

D 93386

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Name.....

Reg. No.....

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

(CBCSS)

Chemistry

CHE 1C 01—QUANTUM MECHANICS AND COMPUTATIONAL CHEMISTRY

(2019 Admissions)

Time : Three Hours

Maximum : 30 Weightage

Section A

Answer any eight questions.

Each question carries a weightage of 1.

1. Write time dependent Schrödinger wave equation. Mention one application.
2. Which of the following are eigen functions of $\frac{d^2}{dx^2}$? Find the corresponding eigen values :
 - (a) $A \sin kx$.
 - (b) e^{x^2} .
 - (c) $\log x$.
 - (d) e^{-ax} .
3. A particle is confined to one dimensional box of length 'a'. What is the degeneracy associated with the level having energy $\frac{14 h^2}{8 ma^2}$.
4. Write recursion formula for a simple harmonic oscillator. Explain its significance.
5. Represent \hat{L}_z in (a) Cartesian co-ordinates ; (b) Spherical polar co-ordinates.
6. Explain with example 'spin orbital'.
7. State and explain independent particle model.
8. What is STO ? Write one example.
9. Explain the concept of force field in computational chemistry.
10. Write Z-matrix for H₂O.

(8 × 1 = 8 weightage)

Turn over

Section B

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

11. Define Hermitian operator. Show that Hermitian operators always have real eigen values.
12. A particle in one-dimensional box of length a is given by the state function $\sqrt{2/a} \sin(\pi/a)x$. Find the average value of momentum along x direction. Justify your answer.
13. Find eigen functions and eigen values for a planar rotor.
14. Is wave function for H atom is Ne^{-r/a_0} . Show that the maximum probability of finding the electron is at $r = a_0$.
15. State and prove variation theorem.
16. Briefly discuss Hartree Fock self consistent field method of solving many electron atoms.
17. Write a brief account of semi empirical methods of computational Chemistry.
18. Briefly discuss structure of a Gaussian input file.

(6 × 2 = 12 weightage)

Section C

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

19. Briefly discuss postulates of quantum mechanics.
20. Apply Schrödinger equation for one dimensional simple harmonic oscillator. Find eigen functions and eigen values.
21. Apply Schrödinger wave equation for H atom transform into spherical polar co-ordinates. Separate the variables. Solve the $\phi(\text{phi})$ equation.
22. Use perturbation method to find the ground state energy for a particle in one dimensional box with slanted bottom.

(2 × 5 = 10 weightage)