Question Bank [4/6/8/10/12 marks]

Module I

1. Derive time independent Schrodinger wave equation.

2. Derive Schrodinger equation for one dimensional box and obtain the Eigen value by solving the equation.

3. Discuss briefly the plots of radial and angular wave functions for 1s orbital of hydrogen atom.

4. What is Linear Combination of Atomic Orbitals (LCAO)? Give the wave function equations for the formation of molecular orbitals by the combination of atomic orbitals?

5. Discuss in detail the features of MO theory with energy level diagram.

6. Differentiate bonding and anti-bonding molecular orbital.

7. Describe the combination of **s-s** orbitals to give bonding and anti-bonding molecular orbitals.

8. Explain why H_2^+ is less stable than H_2 molecule?

9. O2 molecule is paramagnetic while O_2^{2-} ion is diamagnetic

10. CO is diamagnetic. Justify it with MO concept.

11. Explain Heisenberg uncertainty principle.

12. Draw the shape of Molecular Orbitals obtained by overlap of **s** and **p** orbitals.

13. Describe the overlapping of **p-p** orbitals with orbital diagram.

14. Draw and explain the molecular orbital energy level diagram for **hydrogen molecule (H_2)** and calculate the bond order.

15. Draw and explain the molecular orbital energy level diagram for **hydrogen molecular ion (H_2^+)** molecule and calculate the bond order.

16. Draw and explain the molecular orbital energy level diagram for **oxygen molecule (O_2)** molecule and calculate the bond order.

17. Draw and explain the molecular orbital energy level diagram for **CO molecule** and calculate the bond order.

18. Give the salient features of crystal field theory.

19. Discuss the crystal field splitting in octahedral complex.

20. Discus the crystal field splitting in a tetrahedral complex.

21. Explain Huckel's rule on aromatic, Non-aromatic and Anti-aromatic compounds.

22. Identify from the following aromatic, non-aromatic and anti- aromatic compounds.

    a. Cyclopentadienyl anion b. Cyclopentadienyl cation c. Napthalene d. Pyrrole

23. Explain in detail pi molecular orbitals of Benzene and Butadiene.

Module II

1. What is spectrochemical series? Mention its importance.

2. Draw energy level diagrams to show the splitting of d orbitals in an octahedral and tetrahedral ligand field.

3. Draw the energy level diagrams and indicate the occupancy of the orbitals in the following complexes: a) d^6, octahedral, low spin b) d^6, tetrahedral, high spin. Calculate the CFSE in Δ_0 units assuming the ligands to be strong field ligands.

4. Calculate the CFSE for d^8 ion in octahedral and tetrahedral complexes, using Δ_0 in both cases.

5. Calculate the spin only magnetic moment for a d^8 ion in octahedral and tetrahedral high spin complexes.

6. Explain briefly about high spin and low spin complexes with examples.

7. Calculate the magnetic moment for d^4 ion in octahedral and tetrahedral geometries under the influence of strong ligand fields.

8. Write the oxidation number, d-orbital occupation, co-ordination number and expected magnetic moment of the central metal ion in the following complexes: i. $K_3[Co(C_2O_4)_3]$ ii. $[Mn(H_2O)_6]SO_4$ iii. $Ni(CO)_4$ iii. $[Cu(NH_3)_4]SO_4$

9. Identify the following ions as high spin or low spin complexes and calculate the magnetic moment of the complexes. i. $[CoF_6]^{3-}$ ii. $[NiCl_4]^{2-}$ iii. $[Fe(CN)_6]^{3-}$ iv. $[Co(H_2O)_6]^{3+}$

10. What are the different regions of electromagnetic radiations?

11. Explain the characteristics of Electromagnetic radiation.

12. Write a note on the principle of UV- Vis spectroscopy.

13. What is the condition for a molecule to absorb Microwave radiation? Give examples for microwave active and inactive molecule.

14. What is the significance of selection rule in spectroscopy?

15. Write a note on the significance of Hooke's law.

16. What is the major requirement for infra-red absorption? [or] Explain the criteria for a molecule to absorb in IR region.

17. Explain the principle behind the absorption of radio frequency waves. [Or] What are the criteria for a molecule to absorb NMR radiation? [or] What is the resonance condition in NMR spectroscopy?

18. Define the term chemical shift and mention the characteristics of chemical shift.

19. What do you understand by the term "splitting of signals"? Explain with examples.

20. Explain briefly about spin-spin interaction? Explain its effect in NMR spectrum.

21. What is shielding? Explain the effect of shielding on the magnetic field of the spinning nuclei.

22. What is de-shielding? Explain the effect of shielding on the magnetic field of the spinning nuclei.

23. What is Larmor frequency? Give its significance.

24. Explain in detail the influence of electronic environment on the position of signals taking an example in NMR spectroscopy. [Chemical shift and its characteristics].

