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MCH–018

MASTER OF SCIENCE
(CHEMISTRY) /
MASTER OF SCIENCE
(ANALYTICAL CHEMISTRY)
(MSCCHEM/MSCANCHEM)
Term-End Examination
June, 2026

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 :

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

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

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

1. Answer any *five* of the following : 5×2=10

   (a) The ground state energy of a particle in a one-dimensional box cannot be zero. Comment.

   (b) Give the boundary conditions where the wave function for a particle confined to move in a three-dimensional box must be zero.

   (c) Define a radial node and calculate the number of radial nodes for 3*p* orbital.

   (d) What are the basic requirements for the perturbation method to be useful ?

   (e) State Pauli's exclusion principle and give its significance.

(f) Define an irreducible representation.

(g) What are the basic assumptions of the HMO method ?

2. (a) (i) Check whether the function, sin (x) is eigen function of the operator, $\frac{d^2}{dx^2}$. Find corresponding eigen value. 2

(ii) Calculate the de Broglie wavelength for a spherical droplet of water with radius = 0.1 mm, which is moving at a speed of 1 ms^{-1}. The density of the droplet = 1.0×10^{-3} kgm^{-3}. 3

(b) (i) State Heisenberg's uncertainty principle. 2

(ii) What are well behaved functions ?

Find out the function e^{-x^2} is a well-behaved function ? Justify your answer. 3

3. (a) Define a free particle. Give the salient features of the quantum mechanical description of 'Free particle' moving along X dimension. 2

(b) Show that the wave function for $n = 1$ and $n = 2$ energy states of a particle in one-dimensional box are orthogonal. 4

(c) Define degeneracy. Show that the (4, 5, 5) and (1, 4, 7) energy states are degenerate. Also state the type of degeneracy being demonstrated. 4

4. (a) (i) What are the center of mass coordinates ? Write mathematical expression for them. 2

(ii) Formulate the Schrödinger equation for a linear harmonic oscillator and provide the boundary conditions. 3

(b) Calculate the expectation value of (r) for the electron in the (n = 1; l = 0) state of the hydrogen atom. The corresponding wave function is $2\left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0}$. 5

5. (a) (i) Determine the number of possible orientations (degeneracy) of the orbital angular momentum for an electron with l = 3. 2

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

(b) Prove that $[L_x, L_y] = i\hbar L_x$; where L_x and L_y are given as

$$L_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$

$$L_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$$ 5

6. (a) Generate group multipliable table for water molecule. 5

(b) Drive the expression for the exchange integral in the Heitler-London treatment of the hydrogen molecule,

and explain its significance in bond formation. 5

Or

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

7. (a) Show the equivalence between ionic-covalent resonance in VB theory and configuration interaction in MO theory for H_2 molecule. 5

(b) (i) Draw the MO energy level diagram for HF molecule. 2

(ii) Use HMO method to derive the delocalization energy of cyclobutadiene. 3

Or

Apply Hückel Molecular Orbital (HMO) theory to ethylene (C_2H_4) and calculate π-electron energy levels. 3

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