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(FOR THE CANDIDATES ADMITTED DURING THE ACADEMIC YEAR 2024 ONLY) **SUB CODE 24PCY206** **REG.NO. :**

N.G.M. COLLEGE (AUTONOMOUS): POLLACHI

END-OF-SEMESTER EXAMINATIONS: MAY 2025

B.Sc CHEMISTRY **MAXIMUM MARKS: 75**

SEMESTER II **TIME: 3 HOURS**

PART - III

24PCY206 – QUANTUM CHEMISTRY AND NANO CHEMISTRY

SECTION – A (10 X 1 = 10 MARKS)

ANSWER THE FOLLOWING QUESTIONS. (K1)

1. Which experiment led to the discovery of quantized energy levels?

A) Rutherford's scattering B) Photoelectric effect C) Compton effect D) Double-slit experiment

2. Which quantum number determines the energy of an electron in hydrogen?

A) n B) l C) m D) s

3. In the LCAO method, the bonding molecular orbital is formed by:

A) Addition of atomic orbitals B) Subtraction of atomic orbitals C) Direct multiplication of wave functions D) Overlap of core orbitals

4. What is the main environmental concern of nanomaterials?

A) Air pollution B) Water pollution C) Toxicity to organisms D) None of the above

5. In BET analysis, which gas is commonly used for adsorption?

A) Oxygen B) Nitrogen C) Hydrogen D) Carbon Dioxide

ANSWER THE FOLLOWING IN ONE (OR) TWO SENTENCES (K2)

6. Why does classical physics fail at atomic scales?

7. What is the significance of the wave function in quantum mechanics?

8. How is bond order determined from molecular orbital theory?

9. List two methods of nanomaterial preparation

10. Distinguish between AFM and STM

SECTION – B (5 X 5 = 25 MARKS)

ANSWER EITHER (a) OR (b) IN EACH OF THE FOLLOWING QUESTIONS. (K3)

11. a) Explain the operator formalism in quantum mechanics

(OR)

b) Infer the energy levels for a particle in a 3-D box

12. a) Interpret the energy levels of the hydrogen atom using the Schrödinger equation

(OR)

b) Explain the first-order perturbation theory and its application to the hydrogen atom

13. a) Illustrate the LCAO-MO approach for diatomic molecules with an example

(OR)

b) Discuss the significance of charge distributions from HMO theory

14. a) Elucidate any two methods of nanomaterial preparation

(OR)

b) Compare Bottom-Up and Top-Down approaches for nanomaterial synthesis

15. a) How does scanning electron microscopy (SEM) help in studying nanomaterials?

(OR)

b) Compare Atomic Force Microscopy (AFM) and Scanning Tunneling Microscopy (STM)

SECTION – C (5 X 8 = 40 MARKS)

ANSWER EITHER (a) OR (b) IN EACH OF THE FOLLOWING QUESTIONS (K4 (Or) K5)

16. a) Discuss the postulates of quantum mechanics and their significance

(OR)

b) Conclude the Schrödinger equation for a harmonic oscillator and discuss its solutions

17. a) Examine the separation of variables method for solving the Schrödinger equation for H

(OR)

b) Describe the perturbation method in detail

18. a) Determine the HMO treatment for benzene and determine its delocalization energy

(OR)

b) Construct the Slater determinant for a 2-electron system and its note in quantum mechanics

19. a) Estimate the properties of nanomaterials

(OR)

b) What are carbon nanotubes (CNTs)? Explain their structure and properties

20. a) Discuss the importance of XPS (ESCA) in chemical analysis of nanomaterials

(OR)

b) Explain the instrumentation, and applications of Photoluminescence (PL) spectroscopy

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