TB165130D

Reg. No.: .....

Name : .....

B. Sc. DEGREE (C.B.C.S.S.) EXAMINATION, OCTOBER 2018
(2016 Admission Regular & 2015 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. Diagramatically represent the wavefunctions corresponding to quantum numbers n=1,2,3 for particle in a box stationary states.
2. Diagramatically represent Compton scattering.
3. The unit of the force constant is.....
4. Water molecule has ..... normal mode of vibration.
5. Give an example of a molecule belonging to D_{3h}.

(5 × 1 = 5)

PART B

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

6. What are the criteria for forming molecular orbitals from atomic orbitals
7. Given that the fundamental vibrational band for CO is at 2140 cm^{-1}, calculate the force constant of the C-O bond, whose reduced mass is given as 1.1368×10^{-26} kg
8. How will you distinguish between the overtones and hot bands of a spectrum?
9. What is bathochromic effect?
10. Which of the following have a nuclear spin?
    a) $_1H^1$ b) $_6C^{14}$ c) $_9F^{19}$ d) $_7N^{15}$
11. Define an improper rotation axis.
12. What is a dihedral mirror plane?
13. Identify the point group to which H_2O belongs.

(5 × 2 = 10)

PART C

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

14. Give a detailed account on physical picture of bonding and anti-bonding wave functions emerging from the application of the LCAO approximation to the H_2^+ ion.
15. Write a note on the application of Schrodinger wave equation to hydrogen atom.
16. Discuss briefly the quantum mechanical concept of Raman Effect.
17. Derive an expression for rotational energy of a rigid diatomic molecule.
18. The bond length of HBr molecule is 180 pm. Calculate the wave number in cm^{-1} for the transition J=1 to J=2 for this molecule. (H =1.008×10^{-3} kg mol^{-1}; Br = 79.909×10^{-3} kg mol^{-1}).
19. Why do aromatic hydrogen atoms have a higher chemical shift value compared to

aliphatic hydrogen atoms?

20. Sketch the NMR spectrum of 1,1-dibromoethane and explain.
21. How many symmetry elements and symmetry operations exists in NH_3 molecule? Find out the point group to which the molecule belongs.

(5 × 5 = 25)

PART D

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

22. a) Give a detailed account of Plank's quantum hypothesis and Plank's radiation law. Calculate the energies of two radiations one with wavelength 800nm and other 400nm.
    b)State and explain Heisenberg's uncertainity principle. Write a note on its significance.
23. What are quantum numbers. Explain the physical significance of the different types of quantum numbers.
24. a) Discuss the complementary character of IR and Raman spectroscopies
    b) Discuss the application of Raman spectroscopy.
25. a) What is the most common reference compound used in NMR spectroscopy? Why is it advantageous to use it?
    b) How will you distinguish between 1-chloropropane and 2-chloropropane from their proton NMR spectra?

(2 × 10= 20)