REV-01
MSC/32/37

2025/11

SET A

M.Sc. CHEMISTRY
THIRD SEMESTER
APPLICATION OF SPECTROSCOPY-I
MSC – 304

[USE OMR FOR OBJECTIVE PART]

Duration: 1:30 hrs. **Full Marks: 35**

Objective

Time: 15 mins. **Marks: 10**

Choose the correct answer from the following: ***1×10=10***

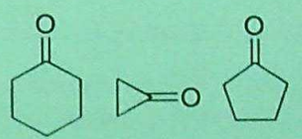
1. Which of the following molecules is IR active?
   a. N_2 b. O_2
   c. Cl_2 d. CO

2. The –OH functional group shows an IR absorption band at approximately
   a. 1600-1700 cm^{-1} b. 2100-2250 cm^{-1}
   c. 3200-3600 cm^{-1} d. 2800-2900 cm^{-1}

3. Which of the following bonds shows the highest stretching frequency in IR spectroscopy?
   a. C=C b. C=N
   c. C=O d. C≡N

4. 'The IR band of -C=C- stretching in trans-2-pentene is more intense than cis-2-pentene' – this statement is
   a. TRUE b. FALSE
   c. Invalid d. Not related

5. The correct order -C=O stretching frequency is



(a) (b) (c)

   a. a < c < b b. a < b < c
   c. c < a < b d. a < c < b

6. Protons in electron-rich environments appear
   a. Upfield b. Downfield
   c. At same δ always d. Broadened peaks

7. A compound gives the following ^1H NMR signals: δ 2.1 (3H, singlet), δ 7.3–7.8 (5H, multiplet). The compound is:
   a. Acetophenone
   b. Benzaldehyde
   c. 1,4-dimethyl benzene
   d. Ethylbenzene

8. According to the Karplus equation, the vicinal coupling constant (^3J) is minimum when the dihedral angle between two protons is approximately
   a. 0°
   b. 60°
   c. 90°
   d. 180°

9. Which methyl group shows a singlet at δ 2.1 ppm in ^1H NMR?
   a. CH_3–F
   b. CH_3–Cl
   c. CH_3–O–
   d. Aromatic –CH_3

10. Which of the following nuclei is *not* NMR active?
   a. ^1H
   b. ^{13}C
   c. ^{16}O
   d. ^{19}F

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Descriptive

Time : 1 hr. 15 mins. **Marks : 25**

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

1. **a.** Determine the stretching frequency of C-H and C-D bond, given force constant $K = 5 \times 10^{5}$ dyne/cm. 2+3=5

   b. What is shielding and deshielding in NMR?

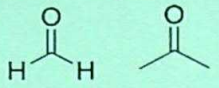
2. **a.** Determine the vibrational degrees of freedom for the following molecules 3+4+2+1 =10
   i. CH_3CHO,
   ii. CO_2,
   iii. NH_3

   b. Arrange the following bonds in order of their increasing vibrational stretching frequencies. Also, give reasons for the order observed.
   (i). C-I, (ii). C-Br, (iii). C-H, (iv). C-Cl, (v). C-D, (vi). C-C

c. What is the prerequisite for a molecule to respond in FT-IR spectroscopy?

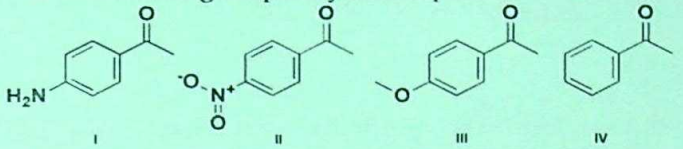
d. Why it is called Fourier-transform infrared (FT-IR) spectroscopy?

3. a. Which of the following molecule will show higher (-C=O) stretching frequency? Explain. **2+2+3+3 =10**



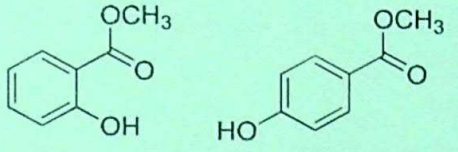
(i) (ii)

b. Arrange the following compounds in order of their increasing -C=O stretching frequency and explain



I II III IV

c. Based on the following two molecules how the dilution will affect the -C=O stretching frequency-Explain

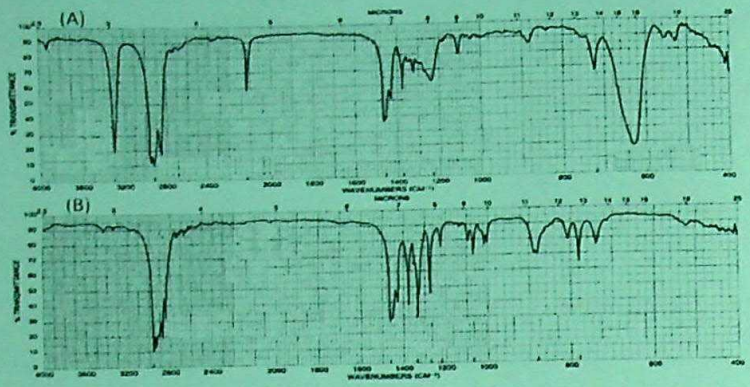


(i) (ii)

d. The FTIR spectra of two isomeric compounds having the molecular formula C_8H_{14} are shown below. Each compound contains one carbon–carbon double bond.

(i) Propose the probable structures corresponding to Spectrum A and Spectrum B.

(ii) Provide a detailed justification for your assignments based on the characteristic IR absorption bands observed in each



spectrum.

4. **a.** How to calculate the coupling constant (J)if the chemical shift of the two peaks of a doublet is 2.516 and 2.535 ppm, and if the NMR was taken at a 300 MHz instrument. **2+2+2+2 +2=10**

b. Why N,N-dimethylformamide (DMF) show two different signals for the methyl group?

c. How can you distinguish methylbenzene and methoxybenzene by ^{1}H-NMR?

d. What is a chiral shift reagent?

e. Why is TMS chosen as an internal standard in NMR?

5. **a.** Both ethyl acetate (CH_3-$COOCH_2CH_3$) and methyl propionate (CH_3-CH_2-$COOCH_3$) have the formula $C_4H_8O_2$. Describe how ^{1}H NMR could distinguish between them. **3+3+2+2 =10**

b. Why is chemical shift measured in ppm?

c. Draw a molecule in which adoublet of doublet (dd) pattern is present.

d. How can you distinguish between ethanol and dimethyl ether using ^{1}H NMR spectroscopy?

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