REV-01
MSC/01/05

2025/06

SET A

M.Sc. CHEMISTRY
SECOND SEMESTER
QUANTUM CHEMISTRY-II
MSC – 204 [REPEAT]

[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. The Born-Oppenheimer approximation is valid when
   a. Nuclear motion is faster than electronic motion
   b. Mass difference between nuclei and electrons is negligible
   c. Electronic motion is much faster than nuclear motion
   d. Both motions are equal

2. The unperturbed Hamiltonian refers to
   a. The exact system
   b. A complicated potential
   c. A linear approximation
   d. A known solvable system

3. According to the variation principle, the calculated energy is
   a. Always less than true ground state energy
   b. Always greater than or equal to the true ground state energy
   c. Equal to the experimental value
   d. Unpredictable

4. The β parameter in Hückel theory represents
   a. Overlap between non-bonding orbitals
   b. Kinetic energy
   c. Resonance or exchange integral
   d. Bond dissociation energy

5. A better trial wavefunction in the variation method gives
   a. Higher energy
   b. Lower energy closer to the exact value
   c. Same energy as a bad one
   d. Complex energy values

6. The radial part of the hydrogen atom wave function depends on which quantum numbers?
   a. Only n
   b. Both n and l
   c. Only l
   d. Both l and m

7. What is the correct expression for the number of angular nodes in a hydrogen orbital?
   a. $n + l$
   b. $n - l - 1$
   c. $n - 1$
   d. l

8. The 2s orbital of hydrogen has how many radial nodes?
   a. 0
   b. 1
   c. 2
   d. 3

9. The main difference between 2s and 2p radial functions is:
   a. 2s has a radial node, 2p does not
   b. 2p is more compact
   c. 2s is always zero at the nucleus
   d. 2s is an angular function

10. If $\Phi_m(\emptyset) = \frac{1}{\sqrt{2\pi}} e^{-2i\emptyset}$, then value of m is
   a. 1
   b. -1
   c. 2
   d. -2

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(Descriptive)

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

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

1. **a.** The quantum state of a particle moving in a circular path in a plane is given by $\Psi_{(m)}(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi}$, $m = 0, \pm1, \pm2, \pm3, \ldots\ldots$ When a perturbation $H_1 = p \cos\phi$ is applied (p is constant), what will be the 1st order correction to the energy of the m^{th} state. **3+2=5**

   b. How can you convert spherical coordinates (r, θ, ∅) to Cartesian coordinates (x, y,z)?

2. **a.** Using Variation theorem, find the energy for a particle in a 1-D box having the wave function $\Psi = \sin(\frac{n\Pi x}{l})$ and find if the wavefunction is acceptable or not? **3+5+2 =10**

   b. Calculate (i) Excitation energy (ii) Total energy (iii) Π-bond formation energy (iv) Delocalization energy of Cyclobutadiene using Huckel Molecular Orbital theory?

   c. Write the postulates of Huckel Molecular Orbital theory.

3. **a.** The unperturbed energy levels of a system are $E_0=0$, $E_1=2$, $E_2=4$. Find the 2nd order correction to energy for 1stexcited state in presence of perturbation V for which $V_{10}=2$, $V_{20}=4$, $V_{12}=6$. **4+3+3 =10**

   b. If a 1-D box ($0 < x < l$) is perturbed by λx, then calculate the 1st order correction to energy.

   c. The wave function $\psi=x^2$ is acceptable or not for a free particle in 1-D box? Find the % error if not acceptable.

4. **a.** Draw the radial wave function plot for 4s and 4d orbitals. **3+5+2 =10**

   b. Derive the most probable and average distance of the electron from the nucleus in H-atom.

   c. Show the spherical coordinates (r, θ, ∅) in a figure.

5. **a.** Give the n, l values and assign the orbital if $R_{nl}(r) = \frac{1}{2\sqrt{6}}\left(\frac{Z}{a_0}\right)^{5/2} re^{-Zr/2a_0}$. **2+2+2+2 +2=10**

b. What is the general form of the hydrogen atom wave function $\Psi(r, \theta, \varphi)$?

c. What are the quantum numbers associated with the radial and angular parts?

d. What is the mathematical form of the angular part of the wave function?

e. If $R = (1 - r)\, e^{-\frac{r}{2a_0}}$, what will be the value of n, l?

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