KAMARAJ COLLEGE (Autonomous)

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(Affiliated to Manonmaniam Sundaranar University, Tirunelveli)

(4 Pages) **Reg. No:……**

Question Code: 26E02203 **Course Code : 24PMCH42**

PG Degree - End Semester Examinations, April 2026

Fourth Semester

M.Sc., CHEMISTRY

Physical Chemistry - II

(For those who joined in July 2024 onwards)

Time : 3Hours **Maximum : 75 Marks**

PART – A (10 × 1 = 10 Marks)

Answer ALL Questions

Choose the correct answer :

CO:1 K:1 1. The minimum energy required to remove an electron from the surface is called

(a) work function (b) threshold frequency

(c) Gibbs free energy (d) Helmholtz free energy

CO:1 K:2 2. Two wave functions are said to be orthogonal if

(a) their sum is zero

(b) their product is zero everywhere

(c) the integral of their product over all space is zero

(d) they have the same eigen value

CO:2 K:2 3. Which orbital has no angular node?

(a) 2p (b) 3d

(c) 1s (d) 4f

CO:2 K:1 4. Pauli's exclusion principle states that

(a) electrons move in circular orbits

(b) no two electrons in an atom can have the same set of four quantum numbers

(c) energy levels are quantized

(d) wave functions must be normalized

CO:3 K:2 5. Pauli's exclusion principle is not applicable to which of the following particles

(a) Electrons (b) Protons

(c) Photons (d) Neutrons

CO:3 K:1 6. In MO theory, the bonding molecular orbital is formed by

(a) destructive overlap (b) sidewise overlap

(c) constructive overlap (d) no overlap

CO:4 K:2 7. The total number of symmetry operations is equal to the _____ of the point group.

(a) order (b) inversion center

(c) class (d) Sub-class

CO:4 K:2 8. Which symmetry element corresponds to the operation σ?

(a) Axis (b) Point

(c) Plane (d) Line

CO:5 K:1 9. The number of normal vibrational modes in a non-linear molecule with *N* atoms is

(a) 3N − 5 (b) 3N

(c) 3N − 6 (d) 2N − 3

CO:5 K:1 10. A vibrational mode is IR active if it

(a) does not change dipole moment (b) changes the dipole moment of the molecule

(c) has a center of inversion (d) is Raman inactive

PART – B (5 X 5 = 25 Marks)

Answer ALL Questions choosing either (a) or (b).

Answer should not exceed 250 words.

CO:1 K:4 11. (a) Analyze the postulates of quantum mechanics.

(OR)

(b) Verify whether f(x)=e^{ax^2} is an Eigen function of the operator (d/dx).

CO:2 K:3 12. (a) Normalize the wave function $\Psi_n(x)$ for a particle in a one-dimensional box of length L. Show the steps of normalization explicitly.

(OR)

(b) Find the degeneracy of the particle of mass m it is confined in a cubic box of energies $9h^2/8ma^2$.

CO:3 K:4 13. (a) Find the slater determinant of helium and lithium atoms.

(OR)

(b) (ii) Highlight the need for approximation method.

(ii) Write the Hamiltonian of helium atom.

CO:4 K:3 14. (a) Illustrate that the set of operations of water molecule given below form a group. E, C_2, σ xz, σ yz

(OR)

(b) Interpret the properties of irreducible representations.

CO:5 K:4 15. (a) Identify the normal modes of vibration of H_2O and determine which of the vibrational modes are IR-active and Raman-active.

(OR)

(b) Analyze the selection rules of IR and Raman Spectroscopy.

PART – C (5 X 8 = 40 Marks)

Answer ALL Questions choosing either (a) or (b).
Answer should not exceed 600 words.

CO:1 K:5 16. (a) (i) Interpret the effect of temperature on a black body.

(ii) Examine the conditions of an acceptable wave function.

(OR)

(b) (i) Derive an expression for de Broglie wavelength of a particle of mass m and velocity v.
(ii) Distinguish matter waves and electromagnetic waves.

CO:2 K:4 17. (a) Formulate and solve the Schrödinger equation for a particle confined to a one-dimensional infinite potential well (zero potential inside the box) and determine the normalized wave functions.

(OR)

(b) Derive the Schrödinger equation for a rigid rotor. Show that the energy levels are quantized and discuss their degeneracy.

CO:3 K:5 18. (a) Evaluate the wave function of H_2^+ molecule using MO theory.

(OR)

(b) Determine the approximate value of the ground-state energy of Helium atom using VB theory.

CO:4 K:4 19. (a) Construct C_3v character table using Great orthogonality theorem.

(OR)

(b) Represent the five symmetry elements E, Cn, σ, i and Sn in matrix form and calculate the character.

CO:5 K:5 20. (a) Determine the delocalization energy for ethylene using HMO calculations.

(OR)

(b) Evaluate whether the electronic transitions n→ π* and π→π* in formaldehyde is symmetry allowed or forbidden with proper explanation.