MODULE 1 : QUANTUM CHEMISTRY

1 . What is the role of doping on the band structures of solids ? YMCA

2. Give the schrodinger wave equation for a particle in one dimensional box. YMCA

3. Draw the pi- molecular orbitals for butdiene. YMCA

4. Give three main postulates of CFT. Expain the splitting of d orbitals under octahedral , tetrahedral and square planar ligand field. YMCA

5. Explain crystal field splitting in octahedral complexes. YMCA

6. Define and explain crystal field theory. YMCA

7. Briefly discuss crystal field splitting in tetrahedral complexes. YMCA

8. What is the significance of Ψ and Ψ^2. YMCA

9. Derive the expression for E and Ψ for a particle in 1 – D box. YMCA

10. Draw and explain molecular orbital diagram of O_2 and compare its bond order and magnetic properties with O_2^+ , O_2^-, O_2^{2-}. YMCA

11. What are intrinsic and extrinsic semiconductors.

12. Write down the MOT electronic configuration and draw molecular orbital energy level diagram for N_2 molecule. YMCA

13. Draw pi- molecular orbitals of 1, 3 – butadiene. Also mention HOMO and LUMO. YMCA

14. Explain the complete LCAO Method.

15. Calculate the $\mu_{effective}$ (magnetic moment) for $\mathbf{Ni^{2+}}$ and $\mathbf{Co^{2+}}$ metal ions.

16. Write Huckel Rules for Aromaticity of compounds

17. Predict whether Tropylium cation , cyclopropenyl cation , cyclopentadiene are aromatic or non- aromatic.

MODULE_2

Intermolecular Forces And Potential Energy Surfaces

1. Discuss the potential energy surface diagram of H_2F and its trajectories . YMCA

2. Give a detailed account for any four intermolecular forces of attraction existing in the molecules. YMCA

3. Derive Vander Waal's equation for the real gases and extend the derivation to critical phenomenon. YMCA

4. Write a short note on PES diagram.Elaborate the saddle point and mountain pass in a potential energy surface diagram. YMCA

5. Write short notes on Vander Waal interaction.

6.Derive expression for the calculation of V_c , P_c and T_c in terms of van der waal's constant. YMCA

7. Explain the deviations of real gases from ideal behaviour. YMCA

8. Explain the Andrew isotherms experiment briefly.

9. What are the limitations of equation PV=RT ?What improvements have suggested by van der waal's? YMCA

10. Derive van der waal's equation of state of n moles of a gas . YMCA

11. How does van der waal's equation explain the behaviour of real gases when : (important)

(a) Pressure is low,

(b) Pressure is high and ,

(c) Temperature is high .

12. Draw the well labelled potential energy surface diagram of $\mathbf{H_3}$ and briefly discuss it . YMCA

13. Discuss stationary points and saddle point briefly. Write some applications of PES. YMCA

MODULE -3-PERIODICITY

1. What do you mean by effective nuclear charge ? Write slater's rule to find out effective nuclear charge. (YMCA)
2. Explain Fajan's rule of polarizability and its significance. (YMCA)
3. Give the geometries possible for coordination number 4. Using VSPER theory predict the shape of a AB_3 molecule having 2 lone pair of electrons on central metal atom A (ANSWER- since the question is saying that AB_3 molecule and 2 lone pair so total it have 2 lone pair and 3 bond pair so electronic geometry becomes 5 which is trigonal bipyramidal. Now in trigonal pyramidal 2 lone pair will be on equatorial position so molecular geometry becomes T-SHAPED) (YMCA)
4. Briefly explain polarization and polarizability. Discuss the factor influencing polarizability and consequences of polarizability. (YMCA)
5. What do you understand by electronegativity ? Explain its variation across its periodic table. How it effect other properties of elements / molecules? (YMCA)
6. Discuss the geometry of ClO_3^- and PCl_5. (YMCA)
7. What do you understand polarizability? How does it differ from polarizing power. Discuss the

Fajans rule for ionic and covalent character of a bond. (YMCA)

8. What is a difference between hard acid and soft acid with example ? (YMCA)
9. What is difference between hard base and soft base with example ? (YMCA)
10. The ionization energy of Al to form Al^+ is less than that of Mg to form Mg^+ ion . Explain.
11. Explain why :

(a) Electron affinities of halogens are very high.

(b) Electron affinities of noble gases are zero.

(C) Successive electron affinities have negative values.

(d) Calculate effective nuclear charge for an electron in 4s orbital of Cr, Co (cobalt) , Ni(nickel) (*important)*

(e) Calculate effective nuclear charge for an electron in 3d orbital of Cr, Co (cobalt) , Ni(nickel) (important)

12. Give reasons for the following :

(a) Electron affinity of fluorine is less than that of chlorine.

