D1ACH2301 **(2 Pages)** **Name.....**
Reg.No.....

FIRST SEMESTER M.Sc. DEGREE EXAMINATION, NOVEMBER 2023

(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. Light with a wavelength of 300 nm is incident on a potassium surface for which the work function ϕ is 2.26 eV. Calculate the kinetic energy of the ejected electrons.
2. Explain Born interpretation of wave function.
3. Write the Z-matrix for NH_3 molecule.
4. What do you meant by symmetry breaking?
5. Draw the radial distribution functions for 2s and 2p.
6. Explain Fock operator.
7. What is the de Broglie wavelength of an electron moving at $\frac{1}{137}$ th the speed of light?
8. What is the eigen value of $\psi(x) = Ae^{ikx} + Be^{-ikx}$ for the operator $\frac{d^2}{dx^2}$?
9. Explain Pauli's anti-symmetry principle.
10. What is associate Legendre polynomial?
11. Differentiate Slater type orbitals and Gaussian type orbitals.
12. Explain Hermitian operator with example.

(8 × 1 = 8 weightage)

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

13. Explain the structure of Gaussian input file. Explain any two key words.
14. Employ perturbation method to derive first order correcting to energy for a particle in a one-dimensional box with slanted bottom.

(P.T.O.)

15. Calculate commutator operator for $[x, P_x]$.

16. Write down Schrödinger equation of hydrogen atom in spherical polar coordinate and separate its variable.

17. Describe the postulate of spin by Uhlenbeck and Goudsmith.

18. State operator postulate and apply this to build the Hamiltonian operator.

19. Explain different types of basis sets.

(4 × 3 = 12 weightage)

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

20. Write notes on various computational chemistry methods.

21. Apply variation treatment on the ground state of Helium atom.

22. Explain self consistent field method for atoms.

23. Arrive at energy expression for SHO by solving its Schrödinger equation.

(2 × 5 = 10 weightage)