

LOYOLA COLLEGE (AUTONOMOUS), CHENNAI – 600 034



B.Sc. DEGREE EXAMINATION – CHEMISTRY

SIXTH SEMESTER – APRIL 2022

16/17UCH6MC01 – QUANTUM CHEMISTRY AND PHYSICAL PROCESSES

Date: 15-06-2022

Dept. No.

Max. : 100 Marks

Time: 01:00 PM - 04:00 PM

Part – A

Answer ALL questions.

(10 × 2= 20)

1. What is threshold frequency?
2. Obtain the Eigen values for $\cos mx \cos ny \cos oz$ for an operator d^2/dx^2 .
3. Determine the point group of the following molecules: (a) CH_3Cl (b) PtCl_4 .
4. What are isomorphous groups? Cite an example.
5. State Grotrian-Draper law.
6. Compare thermal reactions with photochemical reactions (Any two).
7. What is g-value?
8. Calculate the energy of an Einstein of radiation of wavelength 240 nm.
9. Differentiate physisorption from chemisorption.
10. What is coagulation?

Part – B

Answer any EIGHT questions.

(8 × 5= 40)

11. State the postulates of quantum mechanics.
12. (a) Find the accelerating potential for an electron with de Broglie wavelength of 5 \AA .
(b) What are energy separations in kJ/mol and cm^{-1} between the levels $n = 1$ and $n = 2$ by considering the length of the 1-D box is 5 \AA .
13. Identify the point group and construct the group multiplication table for NF_3 molecule.
14. What are classes and Abelian group? Predict whether water is Abelian group or not.
15. State and explain absorption laws.
16. Explain various radiative and non-radiative photophysical processes with the help of Jablonski diagram.
17. At 0°C and 1 atm pressure the volume of N_2 gas required to cover a sample of silica gel assuming Langmuir monolayer adsorption is found to be $85 \text{ cm}^3 \text{ s}^{-1}$ of the gel. Calculate the surface area per gram of silica gel. Given that the area occupied by a N_2 molecule is 0.162 nm^2 .
18. In the photochemical combination of H_2 and Br_2 a quantum efficiency of 1×10^6 has been obtained with a wavelength 4800 \AA . How many moles of HBr would be produced under these conditions per calories of radiant energy absorbed?
19. Explain any five applications of colloids.
20. Give the assumptions and derive Langmuir adsorption isotherm equation.
21. Discuss the optical and mechanical properties of colloids.
22. How is electrophoresis helpful in separating charged particles?

Part – C

Answer any FOUR questions.

(4 × 10= 40)

- 23a. Obtain the mathematical expression for black body radiation using Plank's radiation law.
b. Derive time-independent Schrödinger wave equation. **(5+5)**
- 24a. Illustrate the importance of point group in predicting dipole moment and optical activity of the molecules.
b. What are symmetry operations and symmetry elements? **(6+4)**
- 25a. Write the schematic representation of photosensitized process between Donor (D) and acceptor (A) in the presence of sensitizer.
b. Explain Chemiluminescence and bio-luminescence with suitable examples. **(4+6)**
- 26a. Mention the significance of chemical actinometers? Explain uranyl oxalate actinometer in detail.
b. Derive Stern-Volmer equation. **(5+5)**
- 27a. Discuss the kinetics of following photochemical reaction: $H_2 + Cl_2 \rightarrow 2HCl$. Why is quantum yield for this reaction very high?
b. Predict the ground state term symbol for p^3 ion. **(7+3)**
- 28a. Explain the following: (a) Lyophilic and lyophobic colloids.
(b) Critical Micelle concentration
(c) Gibbs adsorption isotherm **(3+3+4)**

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