STELLA MARIS COLLEGE (AUTONOMOUS), CHENNAI - 600 086

(For candidates admitted from the academic year 2015-16& thereafter)

SUBJECT CODE: 15CH/MC/SP64

B.Sc. DEGREE EXAMINATION, APRIL 2021 BRANCH IV – CHEMISTRY SIXTH SEMESTER

COURSE: MAJOR CORE PAPER: SPECTROSCOPY
TIME: 90 MINUTES MAX.MARKS: 50 SECTION -A
Answer all the questions $(15 \times 1 = 15 \text{ Marks})$
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I. Choose the correct answers
1. If the wavelength of a radiation is 2.85μ , then the corresponding wave number is a) 350.8cm^{-1} b) 3508cm^{-1} c) 402cm^{-1} d) 4028cm^{-1}
2. The number of signals observed in ¹³ C NMR decoupled spectrum of acetaldehyde is a) 2 b) 5 c) 1 d) 3
3. In mass spectrometer the energy required for the electron bombardment is in the range of e a) $1-5$ b) $20-30$ c) $10-15$ d) $50-60$
4. The solvent used in NMR technique is a) hexachloroacetone b) ethanol c) toluene d) tetramethylsilane
5. The selection rule for rotational – vibrational Raman spectra is a) $\Delta V = \pm 1$ and $\Delta J = 0$ b) $\Delta V = \pm 2$ and $\Delta J = 0, \pm 1$ c) $\Delta V = \pm 1$ and $\Delta J = 0, \pm 1$ d) $\Delta V = \pm 1$ and $\Delta J = \pm 1$
II. Fill in the blanks:
6. The number of waves which can pass through a point in one second is called
7. The C-O stretching frequency is for tertiary than primary alcohol
8. The zero point energy in vibrational spectroscopy is
9. The increase in λ_{max} values is called as shift
10. Karplus equation for $\phi = 0^{\circ}$ to 90° is
III. Answer in one or two lines:
11. What is NMR transition?
12. Define Nitrogen rule.
13. What is isosbestic point?
14. What is fermi resonance?

15. What is time-of-flight analyser?

SECTION - B

Answer any three of the following:

 $(3 \times 5 = 15 \text{ Marks})$

16. Discuss the fragmentation pattern and draw the mass spectrum for :

(i)
$$H_3C$$
 CH_3 (ii) CH_3 CH_3

17. Explain Franck - Condon principle.

18. Identify the chemical shift values and spin-spin coupling for the following compounds in 1 H NMR. (2 x 2 $\frac{1}{2}$ = 5 Marks)

(i)
$$H_3C$$
 (ii) H_3C

19a. Calculate the bond length of CO molecule, if it's first rotation spectrum line appears at

$$3.84 \times 10^2 \text{ m}^{-1}$$
 (Atomic weight of C = 12 a.m.u & O = 16 a.m.u) (3 Marks)

b. Compare the relative IR stretching frequencies for C-C, C=C and C≡C bonds. (2 Marks)

20. Explain the solvent and conjugation effects in UV-visible absorption bands.

SECTION - C

Answer any TWO of the following:

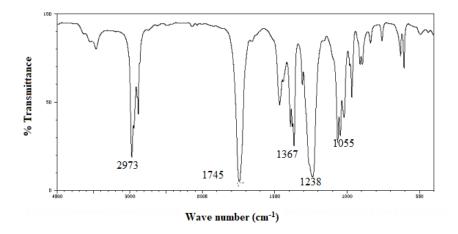
 $(2 \times 10 = 20 \text{ Marks})$

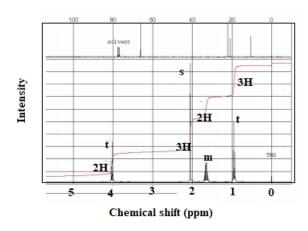
21a. Discuss the principle, instrumentation, sampling and solvents/ standards used in FTIR technique. (7 Marks)

b. Determine the λ_{max} values using Woodward-Fieser rule for the following :(2 x 1 ½ = 3 Marks)

$$(i) \\ H_2N \\ O \\ (ii) \\ H_3C \\ O$$

22a. The IR and 1 H NMR spectra of a compound with the molecular formula $C_{5}H_{10}O_{2}$ are provided below. Major mass spectra fragment peaks are also observed at m/z = 43, 60, and 73. Calculate the m/z for the molecular ion. Deduce the structure of the compound? (2+2+2+1=7 Marks)





b. What is coupling constant? Give its significance.

(3 Marks)

23a. Discuss Mclafferty rearrangement for the given compound:

(2 Marks)

b. What are Stokes and Antistokes lines. Explain.

(5 Marks)

c.The C-H stretching frequency is observed at 3000 cm⁻¹. Calculate the force constant of C-H bond. The atomic mass of C is 12.000 a.m.u and H is 1.008 a.m.u. (3 Marks)
