Chemistry (P.G.)

[CBCS]

M.Sc. Fourth Semester End Examination-2024

(Regular & Supplementary Paper)

PAPER- CEM 401

Advanced Spectroscopy-II (Common Paper)

Full Marks: 40 ***Time: 02 Hrs***

The figures in the right hand margin indicate marks

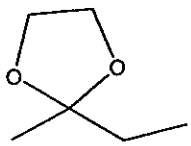
Candidates are required to give their answers in their own words as far as practicable

Illustrate the answers wherever necessary

Group-A

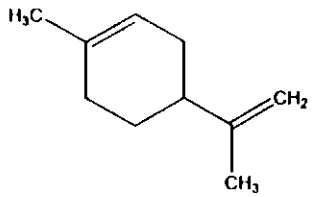
Answer **any four** of the following question 4x2=8

1. Two lines of a doublet in 400 MHz ^{1}H NMR spectrum appear at 2.32 and 2.36 ppm. Calculate the coupling constant.
2. Explain mathematically the difference between specific and molar ellipticity.
3. Write down some significant criteria of sample preparation for CD.
4. Explain the following m/z value in mass spectroscopy



m/z = 116, 101, 87 and 43

5. Assign the mass spectral peak of the following molecule and mention the base peak with explanation



6. Which property makes one nuclei NMR active? Give examples of one NMR active and one NMR inactive nuclei.

7. A compound of molecular formula C_6H_8 show only two types of signals in the ^1H NMR spectra. Identify the compound.

8. What is McLafferty rearrangement?

Group-B

Answer **any four** of the following question 4x8 = 32

9. a). An organic compound having molecular formula $C_4H_6O_2$ shows a very strong IR band at 1720 cm^{-1} and only one singlet signal in its 1H NMR spectra. Draw the structure of the compound.

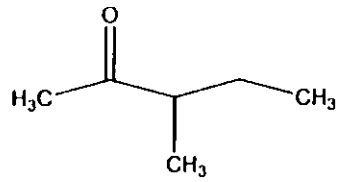
   b). Describe the process of Chemical Ionization process used in mass spectroscopy and explain with a suitable example. 3+5 = 8

10. a). What is positive and negative Cotton effect? Explain graphically with CD and ORD curve.

   b). What does the term molar ellipticity mean in CD? Write down its mathematical expression. (2+2)+(2+2) = 8

11. a). How could you differentiate the following isomeric pair by mass spectrometry

i)



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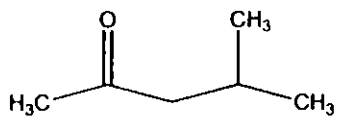
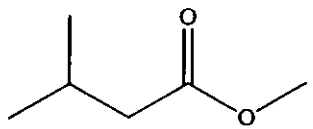


ii)



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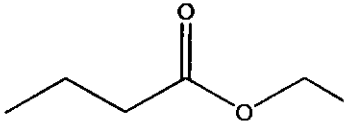


   b). The structure of the compound which displays the following spectral data is

   IR: 1690, 1000 cm^{-1}

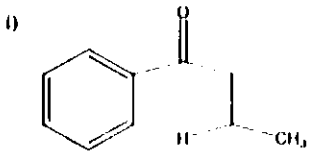
   ^1H NMR: $\delta_{7.8}$ (d, J=8 Hz, 2H), 6.9 (d, J= 8 Hz, 2H), 3.8 (s, 3H), 2.8 (s, 3H)

   ^{13}C NMR: δ_{197}, 165, 130, 129, 114, 56, 26. (2+2)+4=8

12. a). The mass spectrum of 3-butyn-2-ol shows a large peak at m/z = 55. Draw the structure of the fragment and explain why it particularly stable?

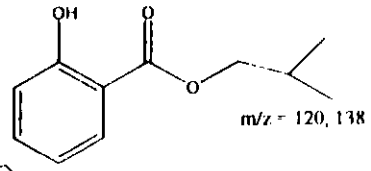
b). Explain the following m/z value in mass spectroscopy indicating base peak (any two)

i)



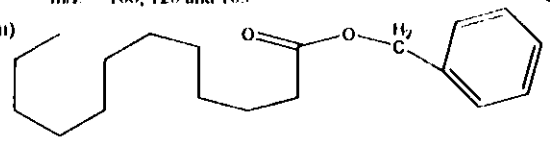
m/z = 106, 120 and 105

iii)



m/z = 120, 138

ii)



m/z = 91, 108, 183

3+2.5X2=8

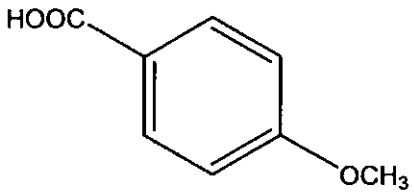
13. a). The compound having molecular formula $C_5H_7NO_2$ shows the following data. Predict the structure of the compound

IR peaks : 2260, 1747 and 1200 cm^{-1}.

^{1}HNMR : $^{\delta}$ppm 4.3(2H, q), 1.3(3H, t) and 3.5(2H, s)

^{13}CNMR : $^{\delta}$ 113, 163, 63, 25 and 14 ppm

b). Explain the following m/z value in mass spectroscopy indicating base peak



m/z = 152, 135 and 107

5+3=8

14. a). Describe the principal of spin-spin splitting origin.

b) What is NOE? Explain it by taking a suitable example. 4+4 =8

15. a). Deduce the structure of compound based on the following data:

Molecular formula: $C_6H_{10}O_2$.

IR (cm^{-1}): 3000, 1735

^{1}H-NMR (δ ppm): 6.97(dq., J = 6.8 & 15.2 Hz, 1H); 5.83(d, J = 15.2 Hz, 1H); 4.17 (q, J = 7.2 Hz, 2H); 1.87 (d, J = 6.8 Hz, 3H); 1.27 (t, J = 7.2 Hz, 3H)

^{13}C-NMR (δppm) : 170, 144, 123, 60, 18, 14.

b). Explain how plane polarised light differs from circularly polarised light.

c). What is the significance of circular birefringence in CD?

4+2+2 = 8
