LOYOLA COLLEGE (AUTONOMOUS), CHENNAI – 600 034

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

FIRST SEMESTER – **APRIL 2016**

CH 1808 - QUANTUM CHEMISTRY & GROUP THEORY

Date: 06-05-2016 Dept. No. Max. : 100 Marks
Time: 01:00-04:00

Part-A

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

1. Which coordinate system is explained by two distances and an angle? Mention its limits.
2. Calculate de Broglie wave length for an electron that has a kinetic energy of 8.01×10^{-18} J.
3. State Bohr's correspondence principle.
4. The infrared spectrum of $^{75}Br^{19}F$ consists of an intense line at a frequency of 1.14×10^{13} s^{-1}. Calculate the force constant of $^{75}Br^{19}F$.
5. Write the Slater determinant for the ground state of helium atom.
6. Draw the radial distribution plot for 3p and 4p orbitals of H-atom and indicate the nodes.
7. Show that the symmetry operations, center of inversion and S_2 bring out the same effect.
8. Predict the number of operations and the number of classes possible for the symmetry element S_4.
9. Mention Born-Oppenheimer approximation with an example.
10. Write down the Hamiltonian for Hydrogen molecule.

Part-B

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

11. In the photoelectric effect, the maximum kinetic energy of electrons emitted from a metal is 1.6×10^{-19} J, when the frequency of radiation is 7.5×10^{14} Hz. Calculate the threshold frequency of the metal and stopping potential of the electrons.
12. Explain the postulates of quantum mechanics.
13. The molecule, $^{12}C^{16}O$ has an equilibrium bond distance of 112.8 pm. Calculate the moment of inertia and the frequency of the photon emitted when the molecule makes rotational transition from $l = 1$ to $l = 0$.
14. What is quantum mechanical tunneling? Explain any two evidences.
15. Write the Schrodinger equation to be solved for H 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.
16. Calculate the average energy for a particle in one dimensional box of length 'a' using perturbation theory if $\psi = \sqrt{\frac{2}{l}}\sin(\frac{\pi x}{l})$ and potential energy, $V = kx$.
17. Show that the operators of any one of the angular momentum component commute with the operator of the square of angular momentum (L^2).
18. Predict the point group and the number of irreducible representations for SO_2 molecule.
19. Obtain the trace of the matrix of the operations i) C_3^2 ii) S_3^5.
20. Outline the construction of the character table for C_{3v} point group.
21. How will you obtain the reducible representation to predict the hybridization of a molecule?
22. Obtain the normalized trial functions for bonding and antibonding orbitals of H_2 molecular ion.

Part-C

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

23a. Derive time-independent Schrodinger wave equation.

b. Show that the wave function describing 1*s* orbital of hydrogen atom is normalized where $\psi_{1s} = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} e^{-\left(\frac{Zr}{a_0}\right)}$ **(7+3)**

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

b. Show that the wave functions corresponding to two different eigenvalues of a Hermitian operator are orthogonal. **(7+3)**

25a. State variation theorem and apply it to the probability of finding the particle in one dimensional box of length '*l*' using the trial wave function, $\psi = x(l-x)$ and compare your result with the true value.

b. Obtain the ground state atomic term symbol for fluorine. **(8+2)**

26a. Identify the symmetry operations of furan and $PFCl_4$ molecules.

b. Find the Huckel molecular orbitals and energies for 1,3-butadiene. **(4+6)**

27a. What is the condition for a molecule to be a member of dihedral group? Give an example.

b. What are coulomb and exchange integrals? How are they obtained? **(4+6)**

28. Highlight the importance of variation method in the determination of energy of MO for Hydrogen molecular ion.

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