LOYOLA COLLEGE (AUTONOMOUS), CHENNAI – 600 034

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

SIXTH SEMESTER – **APRIL 2018**

CH 6612– MOLECULAR DYNAMICS

Date: 17/04/2018 Dept. No. Max. : 100 Marks

Time: 09:00-12:00

PART – A

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

1. Define the term orbit and orbitals.
2. State Pauli's exclusion principle.
3. Calculate the energy of the photon associated with light of wavelength 3000A^o.
4. Define the term degeneracy of an energy level.
5. Find the value of ln100!
6. What are micro states?
7. State Beer-Lambert law.
8. Explain intersystem crossing.
9. The optical density of 0.001 M solution in a cell of 0.1 cm path length is 0.162. Calculate the extinction coefficient.
10. Define quantum yield.

PART – B

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

11. How is photoelectric effect explained by quantum theory?
12. Explain the energy distribution in Black Body radiation.
13. State the postulates of quantum mechanics.
14. Explain the emission spectrum of hydrogen atom.
15. Derive the energy equation for butadiene.
16. Calculate the translational partition function of NO molecule at 300 K in a volume 1000 m^3. Assuming the gas to behave ideally.
17. Calculate S_{trans} for nitrogen gas at one atm. pressure and at 30^{o}C.
18. Explain the primary and secondary processes in a photochemical reaction.
19. Explain chemical actinometers 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 x 10^{-3} mole of HI. Calculate the quantum yield for the dissociation of HI.
21. Discuss the process of photosensitization.

22. In the photochemical combination of hydrogen and chlorine a quantum efficiency of 1×10^6 is obtained with a wavelength of 480 nm. How many moles of hydrogen chloride would be produced under these conditions per joule of radiation energy absorbed?

PART – C

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

23. a) What are quantum numbers? Give its significance. **(5)**

b) Explain Bohr's theory of 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}. **(5)**

b) Derive the expressions for eigen value and eigen function for a particle in one dimensional box. **(5)**

25. Derive Maxwell-Boltzmann statistics. Give its application. **(10)**

26. a) Derive an expression for translation partition function. **(5)**

b) Discuss the kinetics of photochemical reaction of H_2 and Br_2. **(5)**

27. Explain any two of the following:

(i) Phosphorescence (ii) Chemiluminescence

(iii) Relaxation Technique (iv) Jablonski'sdiagram **(10)**

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

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