LOYOLA COLLEGE (AUTONOMOUS), CHENNAI – 600 034

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

SIXTH SEMESTER – **NOVEMBER 2016**

CH 6612 – MOLECULAR DYNAMICS

Date: 12-11-2016   Dept. No.   Max. : 100 Marks
Time: 01:00-04:00

PART-A

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

1. What is black body radiation?
2. What is Zeeman effect?
3. What is the ground state energy for an electron that is confined to a potential well with a width of 0.4 nm?
4. Write the Schrodinger's wave equation for a particle in 1-D box and mention the various terms involved in it.
5. Define the term partition function.
6. What do you mean by thermodynamic probability?
7. Calculate the energy associated with one Einstein of radiation of wavelength 8000Å.
8. Define the term Chemiluminescence.
9. Why is the quantum yield of photochemical combination of H_2 and Cl_2 abnormally high?
10. What is photosensitization?

PART-B

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

11. Explain the theory of classical mechanics and its failures.

12. Explain the emission spectrum of H-atom.

13. Write any five postulates of quantum mechanics.

14. What are quantum mechanical operators? Explain them briefly.

15. 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.

16. What is an ensemble? Explain its various types.

17. Derive the relationship between energy and partition function.

18. Write the mechanism of photosynthesis.

19. Explain the following terms.

    (i)   Vibrational cascade (ii) Bioluminescence.

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

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

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

PART-C

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

23. Write a note on the following: (5+5)

    a) Photoelectric effect b) Pauli's exclusion principle.

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

    b) Derive an expression for the energy of a particle in a one dimensional box.   (5)

25. a) Calculate the relative numbers of distinguishable states in ice and in liquid water at 273K. (Given $\Delta H\ f_{us}$ = 6.0kJ mole^{-1} at 273 K; K = 1.38 x 10^{-23} JK^{-1}).   (6)

    a) Write a note on residual entropy. (4)

26. a) Compare the important features of Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics. (6)

    b) Write the differences between fluorescence and phosphorescence. (4)

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

28. a) Write a note on flash photolysis. (10)

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