LOYOLA COLLEGE (AUTONOMOUS), CHENNAI – 600 034

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

SIXTH SEMESTER – **APRIL 2018**

CH 6606– MOLECULAR DYNAMICS

Date: 21-04-2018   Dept. No.   Max. : 100 Marks
Time: 01:00-04:00

PART – A

Answer ALL the questions.   **(10x2=20)**

1.   Define the terms orbit and orbitals.

2.   State Pauli's exclusion principle.

3.   Define the term degeneracy of an energy level.

4.   What are operators? Give an example.

5.   Find the value of 1n100!

6.   What do you mean by thermodynamic probability?

7.   What is internal conversion?

8.   Define the term Chemiluminescence.

9.   What do you mean by quenching in photochemical process?

10.   What are thermal reactions?   Give an example.

PART – B

Answer any EIGHT questions.   **(8x5=40)**

11.   How is photoelectric effect explained by quantum theory?

12.   Explain the energy distribution in Black Body radiation.

13.   Explain Zeeman effect.

14.   What are Eigen functions and Eigen values of the operator d/dx?

15.   Derive the energy equation for butadiene molecule.

16.   Explain Sackur-Tetrode equation.

17.   Calculate the translational partition function of a molecule of oxygen gas at 1 atm and 298 K moving in a vessel of volume 24.4 dm^3.

18.   Explain the mechanism of photosynthesis.

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

20.   When irradiated with light of 5000 A^o wavelength, 1×10^{-4} mole of a substance is decomposed.   How many photons are absorbed during the reaction if its quantum efficiency is 10.00 (Avogadro number N = 6.02×10^{23}).

21.   Discuss the kinetics of photochemical reaction between H_2 and Cl_2.

22.   Explain the principle and procedure involved in flash photolysis.

PART – C

Answer any FOUR questions: **(4x10=40)**

23. Explain the following : (a) Energy distribution **(5)**

(b) Emission spectrum of 'H' atom. **(5)**

24. (a)For a particle in a one dimensional box with its potential energy zero, deduce the de Broglie relation from its energy expression. **(5)**

(b)Derive an expression for the energy of a particle in a one dimensional box.**(5)**

25. Derive an expression for translation partition function. Mention its significance. **(7+3)**

26. (a) Derive Maxwell-Boltzmann statistics. **(5)**

(b)Enumerate the differences between thermal and photochemical reactions. **(5)**

27. With a neat sketch of Jablonski diagram, explain the various photo physical and photochemical process that occur during a photochemical reaction. **(10)**

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

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