(b) The electron affinity of Be and N are almost zero while that of Ne is zero.

(c) Electrons affinities of halogens are the highest.

(d) Ionization potential decreases down the group but tend to increase across a period.

13. What is co-ordination number ? Give two examples of complexes having co-ordination number of 2 and 4. (YMCA)

14. What do you understand by orbital penetration? On what factors it depends? Give the trend of its variation in the orbital of same shell?

15. Apply VSEPR theory to explain the shape of the following molecules : (YMCA)

(a) BeF_2 (b) BF_3 (c) NH_3

(d) PF_5 (e) SO_2 (f) $SnCl_2$

(g) I_3^- (h) SF_4 (i) Br_3^-

(j) XeF_4 (K) H_2S (l) H_2O

16. Explain the geometry of two molecules in which the central atom is surrounded by the four electron pair in the following two cases: (important)

(a) When all electron pairs are bonding pair.

(b) When one electron pair is non bonding.

(c) when two electron pair is non bonding

17. What do you mean by inert pair effect explain briefly . (YMCA)

18. What do you mean by periodicity and what is modern periodic law .

MODULE-4

Thermodynamics

(ALL BELOW ARE YMCA QUESTIONS)

1. Give the main difference between wet and dry corrosion with examples.

2. Give two points how scale and sludge formation can be prevented in boilers.

3. Explain Ellingham diagram listing its uses and limitations.

4. Give the equation which relates cell potential and Gibbs free energy at equilibrium. Write three main applications of Nernst equation with examples.

5. What is a state function?

6. Why is work not a state function?

7. Why is entropy a state function?

8.What is the difference between solubility and solubility product?

9.What is Gibbs Free energy?

10. Define entropy.

11. Define entropy. Write its units and physical significance.

12. What do you mean by free energy and Work function ? What are their needs in thermodynamics.

13. Explain the criterion for feasibility or spontaneity of a process in terms of entropy and Gibbs free Energy.

14. Define spontaneity and free energy . Describe the relationship between Helmoholtz free energy and Gibb's free energy.

15. What is Nernst equation ? Write its applications.

16.Give Arrhenious definition of an acid and a base.

17. What is meant by 'strong' and 'weak' acids and bases?

18. What is Lewis concept of acid and bases?

19. What is Ellingham diagram? How can it be constructed? What are its important characteristics?

20. Write a short note on :

(a) emf.

(b) potential difference.

(c) Arrhenious acids and bases.

21. What are extensive and intensive properties ?

22. Discuss three methods to prevent corrosion. ?

(i,e galvanic , impressed current and passivation)

23. What is electrochemical series discuss its applications .

24. Write difference between emf and potential Difference.

25. Explain how acetic acid acts as acid in aqueous solution according to Bronsted- lowry acid base concept.

NUMERICALS:

1. The cell in which the following reaction occurs:

$2Fe^{3+}(aq) + 2I^{-}(aq) \longrightarrow 2Fe^{2+}(aq) + I_2(s)$

has E^0_{cell} =0.236 V at 298K. Calculate the standard Gibbs energy and the equilibrium constant of the cell reaction . ***(Formula to be used: $\Delta_r G^0 = -nFE^0_{cell}$ and $\Delta_r G^0 = -2.303RT \log k_c$)***

Ans. ***$\Delta_r G$=*** *$-45.55 kJ\ mol^{-1}$ & $K_c = 9.616 * 10^7$*

2. Calculate the emf of the cell in which the following reaction takes place:

$Ni(s) + 2Ag^{+}(0.002M) \longrightarrow Ni^{2+}(0.160M) + 2Ag(s)$

Given that E^0_{cell}=1.05 V ***(Ans. 0.91V)***

3. Write the Nernst equation and the e.m.f. of the following cells at 298K :

(a) $Mg(s)\ I\ Mg^{2+}(0.001M)\ II\ Cu^{2+}(0.0001M)\ I\ Cu(s)$

(b) $Sn(s)\ I\ Sn^{2+}(0.050M)\ II\ H^{+}(0.020M)\ I\ H_2\ (g)\ (1bar)\ I\ Pt(s)$

Given……$E^{o}_{Mg^{2+}/Mg} = -2.37V$ $E^{o}_{Cu^{2+}/Cu} = +0.34V$

$E^{o}_{Sn^{2+}/Sn} = -0.14V$

Ans. *(a)2.68 V*

(b)0.078 V

4.Calculate the standard cell potentials of galvanic cells in which the following reactions take place:

(a) $2Cr(s) + 3Cd^{2+}(aq) \longrightarrow 2Cr^{3+}(aq) + 3\ Cd\ (s)$

(b) $Fe^{2+}(aq) + Ag^{+}(aq) \longrightarrow Fe^{3+}(aq) + Ag\ (s)$

Given $E^{\circ}_{Cr^{3+}/\ Cr} = -0.74$ V, $E^{\circ}_{Cd^{2+}/\ Cd} = -0.40$ V ,

$E^{\circ}_{Ag^{+}/\ Ag} = 0.80$ V , $E^{\circ}_{Fe^{3+}/\ Fe^{2+}} = 0.77$ V

Also calculate $\Delta_r G^{\circ}$ and equilibrium constants of the reactions.

