

D 93215

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Name.....

Reg. No.....

**FIRST SEMESTER M.Sc. DEGREE (SUPPLEMENTARY) EXAMINATION  
NOVEMBER 2020**

(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. What do you mean by stationary state in quantum mechanics ?
2. Choose the acceptable and non acceptable wave functions with the indicated intervals from the list. Justify your answer in each case.
  - a)  $e^{-x} (0, \infty)$ .
  - b)  $e^{-x} (-\infty, \infty)$ .
  - c)  $\sin^{-1} x (-1, 1)$ .
  - d)  $(\sin x) / x (0, \infty)$ .
  - e)  $e^{-|x|} (-\infty, \infty)$ .
3. Zero point energy of a rigid rotator is zero. Is this against the uncertainty principle ?
4. Show that  $\langle p \rangle = 0$  for all states of a one-dimensional box of length 'a'.
5. Write the Schrodinger equation and Hamiltonian for a particle on a sphere in spherical polar coordinates.
6. Write a note on Kronecker Delta related to wavefunctions.
7. Calculate the energy of an electron in the ground state and first excited state of H atom.
8. Define spin orbital. Write one example.
9. Show that  $120^\circ$  rotation and  $240^\circ$  rotation are conjugate elements of  $C_{3v}$  point group ?
10. Define cyclic groups. Give an example.

**Turn over**

11. Any two irreducible representations are orthogonal. Demonstrate using the character table for  $C_{2v}$  point group.
12. What is the relation between  $S_2$  and  $i$ . Illustrate using an example.

(12 × 1 = 12 weightage)

**Part B**

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

13. Show that Schrodinger wave equation is an Eigenvalue equation.
14. Evaluate the commutator  $[\hat{x}, P\hat{x}]$ . What is the physical significance of a commutator ?
15. Explain the postulate of quantum mechanics that consider the average of measurements of an experiment.
16. Show that the radial distribution of 2p orbital of hydrogen atom exhibits are maximum at  $r = 4a_0$ .
17.  $\beta$ -carotene is a linear polyene in which 10 single and 11 double bonds are in conjugation along a chain of 22 carbon atoms. If we take each C-C bond length to be about 140 pm, then the length of the molecular box in  $\beta$ -carotene is 2.94 nm. Estimate the wavelength of light absorbed by this molecule from its ground state to next higher excited state.
18. Using the first Hermite polynomial expressions show that the vibrational transition from  $v = 0$  to  $v = 1$  is allowed and from  $v = 0$  to  $v = 2$  is forbidden.
19. The bond length of  $^{12}C^{14}N$  is 117 pm and its force constant is  $1630 \text{ Nm}^{-1}$ . Predict the rotation vibration spectrum of  $^{12}C^{14}N$ .
20. Elaborate on the significance of various quantum numbers. Explain the electron spin postulate and angular momentum with the help of Stern Gerlach experiment.
21. Construct the group multiplication table of  $C_{3v}$  Point Group.
22. Apply reduction formula to derive a linear combination of irreducible representations from one of the reducible representation of water.
23. What do you mean by a group. What are the fundamental properties of a group. Illustrate the fundamental properties using the multiplication of elements of a point group.
24. What are the transformation matrices of  $C_{2v}$  point group with a set of 3 vectors as basis (Given a vector has 3 components).

(8 × 2 = 16 weightage)

**Part C**

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

25. (a) Show that the variables in the Schrödinger equation for a cubic box may be separated and the overall wave functions expressed as  $X(x)$ .  $Y(y)$ .  $Z(z)$ .

- (b) Deduce the energy levels and wave functions,
- (c) Show that the wavefunctions are orthonormal
- (d) What is the degeneracy of the level with  $E = 14h^2/8ml^2$ .
26. Describe the postulates of quantum mechanics with necessary explanations for each postulates.
27. Explain the principles of Great Orthogonality Theorem and apply the theorem to derive the character table for  $C_{4V}$  point group.
28. Explain the systematic determination of the point group of a molecule. Draw the flow chart for the systematic determination of point groups of molecules. Give the differences between cyclic and dihedral point groups with examples.

(2 × 4 = 8 weightage)