LOYOLA COLLEGE (AUTONOMOUS), CHENNAI – 600 034

M.Sc. DEGREE EXAMINATION – **CHEMISTRY**

FIRST SEMESTER – **NOVEMBER 2022**

PCH 1503 – QUANTUM CHEMISTRY AND GROUP THEORY

Date: 28-11-2022 Dept. No. Max. : 100 Marks

Time: 01:00 PM - 04:00 PM

Part-A

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

1. A microscope using suitable photons is employed to locate an electron in an atom within a distance of 10 Å. What is the uncertainty in the measure of its velocity?
2. Mention the limits and Laplacian for circular cylindrical coordinates.
3. How many degenerate energy levels lie in $16h^2/8mL^2$ for a particle in a cubic box of length L?
4. Obtain the value of $H_0(q)$.
5. Mention the need for approximation methods.
6. Mention the significance of overlap integral.
7. Write the Hamiltonian for H_2^+ ion.
8. Predict the order for D_{2h} and D_{2d} point groups.
9. Distinguish between vertical and horizontal planes.
10. Obtain the trace of matrix for the operation S_3^1.

Part-B

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

11. (a) Identify the acceptable wave functions among the following and justify:
    (i) $e^{i\varphi}$ (ii) $\tan\theta$.
    (b) Verify d/dx is a linear operator. **(3+2)**
12. State and explain the postulates of quantum mechanics.
13. What is quantum mechanical tunneling? Provide the suitable evidences for tunneling.
14. Calculate the moment of inertia of $^{2}D^{37}Cl$ and $^{1}H^{37}Cl$ which have an equilibrium bond length of 1.275 Å.
15. Obtain Hermite polynomial equation for simple harmonic oscillator.
16. Apply variation theorem and predict the ground state energy of hydrogen atom using the trial wave function, $\psi = e^{-\alpha r}$.
17. Write down the Schrödinger wave equation for hydrogen atom in terms of spherical polar Coordinates and separate them into three independent variables such as R(r), P(θ) and Z(φ).
18. How are the average energy integrals H_{aa} and H_{ab} evaluated?
19. Mention the importance of Huckel's approximations.
20. List the symmetry elements and operations present in BCl_3 molecule.
21. Construct the C_{2v} character table using Great Orthogonality theorem.
22. Obtain the reducible representation relating to the prediction of hybridization scheme in NH_3 molecule.

Part-C

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

23. a. Normalize the following wave function for a particle in a one-dimensional box of length L: $\psi = A\sin(\frac{n\pi x}{L})$.

b. Obtain the mathematical expression for black-body distribution by Planck's distribution law. **(5+5)**

24. a. Derive the expressions for wave function and energy for a particle in 1-D box of length l.

b. Find out the value of $P_0(x)$ and $P_1(x)$. **(6+4)**

25. a. What is a Slater determinant? Write down the determinants for the excited state of He atom.

b. Obtain the Laguerre equation for hydrogen and hydrogen like atoms. **(5+5)**

26. a. Deduce the value of $[L_x^2, L_x]$. Mention its physical significance.

b. What is secular determinant? How is it solved for ethylene molecule? **(5+5)**

27. a. State the variation principle. Using the variation method, determine the energies associated with the trial function $\psi = c_1\psi_{1a} + c_2\psi_{1b}$ in the formation of H_2^+ ion.

b. Calculate the total π-electron energy for 1,3-butadiene. **(6+4)**

28. Identify the symmetries of IR and Raman vibrational modes of trans-2-butene using the C_{2h} character table provided. Verify whether this molecule obeys mutual exclusion principle.

C_{2h}	E	C_2	i	σ_h		
A_g	1	1	1	1	R_z	x^2, y^2, z^2, xy
B_g	1	-1	1	-1	R_x, R_y	xz, yz
A_u	1	1	-1	-1	z	
B_u	1	-1	-1	1	x, y	

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