

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 - APRIL 2025

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 abelian and non-abelian groups.
2. State and explain the Great Orthogonality Theorem.
3. Describe how that hybridization scheme for σ -bonding is determined for CH_4 molecule.
4. Explain the Heisenberg uncertainty principle.
5. Discuss about the Hamiltonian operator.
6. Compare the classical and quantum treatments of the harmonic oscillator.
7. Explain the Schrodinger equation for hydrogen atom.
8. Derive the Huckel molecular orbital equations for ethylene molecule.

Section C

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

9. Construct the character table for the C_{3V} point group.
10. Discuss the application of group theory to electronic spectra of Ethylene and Formaldehyde.
11. Explain the postulates of quantum chemistry.
12. Derive the time-independent Schrödinger equation for a particle in a one-dimensional box.

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

13. Discuss the Hartree-Fock Self-Consistent Field (HF-SCF) method and its role in solving multi-electron wave functions.
