B.SC. CHEMISTRY
FIFTH SEMESTER
PHYSICAL CHEMISTRY-V
BSC - 502
[USE OMR FOR OBJECTIVE PART]

SET A

Duration : 3 hrs. Full Marks : 70

(**PART-A: Objective**)

Time : 30 min. Marks : 20

Choose the correct answer from the following: **1×20=20**

1. The ratio of number of nodes in the 2nd and 1st wave functions of the particle in a 1-D box is?
   a. Infinity
   b. 1
   c. 2
   d. 3

2. The potential used in the Schrodinger wave equation of 1-D linear harmonic oscillator (x = Displacement from equilibrium position, K = Force constant)
   a. $\frac{1}{2}Kx$
   b. $\frac{1}{2}Kx^2$
   c. Kx^2
   d. $\frac{1}{2}K/x^2$

3. The total number of radial nodes of the orbitals of the H-atom is
   a. (n-1)
   b. (n-l-1)
   c. (n-l)
   d. 1

4. A particle is moving on a surface of a sphere, then degeneracy in states is given by
   a. (2l+1)
   b. 2l
   c. (2l-1)
   d. (l+2)

5. The degeneracy of the first excited state of a particle in a cubical box is
   a. 1
   b. 2
   c. 3
   d. 6

6. Two function are orthogonal if their inner product is
   a. 0
   b. 1
   c. -1
   d. h/2

7. In proton NMR, how many signals would you expect for a compound with three different types of protons?
   a. 1
   b. 2
   c. 3
   d. 4

8. Which solvent is commonly used in NMR experiments for organic compounds?
   a. Acetonitrile
   b. Deuterated water (D_2O)
   c. Chloroform-d
   d. Dimethyl sulfoxide (DMSO)

9. Which of the following statements is true about ESR spectroscopy?
   a. It primarily uses X-rays for detection.
   b. It is applicable only to paramagnetic substances.
   c. It measures the absorbance of visible
   d. It is ineffective in studying free

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light.   radicals.

10. Which of the following is a common feature shared by both ESR and NMR spectroscopy?
    a. Detection of protons   b. Utilization of radiofrequency pulses
    c. Study of molecular vibrations   d. Measurement of absorbance

11. The Beer-Lambert Law is applicable to which spectroscopic technique?
    a. NMR   b. Mass Spectrometry
    c. Infrared spectroscopy   d. UV-Vis spectroscopy

12. Which of the following is a forbidden transition in electronic spectroscopy?
    a. Singlet to triplet   b. All of them
    c. Singlet to singlet   d. Triplet to triplet

13. What is the term for the phenomenon where a molecule absorbs light and undergoes a transition to a higher energy state?
    a. Absorption   b. Emission
    c. Fluorescence   d. Phosphorescence

14. What is the term for the phenomenon where a molecule emits light upon returning to its ground state from an excited state?
    a. Absorption   b. Emission
    c. Fluorescence   d. Phosphorescence

15. In a photochemical reaction, what is the significance of the singlet and triplet states?
    a. They represent different reactant   b. They indicate the spin states of
       molecules   molecules
    c. They denote different reaction   d. They signify the energy levels of
       pathways   molecules

16. Which of the following is used for Raman spectroscopy?
    a. LASER   b. X-ray
    c. Radiowave   d. None of the above

17 Which of the following phenomenon is primarily associated with Raman spectroscopy?
    a. Scattering   b. Absorption
    c. Diffraction   d. None of the above

18. The frequency of Rayleigh lines in comparison to incident radiation is
    a. Same   b. Greater than the incident radiation
    c. Less than the incident radiation d. Cannot be commented

19. Number of Raman active mode for H_2O molecules is
    a. 2   b. 3
    c. 1   d. 4

20. Which of the following mode of CO_2 is Raman inactive?
    a. Symmetric Stretching   b. Both of the above
    c. Bending   d. None of the above

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Time : 2 hrs. 30 min.   Marks : 50

[Answer question no.1 & any four (4) from the rest]

1. a. Write down the postulates of Quantum mechanics.   5+2+3
    b. Write the Laws of Photochemistry?   =10
    c. What do you mean by Stokes and anti-Stokes lines?

2. A Particle of mass ' m ' is confined in a one dimensional box of   5+3+2
    length ' a '. The potential inside The box in zero but outside it is =10
    'infinity. Calculate The energy and normalized wave function using
    Schrödinger's wave equation. Why for a free particle energy is
    continuous?

3. a. Mention the Schrödinger equation of a linear harmonic oscillator   6+4=10
       and calculate the energy of it. Draw the wave function and
       probability for the ground state of the S.H.O. What is zero point
       energy?

    b. The wave function of a particle in a one dimensional box of
       length a is given by $\Psi_1 = A \sin \frac{\pi x}{a}$ Calculate the value of A.

4. a. Calculate the expectation value $\langle x \rangle$ of the wave function   4+3+3
       $\psi_n = \sqrt{2/7} \sin \frac{\pi x}{7}$.   =10

    b. Explain the quantum theory of Raman Effect.

    c. How Raman scattering is different from Rayleigh scattering?

5. a. The spacing between rotational like of HF is 40 cm⁻¹. The   3+2+3+2
       corresponding spacing between rotational lines of DF is   =10
       approximately at?

    b. Why TMS is used as a reference compound in NMR technique?

    c. Naphthalene and Anthracene radical will show how many lines
       in ESR Spectra?

    d. What is Fluorescence and Phosphorescence?

6. a. Draw and signify all of the vibrational modes for H_2O and CO_2 molecule? Which of those vibrational modes are belonging to parallel and perpendicular vibrations? For H_2O and CO_2 molecule identify which of the parallel and perpendicular vibrations belong to which branch of lines?

   b. For the molecule BH, ω_e =2368 cm^{-1} and the anharmenicity constant is 49 cm^{-1}. Calculate the vibrational terms of the first three vibrational levels and determine the spacing between them.

   c. What will be the splitting pattern and intensity ratio of proton NMR spectrum of ethyl acetate?

5+3+2 =10

7. a. The percentage transmittance of an aqueous solution of disodium fumarate at 250nm at room temperature is 19.2% for a 5×10^{-4} mol L^{-1} solution in a 1 cm cell. The molar absorption coefficient is?

   b. CH_3-$CH_2\bullet$ and $NH_2\bullet$ radical will show how many fine lines in ESR spectra and what is their intensity ratio?

   c. Write the Frank-Condon principle? Write the decrease in energy order for different electronic transitions? Write the selection rule in electronic spectroscopy.

3+4+3 =10

8. a. Raman spectroscopy is complimentary to IR spectroscopy. Why?
   b. Explain role of mutual exclusion principle with an example.
   c. Show all the Raman active modes of H_2O molecule.
   d. Why intensity of anti-Stokes lines is less than Stokes line?

3+3+2+2 =10

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