

FIRST SEMESTER M.Sc. DEGREE EXAMINATION, NOVEMBER 2024
(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 orthonormalized wave functions?
2. Find the commutator of x and d/dx .
3. Given that the energy of a particle of mass ' m ' in a cubic box of length L is $9 h^2/mL^2$. What are the state functions associated with this energy level? What is the degeneracy?
4. What do you mean by square integrable nature of the wave function?
5. Explain the term *Symmetry breaking*.
6. Where do you find maximum electron density for 1s wave function?
7. Give the sketches of the radial distribution function for 1s, 2s and 3s orbitals.
8. Justify the choice of spherical polar coordinates for solving hydrogen like atom.
9. Why separation of variables is not possible with Schrodinger wave equation of He atom?
10. Write down the Slater determinant of Be atom.
11. Differentiate between a spin orbital and atomic orbital.
12. Write down the z-matrix of HCHO.

(8 × 1 = 8 weightage)

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

13. Show that eigenfunctions of a Hermitian operator are mutually orthogonal.
14. Write briefly on space quantization of angular momentum vector.
15. Apply Schrodinger wave equation for planar rigid rotor. Find eigenfunctions and eigenvalues.
16. Write Rodrigues formula to obtain Laguerre polynomials and evaluate $R_{1,0}$.
17. Differentiate STO and GTO with relevant plots.

(P.T.O.)

18. Elaborate on the concept of parameterization in semi-empirical methods.
19. Explain the concept of force field in molecular mechanics.

(4 × 3 = 12 weightage)

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

20. Apply Schrodinger equation for one-dimensional harmonic oscillator. Find the eigen functions and eigenvalues.
21. State and prove variation theorem. Discuss variation treatment of the ground state of Helium atom.
22. Explain the Hatree-Fock self-consistent field method for the treatment of many electron systems.
23. What are Pople style basis sets? Briefly explain their nomenclature. Correlate these basis sets with CPU time for a particular problem.

(2 × 5 = 10 weightage)