25. Discuss splitting of signals in NMR spectrum with an example. [or] Explain the influence of neighboring nuclei on the signal of NMR spectrum taking an example.

26. Discuss in detail about the selection rule for rotational spectrum of a rigid diatomic molecule.

27. Write note on the vibrational spectrum of a diatomic molecule undergoing simple harmonic motion.

28. Explain in detail the selection rule for Carbon monoxide absorbing in IR region.

29. Discuss the selection rule for H atom in electronic spectroscopy.

30. Write notes on the selection rule for many electron atom based on electronic spectroscopy.

Module III

1. Explain the principle of XPS?

2. Define Miller indices with examples.

3. For the intercepts x, y, and, z with values of 3, 1, and 2 respectively, find the Miller indices.

4. Compute the Miller Indices for a plane intersecting at $x = \frac{1}{4}$, $y = 1$, and $x = 1/2$.

5. Give the expression for Bragg's law and explain the terms involved in it.

6. What is inter-plane spacing's in lattices? Give the expression taking an example.

7. Determine the Miller indices (hkl) of the shaded planes below. Show your work on each step of Miller indices to determine the plane.

a.   b.   c.
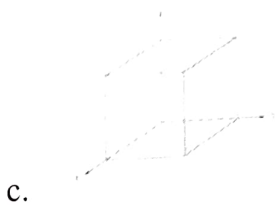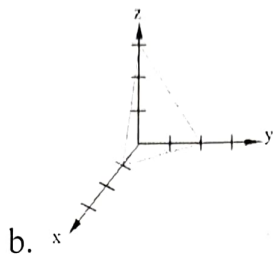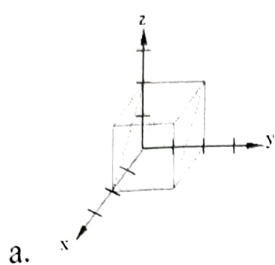
8. State Fajan's Rule. Give examples.

9. First ionization energy of Al is lower than that of Mg. Comment on the statement.

10. How many numbers of geometries are possible in C.N 4? Explain with one example.

11. Write the following equations of state for real gases i. Clausius equation, ii. Berthelot equation.

12. Discuss the principle, instrumentation and applications of XPS.

13. Explain Bragg's law with a neat diagram.

14. Define the terms i. Critical temperature ii. Critical volume iii. Critical pressure.

15. Write notes on dipole-dipole interactions.

16. Explain Vander Waals equation of state with corrections for volume and pressure.

17. Write notes on the factors influencing the Ionization energy and how does it varies along the period and group.

18. What do you understand by the term electronegativity? List out the elements from the following the most electropositive and electronegative element.

Li, Be, B, C, K and Flourine.

19. Why do halogen atoms have a very strong electron affinity? Explain.

20. What is electron affinity? What are the factors influencing it and arrange Br, F, I and Cl in the order of increasing electron affinity.

21. What is screening effect? Calculate shielding constant and Effective nuclear charge for i. 4s electron in Mn ii. 3d electron in Cu.

22. Explain Slater's rule for determining shielding constant. Give the increasing order of effective nuclear charge in Na, Al, Mg and Si atoms based on effective nuclear charge and give reasons.

23. Give reasons for the following

   i. . Ongoing from C to N in the second period, the values of electron affinity decreases instead of increasing.

   ii. Ca^{2+} has a smaller ionic radius than K^+

   iii. Sr has larger atomic size when compared to Mg.

24. What is atomic radii? Give its variation along the period and down the group taking examples. Arrange the following in the increasing order of atomic radii and give reasons: N, S, P and O.

25. What are the factors that influence electronegativity?

26. What is ionic size? Explain with examples how cationic and anionic size varies along the period and group?

27. Give reasons for the following: i. $Mg^{2+} < Mg$, and $Cl^- > Cl$.

28. What is Polarizability and Polarizing power for an ion? Explain the factors that enhance polarizability and polarizing power.

