(c) State Heisenberg's uncertainty principle. Calculate the uncertainty in velocity of an electron if the uncertainty in position & momentum of the electron are equal. **6**

Unit II

4. (a) Derive and discuss the Schrödinger wave equation for a diatomic rigid rotator. Also draw the energy level diagram for the same. **10**

(b) Define space quantization. Pictorially represent the space quantization of angular momentum of a rigid rotator in the $l = 1$ rotational state. **6**

5. (a) Discuss the concept of the degeneracy of quantum mechanical states in a 3D-box. Also brief about accidental degeneracy with a suitable example. **6**

No. of Printed Pages : 07 **Roll No. .....**

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M.Sc. EXAMINATION, 2026

(Second Semester)

(2020-21 Onwards)

(Re-appear Only)

CHEMISTRY

Physical Chemistry-II

Time : 3 Hours] [*Maximum Marks :* 80

Before answering the question-paper, candidates must ensure that they have been supplied with correct and complete question-paper. No complaint, in this regard will be entertained after the examination.

Note : Attempt *Five* questions in all, selecting *one* question from each Unit. Q. No. **1** is compulsory. All questions carry equal marks.

Compulsory Question

1. (a) Find the value of commutator $[x^3, P_x]$. **2**

(b) What are orthonormal wavefunctions ? **2**

(c) What is the degeneracy of the first excited state for a particle present in a 3D-box ? **2**

(d) Define zero point energy. What is its value for 1D-SHO ? **2**

(e) Identify the symmetry elements & point groups for the molecules : **2**

NH_3, H_2O

(f) Define order of a point group. What is the order of the C_{3v} point group ? **2**

(g) Discuss the importance of statistical mechanics. **2**

(h) State the law of equipartition of energy. **2**

Unit I

2. (a) Find the average value, $\langle x \rangle, \langle P_x \rangle, \langle x^2 \rangle, \langle P_x^2 \rangle$ for a particle confined to move in a 1D-box of length 'l' with the normalized wave function : **12**

$$\psi_n = \sqrt{\frac{2}{l}} \sin\left(\frac{n\pi x}{l}\right)$$

(b) By using the above average values, verify Heisenberg's uncertainty principle. **4**

3. (a) Prove that an electron cannot exist inside the nucleus using the uncertainty principle. (Given : Radius of nucleus $\approx 10^{-15}\ m$) **5**

(b) Find the value of $\hat{A}^2$ if $\hat{A} = x - \frac{d}{dx}$. **5**

(b) What are radial distribution functions ? Also explain how you would determine the radius of maximum probability for 1*s*-orbital of a hydrogen atom ? **6**

Given :

$$R_{1,0} = 2\left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0}$$

(c) Find the value of quantum numbers *n*, *l*, and *m* for the given function : **4**

$$\psi_{n,l,m} \propto \frac{2-r}{a_0} e^{\frac{-zr}{na_0}} \cos\theta$$

Unit III

6. (a) State and describe the significance of the Great Orthogonality Theorem (GOT). **8**

(b) Deduce the character table for the C_{3v} point group using GOT. **8**

7. Write notes on the following :

(a) Axis of symmetry and plane of symmetry. **4**

(b) Reducible and irreducible representations. **4**

(c) Work out the multiplication table for C_{2v} point group using H_2O molecule as an example and show how it satisfies all the conditions of a group. **8**

Unit IV

8. (a) Define partition function. Give the physical significance of the partition function. Derive the expression for free energy and entropy in terms of the partition function. **10**

(b) Express the third law of thermodynamics in terms of the partition function. **6**

9. (a) Write short notes on the following : **8**

(i) Microcanonical ensemble

(ii) Canonical ensemble

(iii) Grand canonical ensemble

(iv) Thermodynamic probability

(b) Calculate the number of ways to distribute two indistinguishable particles in three boxes. **4**

(c) Calculate the standard molar entropy of gaseous argon at 25°C. **4**

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