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 - 2023
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. Discuss the following with proper examples
   a) Proper and improper axis of rotation
   b) Inversion and reflection
2. Derive the standard reduction formula for the number of times representation occurs in a reducible representation.
3. Establish the symmetry species of the normal modes of vibration of CH_4 molecules.
4. Which of the three vibrations of an AB_2 molecules are infrared or raman active when it is a) bent b) linear?
5. What are postulates of Quantum Mechanics?
6. The uncertainty in the position and velocity of a particle are 10^{-10} m and 5.27 $\times$ 10^{-24} m sec^{-1} respectively. Calculate the mass of the particle
7. Draw energy level diagram valid for hydrogen and multi-electron atoms.
8. How many electrons are involved in π and σ bonding orbitals in the following molecules: (a) ethylene, (b) ethane, (c) butadiene, and (d) benzene?

Section C

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

9. Illustrate diagrammatically that H_2O molecule is Abelian and NH_3 molecule is non abelian.
10. Verify that the character given in the C_3v point group obey the properties of the irreps K3.
11. Derive Schrödinger wave equation for the wave mechanical model of an atom and discuss its application to hydrogen atom. What is the significance of ψ and $\psi 2$ in it?

Contd...

12. Using variation method solve the schrodinger wave equation for the ground state energy of helium atom.

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

13. Explain valence bond theory. How would you determine the normalized valence bond eigen functions of H_2 Molecule?

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