



LOYOLA COLLEGE (AUTONOMOUS), CHENNAI – 600 034

B.Sc. DEGREE EXAMINATION – CHEMISTRY

SIXTH SEMESTER – APRIL 2015

CH 6612 - MOLECULAR DYNAMICS

Date : 15/04/2015
Time : 09:00-12:00

Dept. No.

Max. : 100 Marks

PART-A

Answer **ALL** Questions:

(10x2=20 marks)

1. What is Zeeman effect?
2. State Pauli's exclusion principle.
3. What are the allowed wave lengths for a particle in a box?
4. What are Eigen functions?
5. What do you mean by thermodynamic probability?
6. Write the Sackur-Tetrode equation? Explain the various terms involved in it.
7. Define the term quantum yield.
8. Define the term Chemiluminescence.
9. What do you mean by quenching in photochemical process?
10. What is photosensitization?

PART-B

Answer any **EIGHT** Questions:

(8x5=40 marks)

11. Explain the theory of classical mechanics and its failures.
12. Write a note on 'photoelectric effect'.
13. What are quantum mechanical operators? Explain them briefly.
14. What are Eigen functions and Eigen values of the operator d/dx ?
15. Derive the energy equation for butadiene molecule.
16. Explain the following terms
 - a) Most probable distribution
 - b) Partition function.
17. 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 .
18. Explain why is the quantum yield of photochemical combination of H_2 and Cl_2 abnormally high?

19. What are chemical actinometers? How are they useful in the determination of quantum yield of a reaction?
20. Explain the mechanism of photosynthesis.
21. Write short notes on biomolecular quenching.
22. Explain the principle and procedure involved in flash photolysis.

PART-C

Answer any **FOUR** Questions:

(4x10=40 marks)

23. Explain the following:
 - a) Energy distribution in black body radiation.
 - b) Emission spectrum of 'H' atom.
24. a) For a particle in a one dimensional box with its potential energy zero, deduce the de Broglie relation from its energy expression.
b) Derive an expression for the energy of a particle in a one dimensional box
25. a) Compare the important features of Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics. (8)
b) What is meant by partition function? (2)
26. With a neat sketch of Jablonski diagram, explain the various photo physical and photochemical processes that occur during a photochemical reaction.
27. a) State and explain the various laws of photochemistry.
b) Enumerate the differences between thermal and photochemical reactions.
28. Derive Stern - Volmer equation. Give its applications.

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