

SHRIMATHI DEVKUNVAR NANALAL BHATT VAISHNAV COLLEGE FOR WOMEN  
(AUTONOMOUS)

(Affiliated to the University of Madras and Re-accredited with 'A+' Grade by NAAC)  
Chromepet, Chennai - 600 044.

M.Sc.Chemistry - END SEMESTER EXAMINATIONS - NOV' 2024  
SEMESTER - II

**22PCHCT2006 - Group theory and Quantum Chemistry**

Total Duration : 2 Hrs. 30 Mins.

Total Marks : 60

**Section B**

Answer any **SIX** questions ( $6 \times 5 = 30$  Marks)

1. Explain the various symmetry elements and operations present in molecules.
2. Discuss the Great Orthogonality Theorem and its applications in constructing character tables.
3. Describe the symmetry of vibrational modes in non-linear molecules like  $\text{CH}_4$  and  $\text{SF}_6$ .
4. Explain the concept of hybridization and its symmetry in molecules like  $\text{BF}_3$  and  $\text{NH}_3$ .
5. List out the postulates of quantum chemistry.
6. Compare classical mechanics and quantum mechanics, focusing on black-body radiation and the photoelectric effect.
7. Discuss the empirical Huckel Molecular Orbital Theory for ethylene.
8. Outline the application of perturbation methods to the hydrogen atom.

**Section C**

I - Answer any **TWO** questions ( $2 \times 10 = 20$  Marks)

9. Construct the character table for  $\text{C}_{3v}$  point group.
10. Using the character table, predict the symmetry of vibrational modes for  $\text{SF}_6$  and  $\text{CH}_4$  molecules.
11. Derive and explain the Schrodinger wave equation.
12. Solve the Schrodinger equation for the hydrogen atom and discuss the quantum numbers.

II - Compulsory question ( $1 \times 10 = 10$  Marks)

13. Evaluate the concept of hybridization and its application in  $sp$  and  $sp^2$  hybridization. Use empirical methods to discuss conjugated molecules like butadiene.

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