TB165130F

Reg. No.: .....

Name : .....

B. Sc. DEGREE (C.B.C.S.S.) EXAMINATION, JANUARY 2019

(2016 Admission Supplementary)

SEMESTER V- CORE COURSE (CHEMISTRY)

CH5B08TB – QUANTUM CHEMISTRY, MOLECULAR SYMMETRY AND SPECTROSCOPY

Time: Three Hours **Maximum Marks: 60**

PART A

I. Answer all questions. Each question carries 1 mark.

1. Comment on the significance of de-Broglie equation.
2. What are the conditions for a wave function to be acceptable?
3. A linear n-atom molecule has ..... normal mode of vibration
4. The frequency of Stokes lines for a molecule are ..... than that of the Rayleigh line
5. What is meant by a symmetry operation?

(5 × 1 = 5)

PART B

II. Answer any five questions. Each question carries 2 marks.

6. Using suitable example, explaineigen value and eigen function of an operator.
7. State the selection rule for the vibrational transitions of a simple harmonic oscillator.
8. Explain the application of group frequency in organic chemistry.
9. Why is TMS used as a standard reference in NMR spectroscopy?
10. If the spin quantum number of a nucleus is 1, how many spin states are possible?
11. Name the elements of the C_{3v} point group.
12. Define a plane of symmetry. What is the associated symmetry operation?
13. How many rotational axes of symmetry are present in $C_5H_5^-$.

(5 × 2 = 10)

PART C

III. Answer any five questions. Each question carries 5 marks.

14. Explain Davisson-Germer experiment on electron diffraction.
15. Draw the MO diagram and calculate the bond order for the following molecules. a)N_2 b)O_2.
16. Sketch the vibrational modes of CO_2 and explain the IR active and IR inactive vibration modes.
17. The bond length of HCl molecule is 120 pm. Calculate the wave number in cm^{-1} for the transitions J=0 to J=1.(Atomic mass: H=1.008 x 10^{-3} kg mol^{-1}; Cl = 35.45 x 10^{-3} $kgmol^{-1}$).
18. Explain briefly a) Fundamental bands, b) overtones and c) hot bands in a vibrational spectrum.
19. Draw a schematic diagram of the proton NMR spectra of pure ethanol and ethanol containing small amount of acid. Label the peaks.
20. Mention the applications of electronic spectroscopy in organic chemistry.

21. How many symmetry operations are there in CH_4 molecule? Explain.

(5 × 5 = 25)

PART D

IV. Answer any two questions. Each question carries 10 marks.

22. a)With the help of black body spectrum explain the concept of blackbody radiation and its energy distribution.
    b)Give a detailed account of Compton effect.
23. Using the concept of particle in a one-dimensional box,derive an expression for the energy and wave function of particle and prove that energy is quantized.Explain its application to π electrons of hexatriene system.
24. Arrive at expressions for (i) the moment of inertia and (ii) expression for rotational energy of a rigid diatomic molecule.
25. Explain the basic principles of NMR spectroscopy.

(2 × 10= 20)