

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. Predict the point group of H_2O , $trans-N_2F_2$, tetrahydrofuran, biphenyl and ethylene.
2. Predict the symmetry of hybridisation of BF_3 .
3. Determine the symmetry of vibrational modes in SF_6 molecule.
4. Describe the postulates of quantum mechanics.
5. Explain commuting and non-commuting operators.
6. The 6^{th} energy level of a particle in a 3D cube box is 6-fold degenerate. What is the energy of the 7^{th} energy level? What is the degeneracy of the 7^{th} energy level ?
7. Explain Hartree-Fock self-consistent field method.
8. Discuss the basic principles of Valence Bond Theory.

Section C

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

9. Construct C_{3v} character table using Great Orthogonality Theorem.
10. Predict the allowed electronic transitions in ethylene and formaldehyde.
11. Derive time-dependent Schrodinger wave equation.
12. Set up and solve the Schrodinger wave equation for rigid rotor.

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

13. Apply variation method to helium atom and derive the value of its energy.
