# LOYOLA COLLEGE (AUTONOMOUS), CHENNAI – 600 034

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

SIXTH SEMESTER – **APRIL 2023**

**UCH 6502 – MOLECULAR DYNAMICS**

Date: 03-05-2023 Dept. No. Max. : 100 Marks

Time: 09:00 AM - 12:00 NOON

## PART – A

**Answer ALL questions.** **(10 x 2 = 20 Marks)**

1. Calculate the energy and wavelength of light of frequency 500 Hz.
2. Verify whether the function $Ae^{-ax}$ is an eigen function of the operator d/dx. Mention the eigen value.
3. Identify the symmetry elements and assign point group for the following

   (i) trans-dichloroethylene (ii) pyridine
4. How will you determine the point group symbol of a molecule?
5. Give examples for high Quantum yield.
6. Calculate the energy of the photon corresponding to wavelength 4800 Å.
7. Mention the importance of actinometers.
8. What is static quenching?
9. What is the effect of temperature on adsorption of gases on liquids?
10. Define Tyndall effect.

## PART – B

**Answer any EIGHT questions.** **(8 x 5 = 40 Marks)**

11. Discuss the duality of photoelectric effect.
12. Applying the postulates of Quantum Mechanics, derive Schrodinger equation.
13. Write about the fundamental laws of black body radiation.
14. Give the applications of group theory to mutual exclusion principle with an example.
15. Discuss the symmetry elements and symmetry operations in $BCl_3$ molecule.
16. Differentiate thermal and photochemical reactions mentioning its industrial uses.
17. Explain the following.

    (a) any two laws of photochemistry (b) bioluminescence.
18. Describe the kinetics of photochemical formation of HBr.
19. Derive Stern Volmer equation.
20. Compare Freundlich and Langmuir isotherm.
21. Give the differences between lyophilic and lyophobic sols with examples.
22. Write the applications of colloids.

## PART – C

**Answer any FOUR questions.** **(4x 10 = 40 Marks)**

23. Derive an expression for the energy of a particle in one-dimensional box and discuss its applications to ethylene molecule.
24. Construct the group multiplication table for $C_{2v}$ point group and verify whether the symmetry operations follow commutative law.
25. (a) What are classes? Identify the classes present in Water molecule. (b) Differentiate fluorescence and phosphorescence.
26. Draw a neat Jablonski diagram and discuss the radiative and non-radiative processes.
27. (a) What are photosensitized reactions? Give examples.

(b) In a photochemical combination of $H_2$ and $Cl_2$ a quantum yield of $1x10^6$ is obtained with a wavelength of 4800 Å. How many moles of HCl would be produced under these conditions per calorie of radiation of energy absorbed? (Energy absorbed = 1 cal = $4.184 \times 10^7$ erg, energy absorbed = $1.196 \times 10^6$).

28. Write a note on electrokinetic phenomenon and critical micelle concentration.

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