LOYOLA COLLEGE (AUTONOMOUS), CHENNAI – 600 034

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

SIXTH SEMESTER – **APRIL 2019**

CH 6612– MOLECULAR DYNAMICS

Date: 04-04-2019   Dept. No.   Max. : 100 Marks
Time: 09:00-12:00

PART-A

Answer **ALL** Questions   (10x2=20 marks)

1. What is Zeeman effect?

2. Mention any two drawbacks of classical mechanics.

3. Consider a particle in a box with the lowest energy (n=1). What is the probability of the particles being between (L/2and0.01L) and (L/2-0.01L)?

4. Write the Schrodinger's wave equation for a particle in 1-D box and mention the various terms involved in it.

5. Give any two differences between macro and micro states.

6. What do you mean by thermodynamic probability?

7. Define the term quantum yield.

8. The molar extinction coefficient of a coordination complex of Fe (II) is $12,000 dm^3 mol^{-1} cm^{-1}$ and the minimum detectable absorbance is 0.01. Calculate the minimum molar concentration of the complex that can be detected in a Beer's law cell of path length 1.00cm.

9. What do you mean by quenching in photochemical process?

10. Why is the quantum yield of photochemical combination of H_2 and Cl_2 abnormally high?

PART-B

Answer any **EIGHT** Questions   (8x5=40 marks)

11. Write a note on 'photoelectric effect'.

12. Determine the energy required for a transition from the $n_x=n_y=n_z = 1$ to $n_x=n_y=n_z = 2$ for an Argon atom (atomic mass = 39.95g) in a cubic container with a 1.0cm side.

13. Write the postulates of quantum mechanics.

14. What are the Eigen functions and Eigen values of the operator d/dx?

15. For a particle in a one dimensional box with its potential energy zero, deduce the de Broglie relation from its energy expression. (5)

16. Explain the following terms

   a) Most probable distribution b) Partition function.

17. Calculate the molar residual entropy of a crystal in which the molecules can adopt 6 orientations of equal energy at 0K.

18. Distinguish between fluorescence and phosphorescence.

19. List out the differences between thermal and photochemical reactions.

20. What are chemical actinometers? How are they useful in the determination of quantum yield of a reaction?

21. Write short notes on bimolecular quenching.

22. Explain the kinetics of photochemical combination of H_2 and Br_2 reaction.

PART-C

Answer any **FOUR** Questions   (4x10=40 marks)

23.) Explain the following (5+5)

    a) Bohr's theory of an atom

    b) Emission spectrum of 'H'atom

24. a) What are quantum mechanical operators? Explain them briefly.

    b) Derive the energy equation for ethylene molecule.

25. Derive Sackur-Tetrode equation. Give its applications

26. a) Calculate the translational partition function of a molecule of oxygen gas at 1 atm and 298K moving in a vessel of volume 24.4dm^3.(5)

    c) Write a note on flash photolysis.(5)

27. With a neat sketch of Jablonski diagram, explain the various photo physical and photochemical processes that occur during a photochemical reaction.

28. Derive Stern - Volmer equation. Give its applications.

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