LOYOLA COLLEGE (AUTONOMOUS), CHENNAI – 600 034

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

SIXTH SEMESTER – **APRIL 2015**

CH 6606/CH 6600 – MOLECULAR DYNAMICS

Date : 24/04/2015   Dept. No.   Max. : 100 Marks
Time : 09:00-12:00

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 3000 A$^\circ$.
3. Define the term degeneracy of an energy level.
4. What are operators? Give an example.
5. What are micro states?
6. Define thermodynamic probability.
7. State Beer-Lambert law.
8. Define quantum yield.
9. State the Grotthus-Draper's law of photochemistry.
10. Give any two differences between thermal and photochemical reactions.

PART – B

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

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

12. What is photoelectric effect? Explain.

13. State the postulates of quantum mechanics.

14. Write the Schrodinger equation.   Explain the terms.

15. Derive the energy equation for butadiene.

16. Derive the equation for translational partition function.

17. Calculate the translational partition function of NO molecule at 300 K in a volume 1000 m^3.

    Assuming the gas to behave ideally.

18. Explain the spin-orbit coupling.

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

20. Explain the mechanism of photosynthesis.

21. Explain Flash photolysis.

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) What are quantum numbers? Give its significance. (5)
    b) Explain the emission spectrum of hydrogen atom. (5)

24. a) Calculate the de Broglie wave length of a body of mass 1 kg moving
       with a velocity of 2100 ms^{-1}. (4)
    b) Derive the expressions for eigen value and eigen function for a particle
       in one dimensional box. (6)

25. Derive the Maxwell-Boltzmann statistics. Give its applications. (10)

26. Derive Sackur-Tetrode equation. Give its applications. (10)

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

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

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