

D 131268

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Name.....

Reg. No.....

**FIRST SEMESTER M.Sc. DEGREE REGULAR/SUPPLEMENTARY
EXAMINATION, NOVEMBER 2025**

(CBCSS)

Chemistry

CHE1C01—QUANTUM MECHANICS AND COMPUTATIONAL CHEMISTRY

(2019 Admission onwards)

Time : Three Hours

Maximum : 30 Weightage

Section A

*Answer any **eight** questions.
Each question carries a weightage of 1.*

1. Explain with example 'Conservative System'.
2. Find the commutator of x and $\frac{d}{dx}$.
3. Explain the term 'Symmetry Breaking'.
4. Write \hat{L}_z in (a) Cartesian coordinates ; (b) Spherical polar coordinates.
5. The 1s wave function for H atom is Ae^{-r/a_0} . Represent the function graphically. Explain
6. Explain with example 'spherical harmonics'.
7. State and explain independent particle model.
8. Write Slater determinantal wave function for L_i atom.
9. Explain the term 'molecular mechanics' in computational Chemistry.
10. Write Z-matrix for methanol.

(8 × 1 = 8 weightage)

Section B

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

11. Show that eigen values of a Hermitian operator are real.
12. Write Rodrigue's formula. Use the formula to find $H_{(X)}$ for $v = 4$ in a simple harmonic oscillator.
13. Is wave function for H atom is Ae^{-r/a_0} . Show that maximum probability of finding the electron is at $r = a_0$.

Turn over

14. Write recursion formula. Discuss its importance.
15. State and prove variation theorem.
16. Briefly discuss the concept of electron correlation.
17. Compare semi empirical and abinitio methods of computational Chemistry.
18. How do you classify basis sets ? Discuss.

(6 × 2 = 12 weightage)

Section C

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

19. Discuss postulates of quantum mechanics.
20. Apply Schrödinger wave equation for H atom. Transform into spherical polar coordinates. Separate the variables and solve the $\Phi(\text{Phi})$ equation.
21. Use variation theorem to find the ground state energy of particle in one dimensional box with slanted bottom.
22. Briefly discuss self Consistent Field Method to solve many electron atoms.

(2 × 5 = 10 weightage)