REV-01
BSC/11/16

2024/11

SET A

B.SC. CHEMISTRY
FIFTH SEMESTER
PHYSICAL CHEMISTRY-III
BSC - 502

[USE OMR FOR OBJECTIVE PART]

Duration: 1:30 hrs. **Full Marks: 35**

(Objective)

Time: 15 mins. **Marks: 10**

Choose the correct answer from the following: ***1×10=10***

1. 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

2. In rotational spectroscopy, which property of a molecule is directly related to the energy levels and transitions observed?
   a. Molecular weight b. Bond length
   c. Molecular shape d. Rotational inertia

3. Which type of vibration involves a change in bond angle within a molecule?
   a. Stretching vibration b. Bending vibration
   c. Torsional vibration d. Rotational vibration

4. Which law describes the relationship between the vibrational frequency of a bond and the reduced mass of the atoms involved?
   a. Hooke's law b. Beer's law
   c. Lambert's law d. Faraday's law

5. Which vibrational mode does a diatomic molecule have?
   a. One stretching mode b. Two stretching modes
   c. One bending mode d. No vibrational modes

6. The linear momentum operator, $\hat{P}_x$ for the x-component is given by

   a. $\frac{h}{2\pi i}\frac{\delta}{\delta x}$ b. $-\frac{h}{2\pi i}\frac{\delta}{\delta x}$

   c. $\frac{h}{2\pi i}\frac{\delta^2}{\delta x^2}$ d. $\frac{ih}{2\pi}\frac{\delta}{\delta x}$

7. Two operators $\hat{A}$ and $\hat{B}$ are said to commute if
   a. $\hat{A}.\hat{B} + \hat{B}.\hat{A} = 0$
   b. $\hat{A}.\hat{B} - \hat{B}.\hat{A} \neq 0$
   c. $[\hat{A}, \hat{B}] \neq 0$
   d. $[\hat{A}, \hat{B}] = 0$

8. The degeneracy of the first excited state of a particle in 2-D square box is
   a. 1
   b. 2
   c. 3
   d. 4

9. The energy of the first excited state of a simple harmonic oscillator in a 1-D box is
   a. $\frac{1}{2}h\upsilon$
   b. $h\upsilon$
   c. $\frac{3}{2}h\upsilon$
   d. $\frac{5}{2}h\upsilon$

10. The operator ∇^2 is called _____ operator
   a. Hamiltonian
   b. Laplacian
   c. Differentiation
   d. Poisson

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Descriptive

Time : 1 hr. 15 mins. **Marks: 25**

[Answer question no.1 & any two (2) from the rest]

1. **a.** Write three postulates of quantum mechanics. **3+2=5**
   b. Explain Beer-Lambert Law.

2. **a.** Draw the P-branch and R-branch of lines in detail for vibrational spectroscopy. **2+3+3+2 =10**
   b. Deduce the expressions for change in energy for: Fundamental vibration, 1st overtone and Hot band.
   c. The rotational spectrum of HI is found to contain a series of lines with a separation of 12.8 cm^{-1}. Calculate the moment of inertia for the molecule.
   d. Calculate the total number of vibrational degrees of freedom for CO_2 molecule? If we substitute one of the O-atom in CO_2 with its isotope, will the molecule become rotational active? Explain.

3. **a.** Draw and signify all of the vibrational modes taking example of a linear and non-linear molecule? Which of those vibrational modes are belonging to parallel and perpendicular vibrations and also identify which of the parallel and perpendicular vibrations belong to which branch of lines. **4+2+2+2 =10**
   b. Calculate the energy for the transition J= 4→5 for rigid rotor and non-rigid rotor?
   c. Calculate the J_{max} for a rigid diatomic molecule for which at 300 K, the rotational constant is **1.566 cm^{-1}**
   d. What is Fluorescence and Phosphorescence?

4. **a.** Find the commutator of the following pair of operators **3+2+3+2 =10**

$$x^3, \frac{d}{dx}$$

b. Prove that $[\hat{A}, \hat{B}\hat{C}] = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}]$

c. Show that position and momentum operator do not commute.

d. Classify the following operators as linear or non-linear.

(i) $\frac{d}{dx}$ (ii) e^x

5. **a.** What is del operator? What is the product of uncertainty in position and velocity for an electron of mass 9.11×10^{-31} kg according to Heisenberg uncertainty principle? **4+3+3 =10**

b. Starting from $\hat{H}\Psi = E\Psi$, derive $\frac{\partial^2\psi}{\partial x^2} + \frac{8\pi^2 m}{h^2}(E - \hat{V}_x)\Psi = 0$ for a particle in 1-D box.

c. What is Born Oppenheimer approximation?

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