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(Pages : 3)

Name.....

Reg. No.....

FIRST SEMESTER M.Sc. DEGREE EXAMINATION, DECEMBER 2019

(CUCSS)

Chemistry

CH 1C 01—QUANTUM CHEMISTRY AND GROUP THEORY

(2015 Admissions)

Time : Three Hours

Maximum : 36 Weightage

Part A

Answer **all** *questions.*
Each question carries a weightage of 1.

1. Calculate the uncertainty in position of an electron moving with a velocity of 2×10^6 ms^{-1}, accurate upto 0.001 %.
2. Define Orthonormal Functions.
3. What do you mean by zero-point energy ? Provide an example for zero-point energy.
4. Sketch the rough graphs of ψ and of ψ^2 for the $n = 4$ and $n = 5$ particle-in-a-box states.
5. Discuss the physical origin of quantisation of energy for a particle confined to move around a ring.
6. What are Hermite polynomials in quantum mechanics ?
7. Define Bohr radius.
8. What are nodes ? How many nodes are there in the plot of radial probability function for a 3*p* orbital ?
9. How do you find the classes of a group ?
10. Explain block diagonalisation.
11. Write a note on Mulliken symbols of character table.
12. Write the transformation matrix obtained from this operation

$$C_2z \begin{bmatrix} x \\ y \\ z \end{bmatrix}.$$

(12 × 1 = 12 weightage)

Turn over

Part B

Answer any **eight** *questions.*
Each question carries a weightage of 2.

13. Elaborate the characters of Hermitian operator by choosing total energy operator in quantum mechanics.

14. What do you mean by a commutator operator ? Commuting operators have common eigen function. Verify.

15. Discuss the physical origin of quantum mechanical tunnelling. Identify two chemical systems where tunnelling might play a role.

16. Set up Schrödinger wave equation for a particle in a three dimensional rectangular box.

17. The $j = 0$ to $j = 1$ transition for carbon monoxide ($^{12}C^{16}O$), occurs at 1.153×10^5 MHz.

    Calculate the value of bond length in carbon monoxide.

18. Explain the exponential decay of wave functions of hydrogen atom wrt. radial distance.

19. Consider the eigen value problem $d^2 \varnothing / d\phi^2 = - m^2 \varnothing$

    Where m is a real number. The two eigen functions of

    $\hat{A} = d^2 / d\phi^2$ are $\varnothing_m (\phi) = e^{im\varnothing}$ and $\varnothing_{-m}(\phi) = e^{-im\varnothing}$. We can easily show that each of these eigen functions has the eigen value $- m^2$. Show that any linear combination of $\varnothing_m (\phi)$ and $\varnothing_{-m}(\phi)$ is also an eigen function of $\hat{A} = d^2 / d\phi^2$.

20. Show explicitly that the first few Hermite polynomials satisfy the recursion formula.

21. Derive the matrix for C_n rotation and S_n rotations considering z-axis as the axis of symmetry. Find the characters of the matrices when $n = 3$.

22. Systematically determine the point group of staggered ferrocene. List the elements of the point group.

23. Decompose the following reducible representations and write it as a combination of irreducible representations

C_{2V}	E	C_2	$\sigma\, xz$	$\sigma\, yz$
Γ (R 1)	12	0	4	0
Γ (R 2)	15	-1	3	3

24. Explain the relation between group theory and quantum mechanics in detail.

(8 × 2 = 16 weightage)

Part C

Answer any **two** *questions.*
Each question carries a weightage of 4.

25. Prove the following relations :

    (a) $\left[\hat{L}_x \hat{L}_y\right] - i\hbar\hat{L}_z$.

    (b) $\left[\hat{L}_y \hat{L}_z\right] - i\hbar\hat{L}_x$.

    (c) $\left[\hat{L}_z \hat{L}_x\right] - i\hbar\hat{L}_y$.

26. Solve the Schrödinger equation for a simple harmonic oscillator to derive expressions for the state functions and energies. Compare the quantum mechanical harmonic oscillator with the classical oscillator.

27. State the Great Orthogonality theorem. Based on the theorem derive the character table for C_{2h} point group. Suggest a molecule belonging to this point group.

28. Explain the improper axis of rotation with suitable examples. Explain the various operations generated by all known S_n axis of rotation where n = odd number and even number.

($2 \times 4 = 8$ weightage)