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MCH–018

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

Term-End Examination

June, 2025

MCH-018 : QUANTUM CHEMISTRY AND GROUP THEORY

Time : 2 Hours *Maximum Marks : 50*

Note : *Attempt any **five** questions. All questions carry equal marks.*

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}

$R_H = 2.17869 \times 10^{-18}$ J

$\mu_H = 0.9995\ m_e$

$\epsilon_0 = 8.854 \times 10^{-12}$ C^2 J^{-1}m^{-1}.

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

   (a) State Heisenberg's uncertainty principle and give its significance for quantum mechanical systems.

   (b) Define Hermitian operators and give their significance.

   (c) Why are the orbitals of a given principal quantum number not degenerate in multi-electron atoms ?

   (d) "Symmetry operations are not same as symmetry elements." Comment.

   (e) What are the ranges of the spherical polar coordinates viz. r, θ and ϕ ?

   (f) State the Born-Oppenheimer approximation and give its importance in the study of molecular systems.

   (g) "The ground state energy of a particle confined to a one-dimentional box cannot be zero." Comment.

2. (a) (i) State the principle of corresponding states. 2

(ii) Evaluate the commutator [A, B], where : 3

$$A = \left(\frac{d}{dx} - x \right) \text{ and } B = \left(\frac{d}{dx} + x \right)$$

(b) (i) Calculate the energy difference between the ground state and the first excited state for an electron confined to a one-dimensional box of length 10 nm. 2

(ii) The longest wave length transition in butadiene is observed at 210 nm. If we assume butadiene to behave like one-dimensional box, calculate the length of the box. 3

3. (a) The Schrödinger wave equation for a particle confined in a three-dimensional box with its walls at infinite potential is given below :

$$\left[\frac{-\hbar^2}{2m} \nabla^2 \right] \psi(x, y, z) = E \psi(x, y, z)$$

Separate this expression into three equations; an equation for each dimension. 5

(b) (i) Using the following recursion relation :

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

along with the values $H_0(x) = 1$ and $H_1(x) = 2x$, determine the expression for $H_2(x)$. 2

(ii) Derive an expression for the moment of inertia for two masses m_1 and m_2 moving on a rigid massless bar about the centre of mass at distances r_1 and r_2 respectively. 3

4. (a) Calculate the energy required to ionise a hydrogen atom in its ground state. 5

(b) (i) What is Russell Saunders' coupling ? How does it help in determining the total angular momentum in a multi-electron atom ? 2

(ii) Draw and describe the radial probability distribution plot for $2s$ orbital of Hydrogen atom. 3

5. (a) What is variation theorem ? Use the trial wave function, $\phi = x(L - x)$ to estimate the ground state energy of a particle of mass m confined to a one-dimensional box of length L. 5

(b) Identify the symmetry elements of H_2O molecule and assign it to a point group. Justify your classification. 5

6. (a) Briefly describe the process of bond formation in hydrogen molecule by valence bond approach. Design the trial wave function for hydrogen molecule according to VBT. 5

(b) Design a trial wave function for hydrogen molecule ion by LCAO approximation. Use variation method for energy minimisation and derive expression for the energy levels. 5

7. (a) Draw the molecular orbital energy level diagram for CO and calculate the bond order. 5

   (b) State the limitations of Hückel's molecules orbital theory and explain how the Extended Hückel's Theory (EHT) addresses some of these limitations. 5

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