT-II **[15 Hours]**

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

UNIT-III **[15 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: Biological functions and toxicology of metals, and medicinal applications; chelate effect and its thermodynamic origin

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

Reaction Mechanisms of Metal Complexes:

Reactivity of metal complexes, inert and labile complexes, Kinetics and mechanisms of substitution reactions, kinetics of substitutions reactions in octahedral complexes, acid hydrolysis, Factors affecting acid hydrolysis, Base hydrolysis, Conjugate base mechanism, Anation reactions, substitution reactions in square planar complexes, Trans effect, Mechanism 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.

Model Question paper
Andhra University, School of Chemistry
M.Sc. Chemistry (Previous) Paper I: General Chemistry-II Semester-II
(w.e.f. 2021-2022 admitted batch)
Time: 3 Hours Answer ALL questionsMaximum marks: 80 (5X16 =80 marks)

(1) (a) i) Derive Schrodinger wave equation?
ii) Explain the postulates of Quantum mechanics
Or
(b) i) Write notes on Hermitian operator and its properties
ii) Explain normalization and orthogonalisation

(2) (a) i) Solve the Schrodinger wave equation for a particle in a one-dimensional box.
ii) Write the factors influencing color
Or
(b) i) Derive the Schrodinger wave equation for a simple harmonic oscillator
ii) Describe the concept of tunneling

(3) (a) i) Explain the solutions of R(r), $\theta(\theta)$ and $\Phi(\phi)$ equations of hydrogen atom
ii) Explain probability density in orbitals
Or
(b) i) Explain the time independent perturbation theory to evaluate the ground state energy of helium atom.
ii) Application of above to ground state energy of hydrogen and helium atom

(4) (a) i) What is variation principle. Write its application to calculation of ground state energy of harmonic oscillator.
ii) Compare Perturbation and variation theorems.
Or
(b) i) Explain Hartee-Fock self-consistent field method for multi electron atoms.
ii) Write a note on Density functional theory(DFT)

(5) (a) i) Explain quantum mechanical approach of molecular orbital theory.
ii) Calculate the ionic and covalent bond contributions in hydrogen molecule
Or
(b) i) Discuss the valence bond approach of H_2 molecule.
ii) Write the electronic transitions in the hydrogen molecule.

MODEL QUESTION PAPER

ANDHRA UNIVERSITY SCHOOL OF CHEMISTRY

M.Sc. Chemistry (Previous)Paper- II: Inorganic Chemistry-IISemester-II

(Effective from 2021-2022 admitted batch)

Time: 3 hours **Answer ALL questionsMax. Marks**: 80 **(5x16=80 Marks)**

1. a) (i) Discuss the structure and magnetic property of $Cu_2(RCOO)_4(H_2O)_2$.
(ii) Write a note on Chevrel phases

OR

(b) (i) Discuss the preparation of, structures of and bonding in $Re_2Cl_8^{2-}$.
(ii) Describe the structures of hexanuclear metal clusters.

2. a) (i) Explain the synthesis, structure and reactions of metal carbonyls.
(ii) Explain Isolobal relationship with suitable examples.

OR

b) (i) Describe the preparation of, structure of and bonding in ferrocene.
(ii) What is 18 electron rules? Illustrate with suitable examples

3. a) (i) Explain the factors affecting the stability of coordination compounds.
(ii) Distinguish between stepwise and overall stability constants.

OR

(b) (i) Describe the Irwing -William's series, Pearson's theory of hard and soft acids and bases (HSAB), (ii) What is chelate effect and discuss its thermodynamic origin

4. a) (i) Discuss a spectrophotometric method for the determination of binary formation constant of a metal complex.
(ii) What are inert and labile complexes?

OR

(b) (i) Describe the pH – metric method for the determination of stability constants.
(ii) Explain inert and labile complexes by using crystal field stabilization energies?

5. a) (i) What is acid hydrolysis reactions? Discuss Factors affecting acid hydrolysis reactions
(ii) What is trans effect? Distinguish between the trans effect and trans influence.

OR

b) (i) Give an account of base hydrolysis of Cobalt (III) complexes.
(ii) Discuss the various factors affecting the rates of substitution reactions of octahedral complexes.