Roll No.

Total No. of Pages : 02

Total No. of Questions : 09

B.Sc. Hons. (Chemistry) (Sem.-5) QUANTUM CHEMISTRY Subject Code : BHCL303-19 M.Code : 90739 Date of Examination : 16-12-22

Time : 3 Hrs.

Max. Marks : 60

INSTRUCTIONS TO CANDIDATES :

- 1. SECTION-A is COMPULSORY consisting of EIGHT questions carrying TWO marks each.
- 2. SECTION-B contains EIGHT questions carrying FOUR marks each and students have to attempt any SIX questions.
- 3. SECTION-C will comprise of two compulsory questions with internal choice in both these questions. Each question carries TEN marks.

SECTION-A

1. Answer Briefly :

- a) Give significance of wave function. How one proceeds to find probability, if Ψ does not come out to be real.
- b) Define force constant for a linear harmonic oscillator.
- c) What is a rigid diatomic rotator? What is its energy for 2^{nd} rotational state?
- d) Calculate the energy of an electron present in second shell for Hydrogen like particles.
- e) What do you mean by luminescence?
- f) Define molar extinction co-efficient.
- g) Write Hamiltonian operator for the K₂ molecule.
- h) Discuss the working of a Thermopile.

SECTION-B

2. Discuss the outcomes from the quantum mechanical treatment of a simple harmonic oscillator.

- 3. Does a moving ball of 100g has a de-Broglie wave associated with it. Justify your answer.
- 4. Compare MOT and VBT.
- 5. Derive equation for Beer's law and give its limitations.
- 6. Explain the concept of quantisation of energy with suitable examples.
- 7. What do you mean by probability distribution curves? What is their shortcoming and how is it overcome? Also draw and discuss radial probability distribution curves for 3rd shell electrons.
- 8. A certain substance in a cell of length 1 absorbs 20% of the incident light. What fraction of the light will be absorbed if the cell is doubled in length.
- 9. What are the conditions for an (a) orthonormal and (b) well behaved wave function.

SECTION-C

- 10. (a) What are operators. What is their role in quantum mechanics and express Schrodinger wave equation in terms of different operators. (7)
 - (b) Calculate the energy required for transition from 131 state to 231 state for an electron in a cubical box with edge length of 2 nm. (3)

OR

10.	(a) Discuss the LCAO-MO treatment for Hydrogen molecule.	(6)
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- (b) Draw MOEL diagram LiH and explain its features. (4)
- 11. (a) Define Quantum yield. Discuss how and why quantum yield varies for different chemical reactions. (5)
 - (b) Draw and explain Jablonski diagram. Which phenomenon involves the change in spin multiplicity.
 (5)

OR

11. Set up the Schrodinger wave equation for Hydrogen atom and solve it to get radial and angular wave functions. How it relates to concept of quantum numbers. (10)

NOTE : Disclosure of Identity by writing Mobile No. or Marking of passing request on any paper of Answer Sheet will lead to UMC against the Student.