M. Sc. DEGREE (C.S.S.) EXAMINATION, NOVEMBER 2021
[2021 Admissions Regular and 2020 Admissions Improvement & Supplementary]
SEMESTER I - CORE COURSE (CHEMISTRY)
CH1C03TM20 - QUANTUM CHEMISTRY AND GROUP THEORY

Time : 3 Hours   Maximum Weight : 30

Part A

I. Answer any Eight questions. Each question carries 1 weight   **(8x1=8)**

1. Determine point group for the following molecules a) PCl5 2) C2H4 3) H2O2

2. Write a note on mathematical group.

3. Write a note on the character of a matrix.

4. Write the standard reduction formula?

5. Explain the significance of zero point energy.

6. Perform the following operation: $\hat{A}(x^2)$, $\hat{A} = d^2/dx^2 + 3d/dx + 4$

7. Sketch the functions Ψ_n and Ψ_n^2 for n = 1, 2, 3 for a particle in a one dimensional box.

8. Explain the significance of Hermite polynomials.

9. Give the quantum mechanical definition of angular momentum.

10. Define space quantization.

Part B

II. Answer any Six questions. Each question carries 2 weight   **(6x2=12)**

11. Explain symmetry elements and symmetry operations.

12. Construct Group multiplication table of C2v.

13. Generate the symmetry adapted linear combination of atomic orbitals for D3h.

14. Generate the character table for C2h.

15. Find out whether $x^2 \frac{d}{dx}$ and $\frac{d^2}{dx^2}$ commute or not.

16. The state of a system is described by the function $\Psi(x,t)$ which is a function of both position and time, but the average value of any physical quantity is independent of time, why?

17. Treating the pi electrons in a conjugated system as particles moving in a one dimensional box, calculate the lowest absorption frequency in cm-1 and the wavelength in nm of absorbed light for the molecule of butadiene. The length of the molecule is 0.56 nm. What is the total ground state energy of the molecule?

18. Discuss the Pauli Exclusion principle.

Part C

III. Answer any Two questions. Each question carries 5 weight   **(2x5=10)**

19. . a) Construct Group multiplication table of C2h.
       b) Show that every symmetry elements in an abelian group forms a separate class by itself.

20. (i) Explain the matrix representation of elements like E,Cn,Sn,i and σ? (ii) State and explain the great orthogonality theorem ?

21. Ladder operators also called raising and lowering operators are defined as

$L_+ = L_x + iL_y \; ; \; L_- = L_x - iL_y$

a) Show that L_+ or L_- commutes with L^2 but not with L_z nor among themselves. b) Show that

$$L^2 = L_+ L_- + L_z^2 - \hbar L_z$$

And

$$L^2 = L_- L_+ + L_z^2 - \hbar L_z$$

22. Illustrate the separation of the variables for hydrogen atom wave functions (r, θ, φ) and arrive at the solutions for the radial and angular parts of the differential equation.