D1ACH2201 **(2 Pages)** **Name.....**
Reg.No.....

FIRST SEMESTER M.Sc. DEGREE EXAMINATION, NOVEMBER 2022

(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. Find the maximum velocity of photoelectrons ejected by an 80 nm radiation if the work function of photoelectrode is 4.73 eV.
2. What is associate Legendre polynomial?
3. Give one example for Hermitian operator.
4. Write the Z-matrix for H_2O molecule.
5. What is the eigen value of e^{-ax} for the operator $\frac{d^2}{dx^2}$.
6. Explain degree of degeneracy.
7. 'Hydrogen atoms tunnel more readily than heavier atoms'. True or false? Justify your answer.
8. Specify the number of radial and angular nodes present in a 4d orbital.
9. What is the de Broglie wavelength of an electron with a kinetic energy of 100 eV?.
10. Write down quantum mechanical operator for the momentum.
11. What are GTO's?
12. Even at E= 0, rigid rotor does not violate uncertainty principle why?

(8 × 1 = 8 weightage)

(P.T.O.)

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

13. Explain Roothaan's concept of basis functions.
14. Prove that the calculated average energy of a trial function x (a-x) is greater than the true energy for particle in a 1D-box.
15. Explain the postulate of spin by Uhlenbeck and Goudsmith.
16. Write the $\Phi(\phi)$ equation for hydrogenic species and give its general solution.
17. A particle of mass 2.00 $x10^{-26}$ g is in a one-dimensional box of length 4.00 nm. Find the frequency and wavelength of the photon emitted when this particle goes from the n = 3 to the n = 2 level.
18. Explain split valence basis set.
19. Write a brief notes on molecular mechanics method.

(4 × 3 = 12 weightage)

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

20. Explain the method of variation applied to Helium atom.
21. Starting from classical wave equation derive an expression for the time-independent Schrödinger wave equation.
22. Outline the important steps used in the Hartree-Fock self-consistent field approach to electronic structure calculations.
23. Discuss the quantum mechanics of one particle rigid rotator.

(2 × 5= 10 weightage)