LOYOLA COLLEGE (AUTONOMOUS), CHENNAI – 600 034

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

SIXTH SEMESTER – **APRIL 2013**

CH 6606/CH 6600 - MOLECULAR DYNAMICS

Date : 25/04/2013   Dept. No.   Max. : 100 Marks
Time : 1:00 - 4:00

PART – A

Answer **ALL** questions: (10 x 2 = 20 marks)

1. State Pauli's exclusion principle.

2. Calculate the energy of the photon associated with light of wavelength 2500 A$^\circ$.

3. What are eigen functions?

4. What are operators?

5. Find the value of ln 100!

6. Define the term partition function.

7. Explain intersystem crossing.

8. What is quantum yield?

9. State the Grotthus-Draper's law of photochemistry.

10. Define molar extinction coefficient.

PART – B

Answer any **EIGHT** questions: (8 x 5 = 40 marks)

11. Explain the difference between classical mechanics and quantum mechanics.

12. Explain the energy distribution in Black Body radiation.

13. Explain the emission spectrum of hydrogen atom.

14. Write the Schrodinger equation.   Explain the terms.

15. Derive the energy equation for butadiene.

16. Calculate S_{trans} for nitrogen gas at one atm. pressure and at $30^{o}C$.

17. Discuss the most probable distribution of particle.

18. Explain the spin-orbit coupling.

19. Explain a chemical actinometer with an example.

20. A sample of gaseous HI was irradiated by light of wave length 253.7 nm when 307 J of energy was found to decompose 1.30×10^{-3} mole of HI.   Calculate the quantum yield for the dissociation of HI.

21. Discuss the process of photosensitization.

22. Discuss the kinetics of photochemical reaction of H_2 and Br_2.

PART – C

Answer ANY **FOUR** questions: (4 x 10 = 40 marks)

23. a) How is photoelectric effect explained by quantum theory?   (4)
    b) Derive the expressions for eigen value and eigen function for a particle
        in one dimensional box.   (6)

24. a) Calculate the de Broglie wave length of a body of mass 1 kg moving
       with a velocity of 2000 m s^{-1}.   (4)
    b) State the postulates of quantum mechanics.   (6)

25. a) Explain Bohr's theory of atom.   (5)
    b) Derive an expression for translation partition function.   (5)

26. Derive Maxwell – Boltzmann statistics.   Give its applications.   (10)

27. Explain any two of the following: (10)
    (i) Fluorescence   (ii) Phosphorescence
    (iii) Chemiluminescence   (iv) Relaxation Technique

28. Derive Stern – Volmer equation.   Give its applications.   (10)

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