



LOYOLA COLLEGE (AUTONOMOUS), CHENNAI – 600 034

B.Sc. DEGREE EXAMINATION – CHEMISTRY

SIXTH SEMESTER – APRIL 2016

CH 6612 – MOLECULAR DYNAMICS

(12th BATCH ONWARDS)

Date: 15-04-2016

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. Calculate the energy of the photon associated with light of wavelength 3000 Å.
3. Define the term degeneracy of an energy level.
4. What are operators? Give an example.
5. Find the value of $\ln 100!$.
6. Define thermodynamic probability.
7. State Beer-Lamberts law.
8. The optical density of 0.001 M solution in a cell of 0.1 cm path length is 0.162.
Calculate the extinction coefficient.
9. Define quantum yield.
10. Explain radiation less transition.

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. State the postulates of quantum mechanics.
14. Write the Schrodinger equation. Explain the terms.
15. Derive the energy equation for butadiene.
16. Calculate the translational partition function of NO molecule at 300 K in a volume 1000 m³. Assuming the gas to behave ideally.
17. Derive Sackur-Tetrode equation and explain the terms involved.
18. Explain the mechanism of photosynthesis.
19. Explain the primary and secondary processes in a photochemical reaction.
20. Explain the spin-orbit coupling.
21. 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?
22. Explain the principle and applications of Flash photolysis.

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 eigenvalue and eigenfunction 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: (10)
(i) Chemical Actinometers (ii) Phosphorescence
(iii) Chemiluminescence (iv) Relaxation Technique.
28. Derive Stern-Volmer equation. Give its applications. (10)

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