

D 51520

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Name.....

Reg. No.....

FIRST SEMESTER M.Sc. DEGREE EXAMINATION, NOVEMBER 2018

(CUCSS—PG)

Chemistry

CH 1C 01—QUANTUM CHEMISTRY AND GROUP THEORY

(2015 Syllabus Year)

Time : Three Hours

Maximum : 36 Weightage

Part A

Answer all questions.

Each question carries a weightage of 1.

1. What is Born interpretation of ψ ?
2. Normalize the wave function $N \exp(im\phi)$.
3. What do you mean by quantum mechanical tunneling ?
4. Calculate the probability that a particle in one-dimensional box of length ' a ' is found to be between 0 and $a/2$.
5. Give the relationship between the Cartesian and polar co-ordinate systems.
6. Define Legendre polynomial. Generate the first two Legendre polynomials.
7. What are radial and angular parts of wave function ?
8. State and explain the spin postulate by Uhlenbeck and Goudsmith.
9. What are Abelian groups ? Give an example.
10. Two matrices A and B are given. Find out if multiplication between them is commutative :

$$A = \begin{bmatrix} 2 & 3 \\ -1 & 5 \end{bmatrix}; B = \begin{bmatrix} 3 & 4 \\ -5 & 1 \end{bmatrix}.$$

11. What are the differences between reducible and irreducible representations of a point group ?
12. Give the reduction formula and explain the terms involved in the expression.

(12 × 1 = 12 weightage)

Turn over

Part B

Answer any eight questions.

Each question carries a weightage of 2.

13. Calculate the commutator $[L^2, L_x]$.
14. Derive the time independent Schrödinger wave equation from classical wave equation?
15. State and prove uncertainty principle using quantum mechanical operators.
16. What chemically significant systems can particle in a box and harmonic oscillator models are used to represent ? Explain.
17. The infrared absorption spectrum of $^1\text{H}^{35}\text{Cl}$ has its strongest band at 8.65×10^{13} Hz. Calculate the force constant of the bond in this molecule, (b) Find the approximate zero-point vibrational energy of $^1\text{H}^{35}\text{Cl}$.
18. Discuss the spherical harmonics in detail.
19. Systematically determine the point group in benzene molecule. Write all the elements correspond to the point group.
20. Construct the group multiplication table of C_{2v} Point Group.
21. Generate transformation matrices of 1, 3 butadiene with a set of orbitals as basis.
22. Decompose RR's to IRR's of C_{2v} point group using similarity transformation.
23. Plot the radial portions of the 4s, 4p, 4d and 4f hydrogen like wave functions.
24. Show that $Y_1^{-1}(\theta, \phi)$ is normalised and that is orthogonal to $Y_2^1(\theta, \phi)$.

(8 × 2 = 16 weightage)

Part C

Answer any two questions.

Each question carries a weightage of 4.

25. Explain the state function postulate and operator postulate in quantum mechanics.
26. Solve the Schrödinger equation for rigid rotator system.
27. State and explain GOT. Prepare C_{3v} character table using GOT.
28. Prove that 3×3 transformation matrices of C_{2v} Point group obey group axioms.

(2 × 4 = 8 weightage)