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(Pages : 2)

Reg. No.....

Name.....

M.Sc. DEGREE (C.S.S.) EXAMINATION, MARCH 2015

First Semester

Faculty of Science

Branch—Chemistry

AN 1C 03/AP 1C 03/CH 1C 03/PH 1C 03/PO H1 C03—QUANTUM CHEMISTRY AND
GROUP THEORY

(Common to all branches of Chemistry)

[2012 Admissions]

Time : Three Hours

Maximum Weight : 30

Section A

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

1. Commuting operators have common eigen function. Verify.
2. What is a well behaved function ? Explain.
3. For a 2 p electron in Hydrogen like atoms. What is the magnitude of orbital angular momentum. What are the possible values of L_z .
4. In a cubic box the energy of free electron is given by $E = \frac{1.125 h^2}{ml^2}$. Give wave function.
5. Write Recursion formula. Explain its significance.
6. Define spin orbital. Write *one* example.
7. Plot the radial portions of the 4s, 4p, 4d and 4f hydrogen like wave functions.
8. Identify the symmetry elements present in the following molecules and assign point group,
(a) Cyclohexane. (Chair form). (b) PCl_5 .
9. Define subgroup. Write the subgroup of C_{3v} point group.
10. Distinguish between reducible and irreducible representation.
11. Write down the matrix representation for the improper rotation axis of symmetry.
12. Explain block diagonalisation.
13. What are the advantages of Raman compared to IR spectroscopy ?

(10 × 1 = 10)

Section B

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

14. Show that $Y_1^{-1}(\theta, \phi)$ is normalised and that it is orthogonal to $Y_2^1(\theta, \phi)$.

Turn over

15. Show that :

- (a) The associated Legendre polynomial $P_e^{|m|}$ vanishes whenever $|m| > e$.
(b) The $P_e^{|m|}$ reduce to Legendre polynomial P_e when $m = 0$.

16. Write equation for \hat{L}^2 and \hat{L}_z in terms of spherical polar co-ordinates.

17. Explain spin postulates.

18. Prove that a cyclic group is always Abelian.

19. Derive a general expression for the matrix representation of $\sigma \hat{v}$ using the basis (x, y, z) . What is the character of this matrix.

20. State great Orthogonality theorem. What are the consequences of the theorem.

21. Alternate lines of P and R branches (IR spectrum) of acetylene are less intense. Why ?

(5 × 2 = 10)

Section C

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

22. Set up the Schrodinger equation and find eigen values and eigen function for a particle moving in a ring.

23. Derive a general expression for the matrix form of rotation operation in the basis of (x, y, z) .

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

25. Outline the essential postulates of quantum mechanics.

(2 × 5 = 10)