

M.Sc. DEGREE (CSS) EXAMINATION, FEBRUARY 2016**First Semester**

Faculty of Science

Branch : Chemistry

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

(2012 Admission onwards)

[Common to all branches of Chemistry]

Time : Three Hours

Maximum : 30 Weightage

Section A*Answer any ten questions.**Each question carries a weight of 1.*

1. Explain the orthogonality and normalisation of wave functions.
2. Explain the terms "eigen function and eigen value".
3. Compare a classical harmonic oscillator with a quantum mechanical oscillator.
4. Define degeneracy. What is the maximum degeneracy possible for a particle in a cube ?
5. Calculate the lowest energy of an electron in a cubic box of side 10^{-8} cm. ($m_e = 9.11 \times 10^{-28}$ g).
6. Ignoring constants write down the angular parts of d_{xz} and $d_{x^2-y^2}$ orbitals.
7. What are Ublerbeck and Goudsmith postulate of spin ?
8. Write group multiplication table for a molecule with E, C_2 , σ and i .
9. What is meant by a cyclic group ? Give an example.
10. Generate matrices for S_3 and i .
11. For a C_{3v} group, what is the direct product of E with itself ?
12. Write the irreducible representation corresponding to rotation about C_2^2 in the case of C_{2v} molecule.
13. Write selection rule for Raman scattering.

(10 × 1 = 10)

Turn over

Section B

*Answer any five questions.
Each question carries a weight of 2.*

14. Evaluate the commutators $[\hat{L}^2, \hat{L}_x]$ and $[\hat{L}_x, \hat{L}_y]$.
15. Apply Schrödinger wave equation for a particle in one-dimensional box. Find the eigen values and eigen function.
16. Define Degeneracy. What is the maximum degeneracy possible for a particle in a cubical box ?
17. Explain Stern-Gerlach experiment.
18. How do you define a point group ? Explain.
19. What is meant by block diagonalisation ? Explain its importance.
20. Derive the reduction formula for reducing a reducible representation into irreducible ones.
21. Comment on vibrational Raman spectra.

(5 × 2 = 10)

Section C

*Answer any two questions.
Each question carries a weight of 5.*

22. Obtain the allowed eigen states and energies of a particle constrained to move within the boundaries of a three-dimensional box.
23. (a) Briefly explain Fortrat diagram.
(b) What are the factors which cause broadening of spectral lines ?
24. Apply orthogonality theorem for C_{3v} point group and derive the character table.
25. Set up Schrödinger wave equation for the hydrogen atom. Transform the co-ordinate and separate the variables.

(2 × 5 = 10)