**Andhra University**

**M.Sc. Chemistry, Semester- I**

**Paper I: General Chemistry**

**(Syllabus for the academic year 2020-2021 only)**

**Basic Quantum Chemistry:**

**Unit I**

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**

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.

**Molecular Spectroscopy:**

**Unit-III**

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 enharmonic oscillators. Selection rules-overtones-combination bands calculation of force constant, enharmonicity constant and zero point energy, Fermi resonance, siumultaneous vibration rotation spectra of diatomic molecules.

***Note: The following highlighted unit shall be studied under self study cum assignment mode by the students & considered for the mid-II examination.***

|  |
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| **Unit-IV**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. |

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MODEL QUESTION PAPER

M.Sc. Chemistry Degree Examination

Paper-I: **General Chemistry I**

**(For the academic year 2020-2021 only)**

Time: 3 hours Max. Marks: 80

 **ANSWER ALL QUESTIONS**

 **5x16=80 Marks**

1. a) Explain the postulates of quantum mechanics.

 Or

 b) Discuss about the Hermitian operator and its properties.

1. a) Explain the wave mechanics of simple harmonic oscillator.

 Or

 b) Derive the wave equation for a particle in three dimentional box and write its solution.

1. a) Describe the stark effect on microwave spectra.

 Or

 b) Discuss the PQR structure of vibrational and rotational spectra.

1. a) Discuss the selection rules for harmonic and anharmonic oscillator.

 Or

 b) Solve the Schrodinger wave equation for a rigid rotor.

1. **ANSWER ANY FOUR QUESTIONS**

 a) Write the properties of wave function.

 b) Write notes on normalisation and orthogonalisation

 c) Discuss the factors influencing colour in particle in a one dimentional box.

 d) Write notes on symmetry arguments in deriving selection rules

 e) What kind of molecules show microwave spectra.

 f) Write a short note on Fermi resonance and accidental degeneracy.

**Andhra University**

**M.Sc. Chemistry, Semester- I**

**Paper II: Inorganic Chemistry-I**

**(Syllabus for the academic year 2020-2021 only)**

 **UNIT-1**

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 pi bonding.

Application of MO theory to square planar (PtCl42-) and Octahedral complexes (CoF63-, Co(NH3)63+).

Walsh diagram for H2O molecule.

**UNIT-II**

Inorganic cage and ring compounds – preparation, structure and reactions of boranes, carboranes, metallocarboranes, boron–nitrogen (H3B3N3H3), phosphorus–nitrogen (N3P3Cl6) and sulphur-nitrogen (S4N4, (SN)x) cyclic compounds.

Electron counting in boranes – Wades rules (Polyhedral skeletal electron pair theory).

Isopoly and heteropoly acids.

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**UNIT-III**

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 effect, nephelauxetic effect – ligand field theory.

 Term symbols – Russell – Sanders coupling – derivation of term symbols for various configurations. Spectroscopic ground states.

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| --- |
| **UNIT- IV : (SELF-STUDY)** Electronic spectra of transition metal complexes: Selection rules, break down of selection rules – Orgel and Tanabe-Sugano diagrams for d1 –d9 octahedral and tetrahedral transition metal complexes of 3d series – Calculation of Dq, B and β parameters. Charge transfer spectra.  Magnetic properties of transition and inner transition metal complexes – spin and orbital moments – quenching of orbital momentum by crystal fields in complexes. |

**Text books**:

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

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

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

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

**Andhra University**

**M.Sc. Chemistry, Semester- I**

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**MODEL QUESTION PAPER**

**M.Sc. Chemistry Degree Examination**

**Paper-II:** **Inorganic Chemistry – I**

**(For the academic year 2020-2021 only)**

Time: 3 hours Max. Marks: 80

**Answer All Questions**

1. a) Explain the geometries of I3-,  XeF4  and ICl3 molecules with the help of VSEPR theory.

 (Or)

 b) Explain the participation of d orbitals in hybridization.

1. a) Give the preparation and structure of N3P3Cl6.

 (Or)

 b) Discuss the difference between Isopoly and Heteropoly acids.

1. a) What is CFSE ? Calculate CFSE in terms of ‘Dq’ for the complex ions, Cr(H2O)6]2+and
 [Fe(CN)6]3-.

 (Or)

 b) Draw the crystal field splitting of ‘d’ orbitals in tetrahedral and square pyramidal

 geometries.

1. a) Explain Nephelauxetic effect. Give the Nephelauxetic series.

 (Or)

 b) Give an account on S-N cyclic compounds.

1. **ANSWER ANY FOUR QUESTIONS**
2. Discuss the rules and applications of Valence Shell Electron Pair Repulsion Theory.

 (Or)

 b) Explain the properties of tetrahedral and square planar complexes using MO energy
 level diagram.

 c) Explain the structures and of Closo , Nido , Arachano , Hypo boranes.

 (Or)

 d) Give a brief account of Inorganic Benzene with structure and properties.

 e) What are the factors affecting crystal field splitting energy in octahedral complexes (Or)

 f) Explain Jahn-Teller effect with suitable examples. What is dynamic Jahn-Teller effect.