



Date: 30-10-2018

Dept. No.

Max. : 100 Marks

Time: 01:00-04:00

Part-A

Answer **ALL** questions:

(10 x 2 = 20)

1. Mention the integral volume and limits for cylindrical coordinates.
2. Show that the function Ae^{-5x} is an eigen function of the operator d^2/dx^2 and obtain the eigen value.
3. Normalize the wave function $\psi = A \sin \frac{n\pi}{l}x$.
4. Calculate the microwave frequency for the $\nu_{3 \rightarrow 2}$ transition in $^{12}\text{C}^{16}\text{O}$ molecule with rotational constant, $B = 1.856 \text{ cm}^{-1}$.
5. Write the Hamiltonian operator for a perturbed system in terms of an unperturbed system. Mention the terms involved.
6. Write the acceptable wave function for He atom.
7. Obtain the ground state term symbol for carbon atom.
8. Prove that associative law is obeyed by the symmetry operations of C_{2v} point group.
9. What is the conjugate of the operation S_5^3 ?
10. $[\text{PtCl}_4]^{2-}$ has a centre of inversion while $[\text{CoCl}_4]^{2-}$ does not have – Justify.

PART-B

Answer any **EIGHT** questions:

(8 x 5 = 40)

11. State and explain the postulates of quantum mechanics.
- 12a. State Bohr's Correspondence principle.
 - b. A cricket ball weighing 200 g is to be located within 0.1 \AA . What is the uncertainty in its velocity?
(3+2)
13. Show that the quantum tunneling transmission coefficient $T = \frac{16 E (V_0 - E)}{V_0^2} e^{-\frac{2a\sqrt{2m(V_0 - E)}}{h^2}}$.
14. Write the Schrodinger wave equation for a rigid rotator and normalize the angular function $\phi(\varphi) = N e^{im\varphi}$.
15. Obtain equations for the radial functions $R_{10}(r)$ and $R_{20}(r)$.
16. Show that the operators L^2 and L_x commute and mention its significance.
17. Point out the salient features of the Huckel's approximation in MO theory.
18. Predict the possible electronic configuration for the ground state term symbol $^4S_{3/2}$.

19. Determine the symmetry point group of 1,3,5-trichlorobenzene. Mention its symmetry elements and operations.
20. Generate the reducible representation for water molecule to find its vibrational modes.
21. How will you prove the presence of S_4 -axis of symmetry in allene and SO_4^{2-} ion?
22. Explain the principle involved in arranging the symmetry operations into different classes.

PART-C

Answer any **FOUR** questions:

(4 x 10 = 40)

- 23a. Derive the Rayleigh-Jean's and Wien's law from Planck's law of radiation. (7+3)
 - b. If $\hat{A} = \frac{d^2}{dx^2}$ and $\hat{B} = x$, find out $[\hat{A}\hat{B} - \hat{B}\hat{A}]f(x)$ and $[\hat{A} + \hat{B}](e^x + \sin x)$.
24. Set up the Hamiltonian for simple harmonic oscillator and obtain the solution by using Hermite polynomial. Evaluate the wave function and energy of SHO for the first three vibrational levels.
- 25a. Write the Schrodinger equation for hydrogen like atoms in spherical coordinates and separate the equation into three independent equations with only one variable each. (7+3)
 - b. Draw the radial distribution function for 1s and 2s orbitals and compare.
- 26a. For a particle in an infinitely deep one dimensional potential box of length L, apply the trial wave function $\psi = N x (L^2 - x^2)$ to calculate the energy and obtain the percentage of error.
 - b. Construct the C_{3v} character table using the Great orthogonality theorem. (5+5)
- 27a. Prove that the wave functions of bonding and anti-bonding orbitals of H_2^+ ion are mutually orthogonal under the condition that the overlap integral is negligibly small. (5+5)
 - b. Calculate the total π -electron energy and delocalization energy for 1,3-butadiene.
28. The molecule $[\text{Co}(\text{en})_3]^{3+}$ belongs to D_3 point group. Predict the number of (i) symmetry operations, (ii) classes, (iii) irreducible representations and their dimensions.
