

M.SC. CHEMISTRY
SECOND SEMESTER
QUANTUM CHEMISTRY-II
MSC – 204 [REPEAT]
[USE OMR FOR OBJECTIVE PART]

**SET
A**

Duration: 1:30 hrs.

Full Marks: 35

Time: 15mins.

(Objective)

Marks: 10

Choose the correct answer from the following:

1×10=10

- Number of radial nodes in 3d orbital is -
 - 4
 - 0
 - 2
 - None of the above
- The value of $[x, x]$ is (where x =position operator)
 - 0
 - 6
 - 5
 - None of the above
- For 1s orbital, the radial distribution plot is -
 - Decayed
 - Ex
 - Depends upon molecule
 - None of the above
- Slater Determinant involves orbital part along with -
 - Spin part
 - Momentum part
 - Energy part
 - None of the above
- Hamiltonian operator is also known as -
 - Total energy operator
 - Kinetic energy operator
 - Potential energy operator
 - Position operator
- What does the Born-Oppenheimer approximation primarily aim to simplify?
 - Electron-electron interactions
 - Electron-nucleus interactions
 - Nuclear-nuclear interactions
 - Electron-spin interactions
- What does the perturbation theorem provide a systematic method for?
 - Finding exact solutions to the Schrödinger equation
 - Solving systems with time-dependent Hamiltonians
 - Calculating corrections to energy levels of a known system
 - Describing the behavior of particles in strong magnetic fields
- According to Huckel theory, what type of orbitals participates in the molecular orbital formation?
 - Atomic orbitals from all atoms in the molecule
 - Only s orbitals from all atoms in the molecule
 - Only p orbitals from all atoms in the molecule
 - Only d orbitals from all atoms in the molecule

9. Which theorem provides a framework for obtaining approximate solutions to the Schrödinger equation by optimizing a trial wavefunction?
- a. Heisenberg Uncertainty Principle
 - b. Variation theorem
 - c. Perturbation theorem
 - d. Pauli's exclusion principle
10. In the context of quantum mechanics, what does the term "anti-symmetry" refer to?
- a. The symmetry of wavefunctions under rotation
 - b. The symmetric behavior of particles in a magnetic field
 - c. The exchange behavior of identical particles
 - d. The behavior of particles under the action of a potential energy field

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(Descriptive)

Time : 1 hr. 15 mins.

Marks : 25

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

1. a. Show that position and momentum doesn't commute on the same Axis. 3+2=5
b. Explain the perturbation theorem and its role in quantum mechanics

2. a. How linear momentum is related with kinetic energy? Show mathematically. 2+2+2+4
=10
b. Find out the angular momentum operator in y-axis using the cross product operation.
c. Draw the radial distribution curve for 3p and 3d orbitals.
d. The unperturbed energy levels of a system are $E_0=0$, $E_1=2$, $E_2=4$. The 2nd order correction to energy for 2nd excited state in presence of perturbation V for which $V_{10}=2$, $V_{20}=4$, $V_{12}=6$ has found to be?

3. a. Find out the value of 'n' and 'l' from the given expression $R=(1-r)e^{-r/3a_0}$ 2+3+5
=10
b. Draw the angular node for 2p and 3d orbital. What is the number of radial node for 4f orbital?
c. Calculate (i) Excitation energy (ii) Total energy (iii) Π -bond formation energy (iv) Delocalization energy of Cyclobutadiene using Huckel Molecular Orbital theory?

4. a. If the right half of the 1-D box is perturbed by a potential 'V'; Calculate the 1st order correction in ground state energy. 3+2+2+2
+1=10
b. Write the volume element for H-atom considering both radial and angular part.

- c. What is the average value of radius vector for 2s orbital for H-atom?
 - d. Define a many-electron wave function and explain its components.
 - e. Explain what Born-Oppenheimer approximation is.
- 5.
- a. Using Variation theorem, find the energy for a particle in a 1-D box having the wave function $\Psi = \sin\left(\frac{n\pi x}{l}\right)$ and find if the wavefunction is acceptable or not?
 - b. What is Laplacian operator? How this operator is involved in total energy operator?
 - c. Find the commutation value for $[x, \sin(p_x)]$

5+3+2
=10

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