REV-01
MSC/66/33/38

2023/06

SET B

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

[USE OMR FOR OBJECTIVE PART]

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

Objective

Time: 15mins. | Marks: 10

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

1. The Born-Oppenheimer approximation separates the motion of
   a. Electrons and nuclei
   b. Electrons and photons
   c. Electrons and protons
   d. Electrons and neutrons

2. Hückel MO theory is most suitable for
   a. Highly symmetric molecules
   b. Molecules with strong electron-electron interactions
   c. Non-planar molecules
   d. Molecules with a large number of atoms

3. Perturbation theory is a mathematical method used to
   a. Determine the structure of molecules
   b. Calculate accurate wave functions and energies
   c. Study the properties of condensed matter
   d. Analyze reaction mechanisms

4. Perturbation theory is often employed when
   a. Analyzing large molecules
   b. Dealing with weak interactions
   c. Solving the Schrödinger equation exactly is not feasible
   d. Considering only strong electron-electron repulsions

5. Non- zero value of radial wave function of hydrogen atom is found at the nucleus for
   a. l = 0
   b. l = 1
   c. l = 2
   d. l = 3

6. Which of the following relation is true for the average kinetic energy (<T>) and average potential energy (<V>) of the electron in the ground state of hydrogen atom
   a. <T> = <V>
   b. 2<T> = - <V>
   c. <T> = - <V>
   d. <T> = -2<V>

7. The degeneracy of a particle moving on a spherical surface is given by
   a. 2l
   b. 2l -1
   c. 2l + 1
   d. l + 2

8. The total number of nodes in 5f orbital of hydrogen atom is
   a. 1 b. 4
   c. 2 d. 3

9. The variational principle in quantum chemistry states that the calculated energy of a trial wavefunction is always
   a. Higher than the exact energy b. Equal to the exact energy
   c. Lower than the exact energy d. Independent of the exact energy

10. The spherical harmonic which is independent of the angle θ and Φ correspond to the value of 'l' and 'm' respectively
   a. 1 and 0 b. 1 and -1
   c. 0 and 0 d. 2 and 0

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(Descriptive)

Time : 1 hr. 15mins. Marks: 25

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

1. a. Define radial probability density and give the expression of it. State the difference between orbit and orbital of the electron in Hydrogen atom. **3+2=5**

   b. What is perturbation theory and when we need apply this theory?

2. a. Define effective potential of the electron in Hydrogen atom and give the expression of it. Discuss how the effective potential of the electron changes with distance from the nucleus for $l = 0$ and $l \neq 0$ **5+5=10**

   b. Write the Schrodinger equation for Hydrogen atom in spherical polar coordinate and give wave function in terms of spherical harmonics. Calculate the normalized $\Phi(\phi)$ function in terms of magnetic quantum number.

3. a. Write the Schrodinger wave equation of a rigid rotator to give the solution of the wave function. Find the expression of energy and calculate the separation of the successive energy levels of the rigid rotator. **5+5=10**

   b. The normalized wave function in the ground state of Hydrogen atom is $\Psi_{1s} = (\Pi a_0^3)^{-1/2} e^{-r/a_0}$. Calculate the most probable distance of the electron from the proton.

4. a. If a 1-D box ($0 < x < l$) is perturbed by λx, then calculate the 1st order correction to energy. What happens if the 1st order correction comes out to be zero? **4+4+2 =10**

b. The unperturbed energy levels of a system are $E_0=0$, $E_1=2$, $E_2=4$. The 2nd order correction to energy for the ground sate in presence of perturbation V for which $V_{10}=2$, $V_{20}=4$, $V_{12}=6$ has found to be?

c. When we need to apply 2nd order correction? The statement "*2nd order correction is always negative*" is true or false.

5. a. 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+6=10**

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

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