D1ACH2501 **(2 Pages)** **Name.....**
Reg. No.....

FIRST SEMESTER M.Sc. DEGREE EXAMINATION, NOVEMBER 2025
(Regular/Improvement/Supplementary)

CHEMISTRY
FCHE1C01- QUANTUM MECHANICS AND COMPUTATIONAL CHEMISTRY

Time: 3 Hours **Maximum Weightage: 30**

Section A: Short answer questions. Answer any *eight* questions. Each carries *one* weightage.

1. What are spin-orbitals? Write the possible spin-functions for a two-electron system.
2. Explain the significance of ladder operators in quantum mechanics.
3. Define spherical harmonics. Plot the polar diagrams for P-functions.
4. Find the most probable distance of the electron from the nucleus of H atom in the 1s state.
5. State and prove variation theorem.
6. Construct Slater determinant for the ground state of Helium atom.
7. What are post HF methods in computational chemistry? Give any two examples.
8. Explain the following terms of computational chemistry.
   i) model chemistry; and ii) geometry optimization.
9. Explain the term electron correlation problem in the context of independent-particle model in quantum mechanics.
10. What are polarization basis sets? When do you use them?
11. Explain briefly single point energy calculation?
12. Write short notes on Pople-style basis sets.

(8 × 1 = 8 weightage)

Section B: Short essay questions. Answer any *four* questions. Each carries *three* weightage.

13. What is a postulate? Explain the prominent postulates of quantum mechanics.
14. Write short notes on Hartree-Fock self-consistent field (HF-SCF) methods.
15. Explain the term *force field* in the context of molecular mechanics.
16. Construct z-matrices for: i) ammonia; and ii) formaldehyde.
17. The eigen functions belonging to different eigen values of a Hermitian operator are orthogonal. Substantiate.

(P.T.O.)

18. a) Explain Roothan's concept of basis functions.
    b) Distinguish between Slater-type and Gaussian-type atomic orbitals.
19. What are ab-initio and semi-empirical methods in computational chemistry? Highlight their basic principles and merits.

(4 × 3 = 12 weightage)

Section C: Essay questions. Answer any *two* questions. Each carries *five* weightage.

20. Arrive at the expressions for the wave functions and energy for a one dimensional quantum harmonic oscillator. Compare classical and quantum mechanical harmonic oscillators.
21. Set up and solve Schrödinger wave equation for a rigid rotor.
22. Solve Schrödinger wave equation for Hydrogen-like systems and arrive at the expressions for wave functions and energy.
23. Use variation theorem to estimate the ground state energy of Helium atom. Compare it with the experimental value.

(2 × 5 = 10 weightage)