

Time: 2.5 hrs]

N.B. (i) Attempt all questions

(ii) All questions carry equal marks

(M.Sc. Chemistry)

[Marks: 70

- Q.1. Answer the following questions. 14
(a) Explain the time independent Schrödinger equation of quantum mechanics.
(b) Prove: If \hat{B} is an operator which commutes with an operator \hat{A} (both being Hermitian), Ψ_1 and Ψ_2 are the eigenfunctions of \hat{A} and a_1 and a_2 are the corresponding eigenvalues respectively, then the integral $\int \Psi_1^* \hat{B} \Psi_2 d\tau = 0$.
(c) Prove that eigen values of a Hermitian operator are real.
- OR**
- Q.1. Answer the following questions. 14
(a) Define Unitary, Laplacian and linear operators with examples.
(b) State first and second postulates of quantum mechanics.
(c) Prove that $[L_x, L_y] = i\hbar L_z$.
- Q.2. Answer the following questions. 14
(a) Find out the values of Ψ and E for a particle moving in a one dimensional box.
(b) Derive the Secular determinant for a molecule having n-number of atoms.
(c) Find out the values of wave function Ψ and energy E for rigid rotator of a diatomic molecule.
- OR**
- Q.2. Answer the following questions. 14
(a) Derive the energy for a particle moving in a three dimensional box.
(b) Applying variation principle to ethylene molecule, find out electron and charge densities and π -bond order. Given: $\psi_1 = \frac{1}{\sqrt{2}} P_1 + \frac{1}{\sqrt{2}} P_2$ & $\psi_2 = \frac{1}{\sqrt{2}} P_1 - \frac{1}{\sqrt{2}} P_2$
(c) State variation principle. Prove that $\bar{E} \geq E$.
- Q.3. Answer the following questions. 14
(a) Find out the bond angle for sp hybridization.
(b) Explain molecular orbital theory for H_2 molecule.
(c) Explain ladder operators.
- OR**
- Q.3. Answer the following questions. 14
(a) Find out the bond angle for sp^2 hybridization.
(b) Explain molecular orbital theory for H_2^+ ion.
(c) Explain Self-Consistent Field (SCF) Method.
- Q.4. Answer the following: 14
(a) Give an account on polymerization of alkenes using Zeigler-Natta catalyst.
(b) Give a brief account on:
(i) Oxidative addition reaction (ii) Insertion reaction (iii) Reductive elimination reactions.

OR

- Q.4. Answer the following: 14
- (a) Explain Lowry-Bronsted Theory of acids and bases. Write the conjugate acids of:
 (i) PH_3 (ii) ClO_4^-
- (b) Define commutator operator and its application with examples.
- (c) Prove that $\hat{L}_+ \hat{L}_- = \hat{L}^2 - \hat{L}_z^2 + \hbar \hat{L}_z$.

- Q.5. Answer the following: 14
- (a) What is K_a ? Derive a relation between ionization constant K_a and the concentration C_0 and H_3O^+ of phenol in the aqueous solution.
- (b) Calculate the pH of 0.01 M solution of CH_3COOH . K_a of CH_3COOH at 298 K is 1.8×10^{-5} .
- (c) Calculate the oxidation number of underlined elements:
 (i) $\text{Na}_2[\underline{\text{Fe}}(\text{CN})_5(\text{NO})]$ (ii) $[\underline{\text{Cr}}(\text{CO})_6]$
- (d) Give the IUPAC of the following:
 (i) $\text{Na}_3[\text{Co}(\text{CN})_6]$ (ii) $\text{K}_4[\text{Cr}(\text{CN})_5(\text{NO})]$
- (e) Give the formula of complexes as shown below:
 (i) Sodium hexanitrito cobaltate (II) (ii) Tris (ethylene diamine) manganese (III) chloride

OR

- Q.5. Answer the following: 14
- (a) What is K_b ? Derive a relation between ionization constant K_b , OH^- and the concentration C_0 of ammonia in the aqueous solution.
- (b) The ionization constant of hydrazine in aqueous solution is 1.0×10^{-6} at 25°C . At this temperature what would be pH of a solution containing 0.096 g of hydrazine in 150 ml solution. Molar mass of hydrazine is 32 g/mol.
- (c) Calculate the oxidation number of underlined elements:
 (i) $[\underline{\text{Cr}}(\text{H}_2\text{O})_4 \text{Cl}_2] \text{Br}$ (ii) $\text{Na}_4[\underline{\text{Co}}(\text{NO}_2)_6]$
- (d) Give the IUPAC of the following:
 (i) $[\text{Pt}(\text{NH}_3)_4(\text{SO}_3)]\text{Br}_2$ (ii) $\text{Zn}_2[\text{Fe}(\text{CN})_6]$
- (e) Give the formula of complexes as shown below:
 (i) Dichloro bis (ethylene diamine) chromium (III) nitrate
 (ii) Carbonato tetraammine cobalt (III) chloride.