



**LOYOLA COLLEGE (AUTONOMOUS), CHENNAI – 600 034**

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

**SIXTH SEMESTER – NOVEMBER 2016**

**CH 6606/CH 6600 – MOLECULAR DYNAMICS**

Date: 03-11-2016

Dept. No.

Max. : 100 Marks

Time: 09:00-12:00

**PART A**

**Answer ALL Questions:**

**(10 x 2 = 20 Marks)**

1. Mention the units of wave number and frequency.
2. State True or False: a) The rest mass of an electron is 0.000548 amu. b) The charge per mass ratio of an electron was determined by J.J.Thompson.
3. What is the possible azimuthal and magnetic quantum number possible for principal quantum number 2?
4. Define radial distribution function.
5. What is Stirling's approximation?
6. Define thermodynamic temperature.
7. What is kasha's rule?
8. State Grothus-Draper law.
9. What is Stern-volmer plot?
10. Define solvent quenching.

**PART B**

**Answer any EIGHT Questions:**

**(8 x 5 = 40 Marks)**

11. For a radiation of wavelength 400 nm calculate 1) Frequency 2) Energy per Einstein.
12. Mention the drawbacks of Bohr's atomic theory.
13. Write i) Schrodinger wave equation ii) de Broglie equation of dualism and explain the terms in these equations.
14. What are the characteristics of wave function  $\psi$ ?
15. For an electron in 4f and 2p orbital, mention the possible values for the quantum numbers l and m.
16. Write a note on the concept of statistical entropy.
17. Explain the following terms: i) Ensemble ii) Population.
18. State Franck-Condon principle and explain the concept of various transitions obtained in organic molecules.
19. What is photosensitization and represent schematically the photosensitized process between Donor (D) and Acceptor (A) in the presence of a sensitizer.
20. Explain the concept of photoelectric effect.
21. Distinguish static quenching from dynamic quenching. How does temperature influence the quenching process?
22. Explain laser flash photolysis technique with a neat sketch.

**PART C**

**Answer any FOUR Questions:**

**(4 x 10 = 40 Marks)**

23. Explain the concept of spectral lines found in atomic hydrogen and quantification of their energies based on Bohr's theory.
24. Derive the energy for a particle in a one dimensional box.
25. Write a note on radial probability distribution curves and angular probability distribution curves.
26. Derive Sackur-Tetrode equation for a mono atomic gas.
27. Sketch Jablonski Diagram and mention the photophysical pathways of an electronically excited molecule.
28. Explain in brief about the various chemical actinometers.

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