Group C

Answer any two bits: 8x2=16

13. (a) Predict the structure of the organic compound which exhibits m/e peaks at 86, 71, 58, 43 (100%) in mass spectrum.

(b) A compound with molecular formula $C_9H_5NO_4$ shows the following bands in its infrared spectrum.

3000-2500 (b), 2225 (m), 1715 (s), 1605, 1518 (s), 1344 (s) and 900-700 cm-1 (s).

In NMR spectrum two bands are formed as (i) 1.1τ (singlet, 5.3 squares) and (ii) unsymmetrical pattern 2.6-2.75τ (21.1 squares). Determine the structural formula of the compound. 3+5

14. Explain the observations.

(i) In the mass spectrum of 3-methylpentane the base peak appears at m/z 57 along with a very small peak at m/z 71, whereas in case of 2-methylpentane the base peak appears at m/z 43 along with a large peak at m/z 71 and a small peak at m/z 57. 4

(ii) In the mass spectrum of cinnamaldehyde, base peak appears at m/z 131 along with a very prominent peak at m/z 103 and m/z 77. 4

15. (i) Calculate the chemical shift in ppm (δ) for a proton that has resonance at 126 Hz downfield from TMS on spectrophotometer that operates at 60 MHz. 3

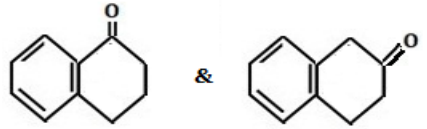
(ii) An organic compound with molecular weight 108 is not acidic in nature but can be easily oxidized to a crystalline compound (melting point 122°C). It gives the following spectral data:

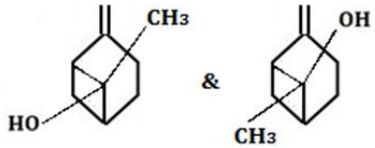
UV: λmax 255 mμ, εmax 202

IR: 3402 (s, b) 3065 (w), 2288 (m), 1499 (w), and 1455 cm-1 (m)

NMR: 2.74τ (singlet, 24.5 squares), 5.4τ (singlet, 9.5 squares), and 6.10τ (singlet, 4.8 squares). Identify the compound. 5

16. How will you differentiate the following pairs by NMR spectroscopy?

(i)  &

(ii) 

(iii) *Cis*-stilbene and *trans*-stilbene. (3+3+2)

2024

M.Sc.

4th Semester Examination

CHEMISTRY

PAPER – CEM-401

Full Marks: 50

Time : 2 Hours

(CEM 401-Advanced Spectroscopy-II)

Group A

Answer any ***four*** bits: 2×4 = 8

1. Why is TMS used as standard for ^1H NMR?
2. What is precessional frequency?
3. What do you mean by Coupling constant?
4. What is Chemical shift?
5. Show the fragmentation pattern of cyclopentanol.
6. Why is vacuum needed in mass spectrometry?

Group B

Answer any ***four*** bits: 4×4 = 16

7. Why is it necessary for a nucleus to behave as a tiny magnet to be studied by NMR spectroscopy?
8. Write down the different ionization methods used in organic mass spectrometry. Explain in detail any one of them.
9. How will you distinguish three isomeric butanols on the basis of mass spectrometry?
10. A compound with molecular formula, $C_6H_{12}O_2$ shows four signals: (i) singlet 1.1 δ (6H), (ii) singlet 2.1 δ (3H), (iii) singlet 2.6 δ (2H), and (iv) singlet 3.9 δ (1H). Propose a structure consistent with the given data. (4)
11. (i) How is CD spectra helpful to understand drug-DNA interaction? (ii) What is the man difference between CD and UV spectroscopy? 2+2
12. Write a short note on McLafferty rearrangement.

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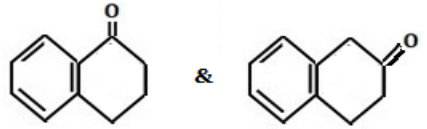
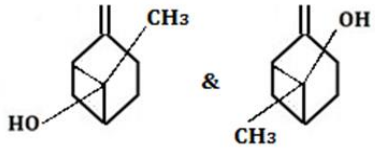
(i)  &

(ii) 

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