

M.Sc. CHEMISTRY
THIRD SEMESTER
APPLICATION OF SPECTROSCOPY-I
MSC – 304 [SPECIAL REPEAT]
[USE OMR FOR OBJECTIVE PART]

**SET
A**

Duration: 1:30 hrs.

Full Marks: 35

Time: 15 mins.

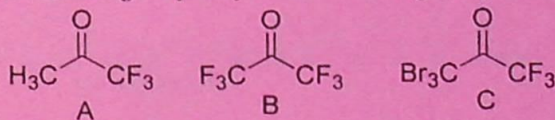
(Objective)

Marks: 10

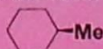
Choose the correct answer from the following:

1×10=10

- 'Stretching frequency is larger than bending frequency' the statement is
 - True
 - False
 - Not related
 - Ambiguous
- The correct order of the force constant (k) is
 - C-N > C≡N > C=N
 - C≡N > C=N > C-N
 - C≡N > C-N > C=N
 - C=N > C≡N > C-N
- The correct order of stretching frequency of the following compounds is

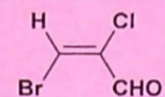


- A > B > C
 - B > A > C
 - A > C > B
 - B > C > A
- The characteristic IR peak of -OH is
 - Sharp and strong
 - Broad and strong
 - Sharp and weak
 - Broad and weak
 - The range of wavelength of the radiation used in FT-IR spectroscopy falls in the range
 - 0.5 to 0.7 μm
 - 2.5 to 25 μm
 - 2.5 to 50 μm
 - 1.5 to 2.5 μm
 - Which kind of nuclei is responsible for the generation of NMR signal?
 - Nuclei at the ground state
 - Nuclei at the higher state
 - excess nuclei at ground state
 - all the nuclei
 - The total number of ^1H NMR signals of the following molecule will be



- 5
- 6
- 7
- 8

8. If a ^1H NMR signal is of quintet type, the correct ratio of peaks will be
 a. 1:2:3:2:1
 b. 1:3:5:3:1
 c. 1:4:6:4:1
 d. 1:3:4:3:1
9. If a peak is of 'dd' type having the peak values 4.010 ppm, 4.014 ppm, 4.060 ppm, and 4.064 ppm in 200 MHz NMR machine. The J values will be
 a. 10 Hz, 0.6 Hz
 b. 8 Hz, 0.6 Hz
 c. 10 Hz, 0.8 Hz
 d. 8 Hz, 0.8 Hz
10. The type of J between the protons will be for the following molecule



- a. 1J
 b. 2J
 c. 3J
 d. 4J

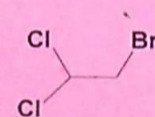
(Descriptive)

Time : 1 hr. 15 mins.

Marks : 25

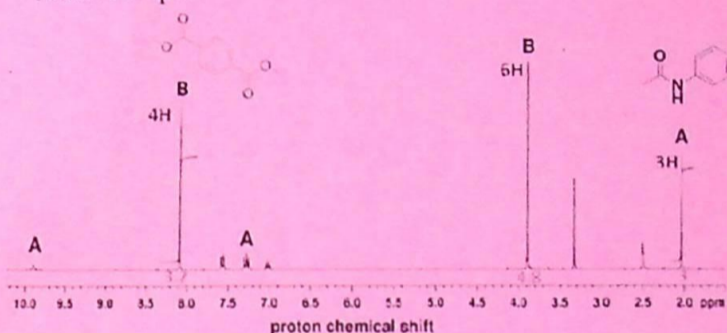
[Answer question no.1 & any two (2) from the rest]

1. a. Workout the spin arrangements and splitting patterns of the following molecule under the ^1H NMR study. 3



- b. Calculate the vibrational frequency of $-\text{C}=\text{C}-$ using Hooke's law in cm^{-1} . Given $K (-\text{C}=\text{C}-) = 10 \times 10^5$ dyne 2
2. a. Calculate the chemical shift value in ppm for a proton having resonance value 1280 Hz downfield from TMS on a spectrometer that operates at 200 MHz? 3+4+3 = 10

b. ^1H NMR spectrum of pure dimethyl terephthalate (B) has been obtained using 100% pure acetanilide (A) as a primary reference standard. The areas of the signals at 8.1 ppm (B) and 2.0 ppm (A) were used for purity calculation. Residual solvent peaks from DMSO- d_6 and water appear at 2.5 and 3.3 ppm, respectively. If the amount of A is of 10 mg what is the amount of B present in the NMR sample?

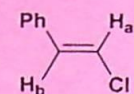


c. What is integration in ^1H NMR? Depict the probable ^1H NMR spectrum of ethyl acetate.

3. a. What is 3J -NMR coupling constant? Explain with example. Find out the coupling constant (J) value of the protons (H_a & H_b) for the given molecule. 4+4+2
= 10

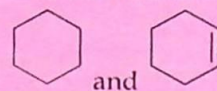
b. A proton of a given compound is showing a doublet peak in ^1H NMR with the peak values as 2.023 ppm and 2.063 ppm. The same NMR machine benzene protons resonate at 2880 Hz with peak value 7.2 ppm. What will be ^1H -NMR machine's frequency and coupling constant value of the proton showing doublet?

- c. Find the chemical shift value of the protons (Ha & Hb) of the given molecule. (Given: δ ppm [Ph_{gem} = 1.35; Ph_{cis} = 0.37; Ph_{trans} = -0.1; Cl_{gem} = 1.08; Cl_{cis} = 0.19; Cl_{trans} = 0.13])



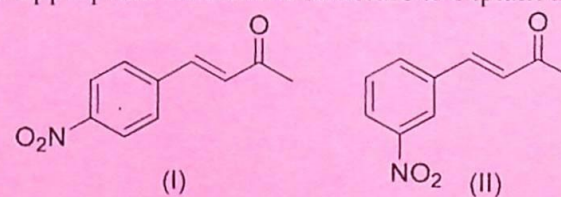
4. a. determine the number of fundamental vibrations in (i) CO₂ and (ii) NH₃
- b. Among CO₂, N₂, Cl₂ which one is IR active and why? Explain
- c. How will you differentiate *cis* and *trans* alkene through FT-IR spectroscopy? Explain with example.
- d. Arrange the following C-H bonds in order of their increasing strength of stretching frequencies \equiv C-H, =C-H, -C-H, and give explanation.
- e. Draw the possible FT-IR spectra of the following compounds and explain the differences

2+2+2
+2+2
=10

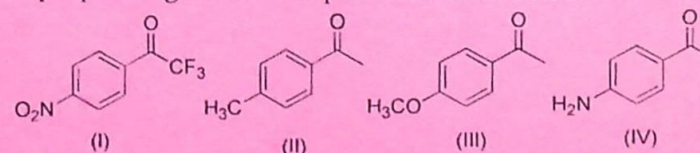


5. a. Which one of the following compounds show higher IR band? Draw the appropriate mesomeric structure to explain the facts.

2+3+3
+2=10



- b. Arrange the following compounds in increasing order of their carbonyl stretching frequencies. Support your explanation with proper diagrammatic representation in detail.



c. What are the three factors that affect vibrational frequency of a compound. Describe with suitable example.

d. Amongst Acetone, Acetophenone and o-Hydroxyacetophenone which one will exhibit highest carbonyl stretching frequency and why? explanation.

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