LOYOLA COLLEGE (AUTONOMOUS), CHENNAI – 600 034

M.Sc. DEGREE EXAMINATION – CHEMISTRY

FIRSTSEMESTER – APRIL 2018

17/16PCH1MC03/CH1814/CH 1808 - QUANTUM CHEMISTRY AND GROUP THEORY

Date: 28-04-2018
Time: 09:00-12:00

Dept. No.

Max. : 100 Marks

Part-A

Answer ALL questions. **(10 × 2= 20)**

1. Show that for a particle in a one dimensional box, the wave functions Ψ_1 and Ψ_2 are orthogonal.

2. The fireball in a thermonuclear explosion can reach temperature of 10^7 K. What value of λ_{max} does it correspond to? In what region of the electromagnetic spectrum is this wavelength found?

3. Calculate zero point energy for a particle of mass 1.68×10^{-27} kg executing simple harmonic oscillation. (Force constant = 10 Nm^{-1})

4. State Bohr's correspondence principle.

5. Draw the radial distribution plot for 2s and 3p orbitals and indicate the nodes.

6. State Pauli's exclusion principle as applied to fermions.

7. Write the Hamiltonian for an atom containing two electrons and mention the terms.

8. Mention the significance of the commutation relationship that exists between operators.

9. Predict the symmetry elements present in chloroform molecule.

10. Give any two examples of point groups for which the mutual exclusion principle is applicable.

Part-B

Answer any EIGHT questions. **(8 × 5= 40)**

11. Derive the time-independent Schrodinger wave equation.

12a Show that Balmer series occurs between 3646 Å and 6563 Å.

  b. Find the value of z in Cartesian coordinate using the elliptical coordinate (6, 1/3, 180º) having major axis (R) 12 units. (3+2)

13. Obtain an expression for the ground state energy of a rigid rotor.

14. Explain quantum mechanical tunneling with suitable evidences.

15. Apply variation theorem to the probability of finding the particle in one dimensional box of length 'a' using the trial wave function, $\psi = x(a - x)$.

16. Show that $[L_x, L_y] = i\hbar L_z$.

17. Write down the Slater determinants for the excited state of He atom.

18. How are the energy integrals evaluated for hydrogen molecular ion?

19. Apply Huckel approximation method to calculate the total energy in ethylene molecule.

20. Bring out the differences between vertical and dihedral planes with examples.

21. Obtain the matrix representation for the reflection operation performed in XY-plane.

22. List out the symmetry elements and operation of D_{2d} point group.

Part-C

Answer any FOUR questions.   **(4 × 10= 40)**

23a. Outline the postulates of quantum mechanics.

  b. The threshold wavelength for a metal is 3800 Å. Calculate the maximum kinetic energy   of photo electrons ejected when the light of wavelength 2500 Å strikes.   (6+4)

24a. Calculate the wavelength of the photon emitted when a particle of mass 2.1×10^{-29} kg in one dimensional box of length 3.98 nm goes from n = 2 to n= 3 level.

  b. Derive the wave function and energy for a particle in a rectangular three dimensional box.

(4+6)

25a. Write the Schrodinger equation to be solved for hydrogen atom and solve it for its energy using a simple solution, which assumes the wave function to depend only on the distance r and not on the angles θ and φ.

  b. Prove that $3e^{-8x}$ is an eigen function of second order differentiation. Find its eigen value.

(7+3)

26 Derive expressions for the bonding and anti-bonding molecular orbitals of H_2^+ using variation method.

27a. Obtain the possible roots of secular determinant for 1,3-butadiene molecule. (5)

  b. Arrive at the possible electronic configuration for the ground state term symbol $^3P_2$ (5)

28a. Construct C_{3v} character table using Great orthogonality theorem. (5)

  b. Prove that $\pi \rightarrow \pi^*$ transition in formaldehyde is electronically allowed. C_{2v} character   table is provided for your reference.(5)

C_{2v}	E	C_2 (z)	σ_v(xz)	σ_v(yz)
A_1	+1	+1	+1	+1
A_2	+1	+1	-1	-1
B_1	+1	-1	+1	-1
B_2	+1	-1	-1	+1

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