2026

M.Sc. 2nd Semester Examination

CHEMISTRY

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Paper : CEMC454X0

(Advanced Spectroscopic Techniques for Structure and Property)

Full Marks : 50 Time : Two Hours

The figures in the margin indicate full marks.
Candidates are required to give their answers in their own words as far as practicable.

Group - A

Answer any ***four*** questions : 2×4=8

1. What is Karplus equation? Show the plot of spin-spin coupling constant *vs* dihedral angle.
2. What is the difference between a base peak and a molecular ion peak in Mass spectroscopy?
3. What is spin-spin coupling?
4. Which reference compound is used for NMR in D_2O? Write its structure.
5. What is chemical exchange in NMR Spectroscopy? Explain with an example.

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6. Arrange the compounds containing Fe(0), Fe(I) and Fe(II) and Fe(III) in order of decreasing isomer shift values in Mössbauer spectra.

Group - B

Answer any ***four*** questions : 4×4=16

7. Isomeric esters D and E have the composition $C_{11}H_{12}O_4$. Spectral data are summarized below : Deduce the structures of D and E and rationalize your answer.

   Compound D: δ 8.49(t, J = 2Hz, 1H), 8.05 (d, J=2Hz, 2H), 2.46 (s, 3H), 3.94 (s, 6H);

   Compound E: δ 8.52(d, J = 2Hz, 1H), 8.00 (dd, J=8, 8Hz, 1H), 7.28 (d, J=8 Hz, 1H), 3.91 (s, 6H), 2.63 (s, 3H).

8. Compound A having the molecular formula $C_6H_{10}O_2$ shows the following spectral data :

   FTIR (cm^{-1}) : 1695

   ^{1}H-NMR(δ) :6.95 (dq, J_1 = 16 Hz and J_2=6.8 Hz, 1H, 5.81 (dq, J_1 = 16Hz, and J_2=1.7 Hz, 1H), 1.88 (dd, J_1=6.8 Hz and J_2=1.7 Hz, 3H), 4.13 (q, J=7 Hz, 2H) and 1.24(t, J=7 Hz, 3H).

   Mass Spectra (important peaks, m/z) : 114 (M+), 69 (base peak) and 41 (w)

   Suggest a probable structure.

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9. A and B are two isomer having molecular formula $C_9H_{10}O_2$. Deduce the structure of the isomers (A & B) with the help of given FTIR and ^{1}H NMR data :

   For isomer A: FTIR:1680 cm^{-1}; ^{1}H NMR (δ):7.6 (d, 2H), 6.9 (d, 2H), 3.9 (s, 3H), 2.0 (s, 3H).

   For isomer B: FTIR:1740 cm^{-1}; ^{1}H NMR (δ):7.2 (s, 5H), 5.0 (s, 2H), 1.98 (s, 3H).

10. Compound C ($C_8H_{12}O_4$) shows the following ^{1}H NMR spectral data :

    ^{1}H-NMR (δ):6.80 (s, 2H), 4.25 (q, J=7 Hz, 4H), 1.30 (t, J = 7 Hz, 6H).

    Suggest a possible structure.

11. An organic compound having molecular formula C_5H_8O shows following spectral data

    UV – Vis – λ_{max} (ETOH) = 277nm, ε_{max} = 4600

    IR (cm^{-1}) 3020, 1685.

    ^{1}H NMR δ (ppm) : 6.2(d, J =17 Hz, 1H), 5.4(m, J =17 Hz, 1H), 2.3 (s, 3H), 1.9 (d, 3H).

    Draw the structure of the compound.

12. Discuss on "nuclear decay scheme" for ^{57}Fe Mössbaur resonance

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P.T.O.

Or,

Explain the Mössbauer spectra of $Na_2[Fe(CN)_5(NO)]$

Group - C

Answer any *two* questions : 8×2=16

13. (a) (i) What is the McLafferty rearrangement in the mass spectral fragmentation of organic compounds?

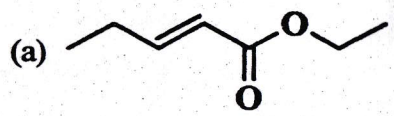
(ii) Give examples.

(iii) Using appropriate deuterium labeled compound prove that in *McLafferty rearrangement* always γ-hydrogen transfer takes place.

