# LOYOLA COLLEGE (AUTONOMOUS) CHENNAI – 600 034

**B.Sc.** DEGREE EXAMINATION – **CHEMISTRY**

SIXTH SEMESTER – **APRIL 2025**

**UCH 6502 – MOLECULAR DYNAMICS**

Date: 26-04-2025 Dept. No. Max. : 100 Marks

Time: 09:00 AM - 12:00 PM

## SECTION A

**Answer ANY FOUR of the following.** **(4 × 10 = 40)**

1. (a) State the major assumptions of classical mechanics.
   (b) A cricket ball weighing100g is to be located within 0.1 Å. What is the uncertainty in its velocity? (6+4)
2. (a) State the postulates of quantum mechanics.
   (b) Identify the acceptable wave function and justify: (i) $-x^2$ (ii) $\cos\theta$. (5+5)
3. (a) Write the group multiplication table for $C_{3v}$ point group.
   (b) What are abelian point groups? Cite an example. (6+4)
4. (a) State and explain laws of photochemistry.
   (b) What is meant by chemiluminescence? Cite an example. (6+4)
5. (a) Explain the mechanism of photosynthesis.
   (b) A sample of gaseous HI was irradiated by light of wavelength 275 nm when 310 J of energy was found to decompose $1.8 \times 10^{-3}$ mole of HI. Calculate the quantum yield for the dissociation of HI. (6+4)
6. Discuss the kinetics of the following photochemical reaction: $H_2(g) + Cl_2(g) \rightarrow 2\,HCl$.
7. How will you determine the surface area using Langmuir and BET adsorption isotherm?
8. Explain the following:
   (i) Brownian motion (ii) Critical Micelle concentration (iii) Schultz-Hardy rule.

## SECTION B

**Answer ANY THREE of the following.** **(3 x 20 = 60)**

9. (a) Derive time-independent Schrodinger wave equation.
   (b) Explain quantum theory of radiation using Planck's theory. (10+10)
10. (a) Predict the point group for the following molecules and determine molecules with significant dipole moment values: (i) Benzene (ii) $NH_3$ (iii) $CO_2$
    (b) What are the rules for forming the groups? What are isomorphic groups? (10+10)
11. (a) Derive the expressions for wave function and energy for a particle in 1-D box of length 1.
    (b) What are classes? Identify the order and number of classes present in the $CHCl_3$ molecule.
    (c) What are symmetry elements and symmetry operations? (10+5+5)
12. (a) Describe the various factors that affect fluorescence emission.
    (b) With a neat sketch of Jablonski diagram, explain the various radiative and non-radiative processes.
    (c) Illustrate the differences between photochemical and thermal reactions. (6+10+4)
13. (a) Derive Stern-Volmer equation for quenching of fluorescence. Mention its significance.
    (b) Explain the salient features of uranyl oxalate and ferric oxalate actinometers in predicting quantum yield. (10+10)
14. (a) Explain the postulates of Langmuir's unimolecular theory of adsorption and derive an expression for Langmuir adsorption isotherm.
    (b) Discuss the applications of colloids in detail. (10+10)

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