

**M. SC. (CHEMISTRY)/
M. SC. (ANALYTICAL CHEMISTRY)
(MSCCHEM/MSCANCHEM)**

Term-End Examination

December, 2025

**MCH-018 : QUANTUM CHEMISTRY AND
GROUP THEORY**

Time : 2 Hours

Maximum Marks : 50

Note : (i) *Attempt any **five** questions.*

(ii) *All questions carry equal marks.*

(iii) *You may use the following, wherever required :*

$$h = 6.626 \times 10^{-34} \text{ Js}$$

$$m_e = 9.11 \times 10^{-31} \text{ kg}$$

$$c = 3.0 \times 10^8 \text{ ms}^{-1}$$

$$R_H = 109,667.58 \text{ cm}^{-1}$$

1. Answer any *five* parts : 5×2=10

- (a) de Broglie formulated an important consequence of quantum mechanical nature of matter. State his idea and give its significance.
- (b) What is meant by orthonormal set of wave functions ?
- (c) Give the energy expression for a particle confined in a one-dimensional box and name the terms involved in it.
- (d) What is the main difference between the spin and orbital angular momentum ?
- (e) Why do we need to use approximation methods to solve the SWE for Helium atom ?

- (f) List the basic requirements for linear combination of atomic orbitals to generate molecular orbitals.
- (g) Give the difference between symmetry element and symmetry operation.

2. (a) (i) What are Hermitian operators ?

Show that $i\frac{d}{dx}$ is a Hermitian operator. 2

(ii) What are linear operators ? If $\hat{A}$, $\hat{B}$ and $\hat{C}$ are three linear operators, prove that $[\hat{A}, \hat{B}]\hat{C} = \hat{A}[\hat{B}, \hat{C}]$. 3

(b) (i) Calculate the energies of the ground state and the first excited state for a particle of mass $= 1.67 \times 10^{-27}$ kg confined to a one-dimensional box with $L = 10$ nm. 3

(ii) Differentiate between probability density and probability. 2

3. (a) (i) What is accidental degeneracy ?
Give an example. 2

(ii) A particle in a three-dimensional cubic box of length $= 2.0 \times 10^{-11}$ m has an energy of 6.0×10^{-20} J in (2, 2, 2) state. Calculate the zero-point energy of the particle. 3

(b) (i) Why are the vibrational energy levels non-degenerate ? 2

(ii) Use the following recursion relation to calculate the expression for $H_2(x)$: 3

$$H_{n+1}(x) = 2x H_n(x) - 2n H_{n-1}(x)$$

Given that $H_0(x) = 1$ and

$$H_1(x) = 2x .$$

4. (a) Determine the wave number of light emitted when an electron in hydrogen atom makes a transition from the $n = 2$ level to ground state. 2
- (b) Derive an expression for the moment of inertia for a diatomic molecule with nuclei of masses m_1 and m_2 at distances r_1 and r_2 , respectively from the center of mass. You may take the internuclear distance as R . 4
- (c) What is group ? Discuss the characteristics of groups in brief. 4
5. (a) The normalized radial wave function for the ground state of hydrogen atom is :

$$2\left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0}.$$

Calculate the average value of the distance of the electron in 1s orbital of hydrogen atom. 5

(b) (i) What is meant by hydrogen like ions ? Explain with an example. 2

(ii) Formulate the Schrödinger wave equation for a Helium atom. Explain the difficulty in solving the equation. 3

6. (a) State and prove variational theorem. How is it used to estimate the ground state energy of a system ? 5

(b) (i) State Born-Oppenheimer's approximation and outline its significance. 2

- (ii) Describe the process of covalent bond formation according to the valence bond theory taking hydrogen molecule as an example. 3

7. (a) (i) Hydrogen molecule ion plays the same role in understanding molecular structure as is played by hydrogen atom for atomic structure. Comment. 2

- (ii) A molecular orbital is given by the following wave function :

$$\Psi = 0.95\phi_A + 0.32\phi_B$$

Calculate the proportion of each atomic orbital in this molecular orbital. 3

- (b) Give the assumptions of Hückel Molecular Orbital (HMO) theory for conjugated molecules. Determine the expression for the energy levels for ethylene molecule by using HMO. 5

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