LOYOLA COLLEGE (AUTONOMOUS), CHENNAI – 600 034

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

SIXTH SEMESTER – **APRIL 2012**

# CH 6606/CH 6600 - MOLECULAR DYNAMICS

 Date : 16-04-2012 Dept. No. Max. : 100 Marks

 Time : 1:00 - 4:00

**PART – A**

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

1. Define the terms orbit and orbitals.

2. Calculate the energy of the photon associated with light of wavelength 3200 Ao.

3. Define the term degeneracy of an energy level.

4. What are operators? Give an example.

5. What are microstates?

6. Define the term partition function.

7. Explain internal conversion.

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 Zeeman effect.

14. State the postulates of quantum mechanics.

15. Explain the significance of eigen functions.

16. Derive Sackur-Tetrode equation and explain the terms involved.

17. Discuss the most probable distribution of particles.

18. Explain the spin-orbit coupling.

19. Explain the primary and secondary processes in a photochemical reaction.

20. Radiation of wave length 2500 Ǻ was passed through a cell containing 10 ml of a

 solution which was 0.05 molar in oxalic acid and 0.01 molar in uranyl sulphate. After absorption of

 80 Joules of radiation energy, the concentration of oxalic acid was reduced to 0.04 molar. Calculate

 the quantum yield for the photochemical decomposition of oxalic acid at the given wave length.

21. Explain the kinetics of fast reaction by relaxation techniques.

22. Discuss the kinetics of photochemical reaction between H2 and Br2.

**PART – C**

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

23. (i) What are quantum numbers? Give its significance.

 (ii) A photon of wave length 4000 Ǻ strikes a metal surface, the work function of the

 metal being 2.13 eV. Calculate the energy of the photon in eV.

24. (i) State Pauli’s exclusion principle and explain.

 (ii) Derive the expressions for eigen value and eigen function for a particle in one

dimensional box.

25. Explain the separation of partition functions and its significance.

26. Derive Maxwell-Boltzmann statistics.

27. Explain any two of the following:

 (i) Chemical Actinometers (ii) Fluorescence

 (iii) Chemiluminescence (iv) Flash photolysis

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

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