



LOYOLA COLLEGE (AUTONOMOUS), CHENNAI – 600 034

B.Sc. DEGREE EXAMINATION – CHEMISTRY

SIXTH SEMESTER – APRIL 2017

CH 6612- MOLECULAR DYNAMICS

Date: 18-04-2017
Time: 09:00-12:00

Dept. No.

Max. : 100 Marks

PART-A

Answer ALL Questions:

(10 x 2 = 20 marks)

- 01) State Wien's displacement law.
- 02) The distance between Chennai to Delhi is approximately 2000 Km. How long will it take from Chennai to Delhi if you travel in a vehicle which moves with a constant speed equal to that of an electron in the first orbit of Hydrogen atom?
- 03) $\Psi = 3xe^{-4x}$ is an eigen function of the operator d^2/dx^2 . Find the eigen value corresponding to the operator.
- 04) Write the boundary conditions for a particle confined to move in a one dimensional box.
- 05) A system has a partition function equal to $\frac{1}{2}$. What do you understand from this value?
- 06) Translational partition function of a gas increases as the volume of the gas increases. Give reason.
- 07) Distinguish between Internal conversion and Inter system crossing.
- 08) Solutions that are used in photochemical studies must be deoxygenated before the commencement of reaction. Give reason.
- 09) What are fast reactions? Give an example.
- 10) Write the mechanism of photochemical reactions between H_2 and Cl_2 .

PART-B

Answer any EIGHT Questions:

(8 x 5 = 40 marks)

- 11) Calculate the wavelength (in nm) of the longest wavelength radiation emitted in Brackett series of Hydrogen spectrum.
- 12) For the 100 face of silver metal the velocity of electrons emitted using 200nm photons is $7.42 \times 10^5 \text{ ms}^{-1}$. Calculate the work function of this face in eV.
- 13) Find the values of the following
 - a) $\Delta x \cdot \Delta p_x$
 - b) $\Delta x \cdot \Delta p_y$
 - c) $\Delta x \cdot \Delta p_z$
- 14) Write the postulates of quantum mechanics.
- 15) Calculate the energy of the first excited state of an electron confined to move in a one dimensional nanowire of length 10 nm.
- 16) Derive the relation between partition function and internal energy of a system.
- 17) Write short account on the concept of Residual entropy.
- 18) State (a) Grotthus-Drappers' law and (b) Einstein's law of photochemical equivalence.
- 19) Write notes on the Mechanism of photosynthesis.
- 20) Distinguish between Fluorescence and Phosphorescence.
- 21) Describe the kinetics of photochemical reaction between H_2 and Br_2 .
- 22) Elaborate the reasons for obtaining low and high quantum efficiencies.

PART-C

Answer any FOUR Questions:

(4 x 10 = 40 marks)

- 23) a) Explain Einstein's view on "Photoelectric emission" (6)
b) What is Zeemann effect? Give its significance. (4)
- 24) Derive the expression for the energy and wavefunction for a particle confined to move in a one dimensional box of length 'L' and infinite potential barrier. (10)
- 25) a) Evaluate translational partition function for oxygen atoms at 300K contained in a volume of 22.4 dm³. (5)
b) Explain the significance of the Boltzmann distribution. What does this distribution describe? (5)
- 26) a) Explain the depopulation pathways that occur between the first excited singlet state and the first excited triplet state.
b) Write notes on chemiluminescence. (5)
- 27) Describe in detail flash photolysis. (10)
- 28) a) Show that the molecular partition function of a diatomic molecule is given by $q = q_t q_r q_v q_e$ (5)
b) Explain in detail 'Photosensitization'. (5)
