M.Sc. DEGREE (C.S.S.) EXAMINATION, FEBRUARY 2014

First Semester

Faculty of Science

Branch : Chemistry

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

(Common to all branches of Chemistry)

(2012 Admission onwards)

Time : Three Hours   Maximum Weight : 30

Section A

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

1. What are the conditions for acceptable wave function ?

2. What is "commutator operator" ?

3. Explain the utility of the particle in a box model.

4. What is meant by space quantization ?

5. If r is expressed in atomic unit what will be the first radial function and lowest energy level for H-atom ?

6. Give the postulate of spin by Uhlenbeck.

7. Explain the term abelian group. Give an example.

8. Show whether the following matrices commute

$$\begin{bmatrix} 2 & 0 \\ 1 & 1 \end{bmatrix} \text{ and } \begin{bmatrix} 1 & 2 \\ 0 & 1 \end{bmatrix}.$$

9. Differentiate between reducible and irreducible representations.

10. What are the conditions for molecule to be optically active ?

11. What are the polarised and dipolarised lines in Raman spectra ?

12. List the space groups in the triclinic crystal system.

13. What is statement of GOT ?

$(10 \times 1 = 10)$

Turn over

Section B

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

14. Deduce the time independent Schrodinger wave equation.

15. Evaluate the commutator $[\hat{L}^2, \hat{L}_x]$ and $[\hat{L}_{xy}\ \hat{L}_y]$.

16. Write Schrodinger wave equation for H-atom. Transforms into spherical polar co-ordinates and separate the variables.

17. Explain what are block diagonalisation ?

18. List the symmetry elements of benzene molecule and assign symmetry group.

19. Set up group multiplication table for a $C_3 v$ point group.

20. Sketch the normal modes of vibrations of Co_2 and predict their I.R. and Raman activity.

21. What is Frank-Condon principle ? Explain its importance in understanding electronic spectra of diatomic molecules.

$$(5 \times 2 = 10)$$

Section C

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

22. Derive C_3 character table using great orthogonality theorem.

23. What are the possible electronic transitions in a molecule ? Comment on the selection rules in electronic spectroscopy.

24. Apply the Schrodinger equation for a particle in a one dimensional box.

25. Discuss briefly the postulates of quantum mechanics.

$$(2 \times 5 = 10)$$