No. of Printed Pages : 7 **MPH–016**

M. SC. (PHYSICS) (MSCPH)

Term-End Examination

June, 2025

MPH-016 : ATOMIC AND MOLECULAR PHYSICS

Time : 2 Hours *Maximum Marks : 50*

Note : *Attempt any* ***five*** *questions. Marks are indicated against each question. You may use a calculator. Symbols have their usual meanings. The values of physical constants are given at the end.*

1. (a) Write any *two* properties of a Hermitian operator. 2

(b) Determine the speed of electron in the second Bohr orbit for $Z = 3$ and compare it with the speed of light. 3

(c) Consider a plane wave defined as :

$$\psi_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx}$$

Prove the orthonormality condition : 5

$$\int \psi_k(x)\, \psi_k^*(x')\, dk = \delta(x - x')$$

2. (a) Write down the selection rules under dipole approximation in atomic spectroscopy for the quantum numbers l and m. 2

(b) Determine the shift in energy (ΔE_3) due to Darwin term for n = 3 level of hydrogen atom. 3

(c) What is the origin of hyperfine structure in hydrogen atom ? Write down the expression for ΔE_{hfs} in terms of C, $\vec{F}$, $\vec{I}$, $\vec{J}$, where $\vec{I}$ is the total angular momentum of the nucleus, $\vec{J}$ is the total angular momentum of the electron, $\vec{F}$ is the total angular momentum of the atom and C is the strength of coupling between $\vec{I}$ and $\vec{J}$. What are the possible values of quantum number F for $J = \frac{5}{2}$ and $I = \frac{1}{2}$? 5

3. (a) Write the ground state electronic configuration for carbon atom. Determine the term symbols for $2p^2$ configuration and identify the term symbol for the ground state using Hund's rule. 1+5

(b) Derive the expression for the unperturbed energies when the external magnetic field is much greater than the spin-orbit interaction. 4

4. (a) Obtain the approximate internal energy of a diatomic molecule with $M_N \approx 16 m_p$ and $R_{eq} = 1.21 \text{ Å}$. Here m_p is the mass of proton and M_N is mass of nucleus. 6

(b) The ground vibrational state dissociation energy of a diatomic molecule is 2.48 eV, and its fundamental vibrational frequency is 559 cm^{-1}. Determine the equilibrium dissociation energy of the molecule. 4

5. (a) Write the electronic Hamiltonian for the H_2^+ molecular ion. 1

(b) Write the expression for variational integral and hence define Coulomb integral and overlap integral for this system. 5

(c) Prove that for the resonance integrals of H_2^+ ion, $H_{ab} = H_{ba}$. 4

6. (a) The fundamental and first overtone absorption transitions of a diatomic molecule are centered at 1285.1 cm^{-1} and 2551.50 cm^{-1}, respectively. Determine the equilibrium vibrational frequency $(\bar{\omega}_e)$, the anharmonicity constant (χ_e) and the zero point energy of the molecule. 8

(b) Give *two* differences between Nuclear Magnetic Resonance (NMR) and Electron Spin Resonance (ESR). 2

7. (a) If the bond length of HCl molecule is 1.27 Å, obtain the wave numbers for the first three rotational transitions. Given that the atomic masses of H and Cl are 1.008 a.m.u. and 35.45 a.m.u., respectively. 6

   (b) If the Stokes line of pure rotational Raman spectrum of H_2 molecule for a transition from $J = 1 \rightarrow J = 3$ is shifted from the excited radiation by 580 cm^{-1}, determine the bond length of the H_2 molecule. 4

8. (a) Compute the Doppler broadening, at 300 K, for the laser transition in the He-Ne laser which is centered at 632.8 nm. Obtain the ratio between the Doppler width and the natural line width for a lifetime of 30 ns. Assume

that ^{20}Ne is the only isotope present in the Laser. Given that atomic mass of Neon is 20 a.m.u. 8

(b) Give an example each of a gas-phase laser and a solid state laser. 2

Physical Constants :

$$\alpha = \frac{1}{4\pi \in_0} \times \frac{e^2}{\hbar c} \approx \frac{1}{137}$$

$\hbar = 1.06 \times 10^{-34}$ Js

$m_e = 9.10 \times 10^{-31}$ kg

1 a.m.u. = 1.66×10^{-27} kg

1 $cm^{-1} = 1.2398 \times 10^{-4}$ eV

$k_B = 1.3806 \times 10^{-23} JK^{-1}$

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