

M.Sc. DEGREE (C.S.S.) EXAMINATION, JANUARY/FEBRUARY 2017**First Semester**

Faculty of Science

Branch : Chemistry

ANI C03/API C03/CHI C03/PHI C03/POHI C03—QUANTUM CHEMISTRY AND GROUP THEORY

(Common to all branches of Chemistry)

[2012 Admission onwards]

Maximum Weight : 30

Time : Three Hours

Section A

Answer any ten questions.
Each question carries 1 weight.

1. Define Orthonormal functions.

2. Given below are certain functions, State which of them are eigen function of $\frac{d^2}{dx^2}$. If so give the eigen values :(a) $A + B \sin ax$; (b) $A \cos ax$; (c) Ae^{ax^2} .

3. Explain the term spherical harmonics.

4. Express Laplacian operator and volume element in spherical polar co-ordinates.

5. Explain Ladder operators.

6. What are nodes ? How many nodes are there in the plot of radial probability function for a $3p$ orbital ?7. Plot the radial portions of the $4s$, $4p$, $4d$ and $4f$ hydrogen like wave functions.

8. What is meant by "abelian group" ? Give one example.

9. For a C_{3v} group, what is the direct product of E with itself ?

10. What is meant by block diagonalisation ? Explain its importance.

11. Write matrices for the following operations (i) C_3^2 ; (ii) S_4^2 .

Turn over

12. Find the inverse of the matrix :

$$\begin{bmatrix} -1 & 2 & 4 \\ 0 & 1 & 1 \\ 5 & 2 & 3 \end{bmatrix}$$

13. State Franck-Condon principle.

(10 × 1 = 10)

Section B

Answer any five questions.

Each question carries 2 weight.

14. Show that the eigen functions corresponding to different eigen values of a Hermitian operators are always orthogonal.
15. Apply Schrödinger wave equation for a particle in one-dimensional box. Find the eigen values and eigen functions.
16. Show that \hat{L}^2 and \hat{L}_x commute.
17. Show that the radial distribution of 2p orbital of hydrogen atom exhibits are maximum at $r = 4a_0$.
18. List the symmetry elements of benzene molecule and assign symmetry group.
19. Obtain the general matrix C_n rotation and arrive at the matrix for L_3 .
20. State Great orthogonality theorem. What are the consequences of the theorem ?
21. Alternate lines of P and R branches (IR spectrum) of acetylene are less intense. Why ?

(5 × 2 = 10)

Section C

Answer any two questions.

Each question carries 5 weight.

22. What are Hermite polynomials ? How are they used in solving the Schrödinger equation for a harmonic oscillator ?
23. Show that the normalised wave function for a particle in a 3-D box with sides of length a , b and c is $\psi(x, y, z) = \left(\frac{8}{abc}\right)^{1/2} \sin\left(n_x \frac{\pi x}{a}\right) \sin\left(n_y \frac{\pi y}{b}\right) \sin\left(n_z \frac{\pi z}{c}\right)$ and discuss the degeneracies of the first few energy levels.
24. What are character tables ? Construct the character table for C_{2v} point group. Discuss the significance of each area of the table.
25. What are the possible electronic transition in a molecule ? Comment on the selection rules in electronic spectroscopy.

(2 × 5 = 10)