

D 13102

(Pages : 2)

Name.....

Reg. No.....

**FIRST SEMESTER M.Sc. DEGREE (REGULAR/SUPPLEMENTARY)
EXAMINATION, NOVEMBER 2021**

(CBCSS)

Chemistry

CHE 1C 01—QUANTUM MECHANICS AND COMPUTATIONAL CHEMISTRY

(2019 Admission onwards)

Time : Three Hours

Maximum : 30 Weightage

General Instructions

1. In cases where choices are provided, students can attend **all** questions in each section.
2. The minimum number of questions to be attended from the Section / Part shall remain the same.
3. The instruction if any, to attend a minimum number of questions from each sub section / sub part / sub division may be ignored.
4. There will be an overall ceiling for each Section / Part that is equivalent to the maximum weightage of the Section / Part.

Section AAnswer **eight** questions.

Each question carries a weightage of 1.

1. Which of the following are well behaved functions. Justify your answer :
(a) $A \sin kx$; (b) $A \sin^{-1}x$; (c) e^{ix} ; and (d) e^{9x^2} .
2. Find the commutator of x and $\frac{d}{dx}$.
3. Explain quantum mechanical tunneling.
4. Write Rodrigue's formula for $H_{(x)}$ (Simple harmonic oscillator).
5. Explain with example spherical harmonics.
6. Is orbital for H atom is given by $\psi = Ne^{-r/a_0}$. Represent graphically. Explain.
7. State and explain variation theorem.

Turn over

8. Write Slater determinantal wave function for Li atom.
9. What are the assumptions of molecular mechanics approach of computational chemistry?
10. Explain the term 'split valence' basis set.

(8 × 1 = 8 weightage)

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

11. Show that eigen functions of a Hermitian operator are mutually orthogonal.
12. Apply Schrödinger wave equation for a particle in one dimensional box. Find eigen functions and eigen values.
13. Show that \hat{L}_x and \hat{L}_y do not commute.
14. One of the solutions of H atom is $N(3 \cos^2 \theta - 1)$. Draw polar plot. Explain.
15. Find the ground state energy of He by perturbation method.
16. What are the modifications suggested by Fock in Hartree's SCF method? Discuss.
17. Compare ab initio and semi empirical methods of computational Chemistry.
18. Write a brief account of classification of basis sets.

(6 × 2 = 12 weightage)

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

19. Apply Schrödinger wave equation for a non-planar rotator. Find eigen functions and eigen values.
20. Use variation theorem to find the ground state energy of particle in one-dimensional box of length ' a '. Use the trial function $\Phi = x(a - x)$.
21. (a) Show that if the operators commute they will have the same set of eigen functions and eigen values. Use the theorem to rationalise Heisenberg uncertainty principle.
(b) State and discuss expectation value postulate of quantum mechanics.
22. Discuss briefly :
(a) Symmetry breaking.
(b) Space quantization.

(2 × 5 = 10 weightage)