Roll No. | | | | | | | | | | | | | **Total No. of Pages : 02**

Total No. of Questions : 09

M.Sc.(Chemistry) (2015 to 2017) (Sem.–2)

QUANTUM CHEMISTRY

Subject Code : MSCH-204

Paper ID : [A2803]

Time : 3 Hrs. **Max. Marks : 100**

INSTRUCTION TO CANDIDATES :

1. **Atttempt FIVE questions in all selecting ONE question from each section. All questions carry equal marks.**

SECTION-A

1. a) State and explain postulates of quantum mechanics. (8)

   b) What are Hermitian operators? Show that the operator $\hat{p}_x$ for the linear momentum is Hermitian. (12)

2. a) Solve the differential equation, $\frac{d^2\psi}{dx^2} + 4\frac{\pi^2}{\lambda^2}\psi = 0$, for a stationary wave in a clamped string. (10)

   b) Explain the following :

      i) Addition of matrices.

      ii) Hamilton equation of motion.

      iii) Uncertainty principle. (10)

SECTION-B

3. a) Set up Schrodinger equation for the hydrogen atom in polar form and solve it for the radial part. (12)

   b) Derive different term symbols for p^2 configuration. (8)

4. Explain the following :

   a) Angular momentum. (5)

   b) Spin-Orbit coupling. (5)

   c) Expectation values. (5)

   d) Virial theorem. (5)

SECTION-C

5. a) Discuss the time independent perturbation method for the calculation of energy and wave function of a perturbed system having non-degenerate states. (12)

   b) Calculate the energy and normalized wave function for the ground state of hydrogen atom by applying variation method. (8)

6. a) Give a brief account of LCAO-MO approximation. (8)

   b) Explain the following :

      i) Configuration interaction.

      ii) Hartee-Fock equations.

      iii) Gaussian orbital. (12)

SECTION-D

7. a) Give a comparison between valence bond and molecular orbital approaches of chemical bonding. (10)

   b) Write a short note on the electronic states of polyatomic molecules. (10)

8. a) Explain π electron approximation in conjugated systems. (5)

   b) Set up the secular determinant for benzene molecule. Solve it for the energy and wave functions of different molecular orbitals. (15)

SECTION-E

9. Answer briefly : (10 × 2)

a) Explain gradient and curl in vectors.

b) Evaluate the commutator; [x, d/dx].

c) Sketch the first four wave functions of linear harmonic oscillator.

d) Explain why the s orbital is spherical in shape.

e) Determine the effective nuclear charge for the 2s electron in carbon atom.

f) A hydrogen torm is subjected to an electric field of strength F in the z direction. Calculate the first order correction to the energy for the ground state of the atom.

g) What is the basic difference between variation and perturbation methods?

h) Write the ground state anti-symmetric wave function for the helium atom in the determinant form.

i) What are the molecular orbital wave functions of H_2 and N_2 molecules?

j) What is the physical significance of the HMO coefficients?