LOYOLA COLLEGE (AUTONOMOUS), CHENNAI - 600 034



B.Sc. DEGREE EXAMINATION - CHEMISTRY

SIXTHSEMESTER - APRIL 2017

CH 6606- MOLECULAR DYNAMICS

Date: 20-04-2017 Dept. No. Max.: 100 Marks

Time:09:00-12:00

PART- A

Answer **ALL** questions

10X2 = 20 marks

- 1. State photoelectric effect.
- 2. Define Paulis's exclusion principle.
- 3. What is Schrodinger equation.
- 4. Mention the operators used in quantum mechanics.
- 5. What is residual energy?
- 6. What are macro and micro states?
- 7. State chemiluminescence.
- 8. What is meant by photosensitization?
- 9. Define rate law.
- 10. What do you mean by bimolecular quenching?

PART- B

Answer any **EIGHT** questions

8x5 = 40 marks

- 11. Mention any five differences between classical mechanics and quantum mechanics.
- 12. Give a brief account on black body radiation.
- 13. Derive the energy equation for butadiene.
- 14. Enumerate any five postulates of quantum mechanics.
- 15. Derive an expression for eigen value and eigen function.
- 16. Derive Sackur Tetrode equation.
- 17. Derive the relation between partition function and energy.
- 18. Write notes on spin- orbit coupling.
- 19. State and explain the laws of photochemistry.
- 20. Write notes on chemical actinometer.
- 21. Derive Stern-Volmer equation.
- 22. Write notes on flash photolysis.

PART- C

Answer any FOUR questions

4x10 = 40 marks

23. (i). Explain the emission spectrum of hydrogen atom. (6)

(ii). State and explain Zeemann effect. (4)

24. Derive an energy expression for a particle in one dimensional box.

25. (i). What are quantum numbers? Explain. (5)

(ii). Explain how quantum mechanics is applicable to ethylene. (5)

26. Derive Maxwell-Boltzmann statistics. Mention its significances.

27. (i). Give a brief account on Jablonski energy level diagram. (6)

(ii). Discuss the mechanism of photosynthesis. (4)

28. (i). Arrive at an expression for the photochemical rate law. (5)

(ii). Explain the kinetics of the photochemical reaction between hydrogen and chlorine. (5)