(Formula to be used: $\Delta_r G^0 = -nFE^0_{cell}$

and $\Delta_r G^0 = -2.303RT \log k_c$)

Ans. (a) *E°_{cell} = 0.34 V , $\Delta_r G°$= -196.86 KJ mol^{-1} ,*

K= 3.192 x 10^{24}

(b) $E°_{cell}$= 0.03 V , $\Delta_r G°$= -2.895 KJ mol^{-1} , K= 3.22

MODULE 5 : SPECTROSCOPY

1. What is hypsochromic shift ? - **YMCA**

2. What do you mean by IR active molecule? - **YMCA**

3.Explain the theory of UV- visible spectroscopy using various type of electronic transitions. - **YMCA**

4. Write short note on the following : - **YMCA**

(a) Chemical shift.

(b) Beer-Lambert's law.

(c) Fundamental vibrations and overtones.

(d) Fluorescence.

(e) Fermi Resonance

(g) Franck Codon Priniple.

5. Define nmr spectroscopy. - **YMCA**

6. What is the principle of vibrational spectroscopy? **YMCA**

7. Define the term fluorescence and give its application in medicines. – **YMCA**

8.What do you mean by term " Spectroscopy". Discuss the various selection rules governing spectroscopy. **YMCA**

9. Give the structural formula of C_3H_6O which gives one signal in ^1H NMR . - **YMCA**

10. Give the selection rule for IR spectroscopy. Explain stretching and bending vibrations in AB_2 type nonlinear molecule. - **YMCA**

11. Write short note on shielding and de-shielding of protons in NMR spectroscopy. - **YMCA**

12. Discuss the principle of electronic spectroscopy. Explain with reference to butadiene and carbonyl compounds. - **YMCA**

13. What do you mean by Finger print region in IR spectroscopy and why it is important?

14. Draw the rough graph of UV , NMR and IR spectroscopy.

15. Explain JABLONSKI diagram.

16. Explain stretching and bending vibration for a linear molecule CO_2 in IR spectroscopy.

17.Discuss the factors on which chemical shift depends

18. What do you mean by Larmor frequency .

19. What is transmittance.

20. What do you mean by RED and BLUE shift in UV spectroscopy.

21 What is MRI and write its application. Also distinguish between Diffraction and Scattering.

22. Name 5 different surface characterisation techniques.

MODULE 7 : STEREOCHEMISTRY

1. Discuss taking examples of organic molecules types of structural and streoisomerism

2. Draw the fischer projection formula for (2R)-2-Bromobutane.

3. Draw and discuss energy diagram for different conformational isomers of butane.

4. Discuss stereoisomerism in transitional metal compound with suitable examples.

5. What are optical active compounds ? Discuss the essential conditions for optical isomerism , elaborate with example.

6. Differentiate between enantiomers and diasteromers.

7. Define the following terms :

(a) Anomers.

(b) Chirality.

(c) Chiral axis.

8. Discuss the different types of isomerism possible in transition metal compounds.

Module _7_ organic chemistry

(All below are YMCA questions)

1. Discuss the synthesis of a commonly used analgesic drug molecule taking a suitable example.

2. Nucleophilic substitution and elimination reactions often compete with each other. Justify this statement giving the conditions when substitution is preferred over elimination.

3. Allyl halides rapidly undergo nucleophilic substitution while vinyl halides not. Explain.

4. Give the synthesis of aspirin and its medical uses.

5. Explain elimination reaction with detailed mechanism by taking suitable example along with the rule governing major product formation. Describe how elimination reaction competes with substitution reaction.

6. Give synthesis of an antihistamine and antipyretic drug.

7. Give the product when 2-chloro butane reacts with alcoholic and aqueous KOH .

8. What do you mean by Ambident nucleophiles . Give Examples.

9. Give the product when 2- bromo- propane reacts with AgCN and KCN.

10. Write short notes on Cyclization reactions .

11. Briefly explain : Diels Alder reaction .

12. Write oxidation and reduction reaction of alkene , alkyne , aldehyde and ketone .

13. Why Friedel craft acylation is preferred over friedel craft alkylation .

14 .Though halogens are ortho para activator but why it is weakly deactivating . Explain .

15. Explain difference between SN_1 and SN_2 reactions.

16. Explain difference between E_1 and E_2 reactions.

17. Why benzyl carbocation is more stable . Explain with help of resonance structures .