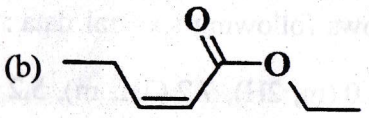
(b) In the Mass spectrum of an unknown organic compound, a base peak is obtained at m/z = 91. What kind of molecules can give such a peak? Show the mechanism of its formation. 4×2=8

14. (a) An organic compound having molecular formula ($C_7H_{12}O_2$) exhibits following ^1H NMR data-δ (ppm):

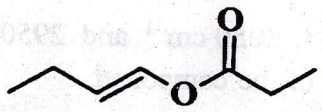
7.10 (dt, J_1=16 Hz, J_2=7.2 Hz, 1H) 5.90 (dt, J_1=16 Hz, J_2=2 Hz, 1H), 4.1 (q, J=7.2 Hz, 2H), 2.10 (m, 2H), 1.25 (t, J=7.2 Hz, 3H), 0.90 (t, J=7.2 Hz, 3H).

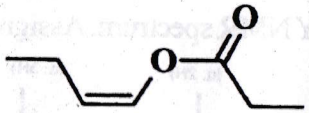
(a) 

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(b) 

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(c) 

(d) 

Identify the correct structure with justification.

(b) A organic compound having molecular formula ($C_9H_{10}O_2$) exhibits following spectral data-FTIR (cm^{-1}) = 1690;

^1H NMR-δ (ppm): 7.8(d, J=8 Hz, 2H), 6.9(d, J=8 Hz, 2H), 3.8 (s, 3H), 2.5 (s, 3H).

^{13}C NMR-δ (ppm): 197, 165, 130, 129, 114, 56, 26.

Suggest a suitable structure. 4×2=8

15. (a) An organic compound having molecular formula $C_9H_8O_2$ shows following spectral data :

^1H NMR-δ :12.7(brs, 1H), 7.8 (d, J=18 Hz, 1H), 7.56 (m, 5H), 6.45(d, J=18 Hz, 1H), IR-1680 cm^{-1}, 2520-3070 cm^{-1} (broad). Draw the structure of the compound.

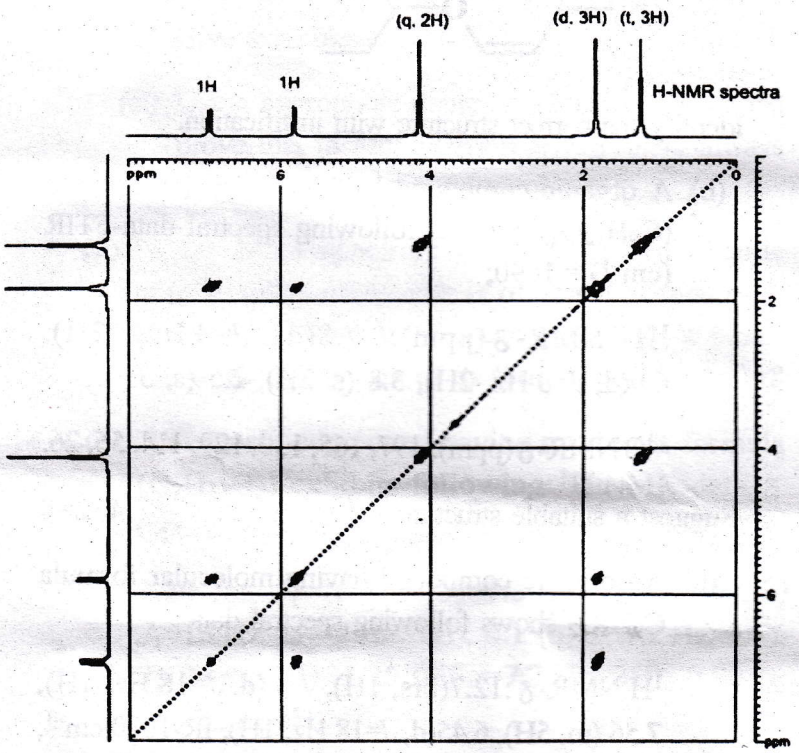
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(b) An organic compound having molecular formula $C_{10}H_{12}O_2$ shows following spectral data :

^1H NMR-δ:8.0 (m, 2H), 7.2 (3H, m), 5.2 (m, 1H), 1.3 (d, 6H)

IR-1730 cm^{-1}, 3050 cm^{-1} and 2950 cm^{-1}. Draw the structure of the compound. 4×2=8

16. A compound having molecular formula $C_6H_{10}O_2$ shows the following 2D COSY NMR spectrum. Assign the structure.



[Internal Assessment : 10 marks]

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