LOYOLA COLLEGE (AUTONOMOUS), CHENNAI – 600 034

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

SIXTH SEMESTER – **NOVEMBER 2022**

UCH 6502 – MOLECULAR DYNAMICS

Date: 02-12-2022 Dept. No. Max. : 100 Marks

Time: 01:00 PM - 04:00 PM

Part – A

Answer ALL questions. **(10 × 2 = 20)**

1. Calculate the energy of the photon associated with wavelength 3000 Å.
2. Show that e^{-5x} is an eigen function of d^2/dx^2. Find the eigen value.
3. Give two examples for D_{2h} point group.
4. Write the symmetry elements for the C_{3V} point group.
5. Distinguish between thermal and photochemical reactions.
6. What are photosensitizers? Cite an example.
7. What do you mean by quenching a photochemical process?
8. Why is the quantum yield for the photochemical combination of H_2 and Cl_2 abnormally high?
9. Define zeta potential.
10. Write the BET equation and mention the terms involved in it.

Part – B

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

11. How is photoelectric effect explained by quantum theory?
12. Derive the energy equation for ethylene molecule.
13. Identify the point group and list out the symmetry elements present in the following molecules: OF_2 and $CHCl_3$.
14. Obtain the group multiplication table for water molecule.
15. A sample of gaseous HI was irradiated by light of wave length 253.7 nm when 307 J of energy was found to decompose 1.30 x 10^{-3} mole of HI. Calculate the quantum yield for the dissociation of HI.
16. State (a) Grotthus-Draper's law and (b) Einstein's law of photochemical equivalence.
17. Write short notes on chemiluminescence.
18. Discuss the kinetics of photochemical reaction between H_2 and Br_2.
19. What are chemical actinometers? Explain any one actinometer in detail.
20. Mention any five differences between chemisorption and physisorption.
21. How is the surface area of solid adsorbent determined using BET equation?
22. Discuss any five applications of colloids.

Part - C

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

23. a. State the postulates of quantum mechanics.
    b. Derive time-independent Schrodinger wave equation. (5+5)
24. a. Mention the order of symmetry operations and the number of classes of operations in NH_3.
    b. Illustrate the importance of point group in predicting dipole moment and optical activity of molecules.
    (5+5)
25. a. Explain the mechanism of photosynthesis.
    b. Calculate the energy of the first excited state of an electron confined to move in a one-dimensional box of length 6Å.
    (6+4)
26. Sketch Jablonski diagram and explain radiative and non-radiative processes.
27. Derive Stern-Volmer equation. Give its applications.
28. a. Give the assumptions and derive Langmuir adsorption isotherm equation.

b. Explain the stability of colloids using Schulze-Hardy rule for Coagulation. (5+5)

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