28. Give the oxidation state for the following:

   i. Cr in CrO_4^{2-} ii. S in $S_2O_3^{2-}$ iii. Fe in $FeCl_3$ iv. Mn in $KMnO_4$

Module IV

1. Give the differences between hard and soft acids.

2. Write notes on hard and soft bases with examples for each.

3. Define the terms i. Entropy ii. Enthalpy and iii. Internal energy.

4. What is the relation between enthalpy and Internal energy?

5. What is entropy? Explain its significance.

6. What is the significance of Gibb's free energy?

7. What is the significance of Helmoltz free energy?

8. Comment on the statement, '' the entropy of the Universe is always increasing''.

9. Explain how Nernst equation is applied in determining potential of a redox reaction?

10. How pH for acid-base reaction is determined using cell potential?

11. Explain how Gibb's free energy for water formation is determined?

12. Define corrosion. Explain its types.

13. Explain the free energy for corrosion reaction.

14. How the E.M.F of a reversible cell is determined using Gibb's-Helmoltz equation?

15. Define Solubility product [K_{sp}]. Explain with an example.

16. What is an Electrochemical cell or Galvanic cell? Give its representation.

17. Define Single electrode potential. Write the mathematical expression for Nernst equation for : $Zn_{(s)}/Zn^{2+}(aq)// Cu^{2+}(aq)/Cu_{(s)}$

18. In an electrochemical cell, the anode is given a negative charge and cathode is given a positive charge. Give reasons.

19. With a neat sketch explain Pourbaix diagram for Iron.

20. Define the following with example.

   a) Plane of symmetry

   b) Centre of symmetry

c) Alternating axis of symmetry

21. Write a note on Geometrical isomerism.

22. Mention the specific type of isomerism exhibited by each of the following pairs:

i) Maleic acid and Fumaric acid

ii) n-Butyl alcohol and Diethyl ether

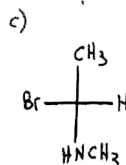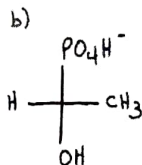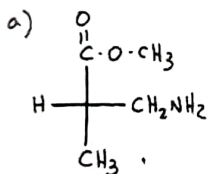iii) Diethyl ether and Methyl propyl ether

23. What is Chirality? Differentiate Chirality and Achirality with example.
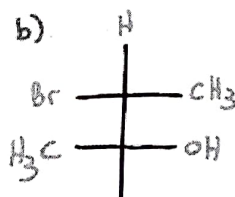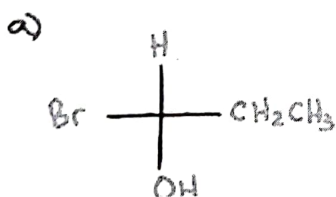
24. Differentiate between Enantiomers and Diastereomers.

25. Explain Sawhorse projection with an example.

26. Draw the Fischer projection of (S)-2-hydroxybutanoic Acid, $CH_3 CH_2 CH(OH)COOH$.

Find R/S for each of the following Fischer Projections

27. Convert the following Fischer projections to Newman Projections

28. Write notes on Structural isomerism with its types and give examples.

29. Explain Newman projection with an example.

30. Write notes on Fischer projection.

31. Discuss the theory behind the electrode potential for an electrochemical cell.

32. Prove $-\Delta A = W_{max}$ and $-\Delta G = W_{useful}$

Module V

1. What are electrophilic reagents? Explain its types.

2. What are nucleophilic reagents? Explain its types.

3. Explain SN_1 mechanism of nucleophilic substitution reactions.

4. Explain SN_2 mechanism of nucleophilic substitution reactions.

5. Give a brief account on electrophilic mechanism of addition reactions.

6. Give a brief account on nucleophilic mechanism of addition reactions.

7. Give a brief account on free radical mechanism of addition reactions.

8. What is the mechanism followed for anti-Markovnikov product? Explain.

9. With an example explain E_1 mechanism of elimination reactions.

10. Explain E_2 mechanism of elimination reactions.

11. What is E_{1cb} mechanism in elimination reactions? What are its criteria?

12. How alkenes are oxidized using $KMnO_4$ reagent?

13. With examples write the oxidation reactions of $K_2Cr_2O_7$ and OsO_4.

14. What is PCC? How is useful for the oxidation of alcohols?

15. What is a reducing agent? Give an example with an equation.

16. What is the reaction of the following with Cyclopropane?

   i. Halogens ii. HI iii. sulphuric acid iv. Hydrogen

17. What is a drug? Give the use of Aspirin and Paracetamol.

18. Explain the role of the following reagents in reduction reactions.

   a) $NaBH_4$

   b) Li/Na in liq.NH_3

   c) Raney Ni

   d) $LiAlH_4$

19. Explain Dieckmann condensation with an example.

20. Explain the mechanism involved in the synthesis of Paraetamol.

21. Explain the mechanism involved in the synthesis of Aspirin.

22. Write a brief account on optical activity in organic compounds with examples. Explain dextro rotatory, laevo rotatory, racemic, and meso as applied to optical isomers.

23. Explain Cahn-Ingold Prelog rules to determine R/S on a chiral center taking an example.

24. Explain in detail the conformational analysis of n-butane with potential energy diagram.

25. How is isomerism exhibited in transition metal compounds? Explain its types with an example.