2023

M.Sc.

4th Semester Examination

CHEMISTRY

PAPER – CEM-401

Full Marks: 50

Time : 2 Hours

(CEM 401-Advanced Spectroscopy-II)

1. Answer any ***four*** bits: 2×4 = 8

(a) What do you mean by local diamagnetic effect?

(b) What is Chemical shift?

(c) Show the fragmentation pattern of cyclopentanol.

(d) Write down the main principle of CD spectroscopy.

(e) What is precessional orbit?

(f) What is called resolution (R) in mass spectrometry?

2. Answer any ***four*** bits: 4×4 = 16

(a) 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)

(b) Predict the structure of the organic compound which exhibits m/e peaks at 86, 71, 58, 43 (100%) in mass spectrum. (4)

(c) How will you distinguish three isomeric butanols on the basis of mass spectrometry? (4)

(d) Write down the different ionization methods used in organic mass spectrometry. Explain in detail any one of them. (4)

(e) Explain diamagnetic anisotropy with example. (4)

(f) (i) Why is it necessary for a nucleus to behave as a tiny magnet to be studied by NMR spectroscopy? (ii) 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. (2+2)

3. Answer any ***two*** questions 2×8 = 16

(a) (i) In the mass spectrum of n-butylbenzene the base peak appears at *m/z* 91 along with a large peak at *m/z* 92 and a small peak at *m/z* 65. Explain the observation.

(ii) 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)

(b) (i) Why is it necessary for a nucleus to behave as a tiny magnet to be studied by NMR spectroscopy?

(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: λ_{max} 255 mμ, ε_{max} 202

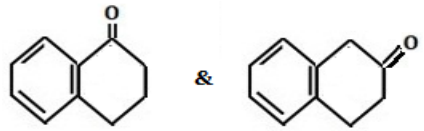
IR: 3402 (s, b) 3065 (w), 2288 (m), 1499 (w), and 1455 cm^{-1} (m)

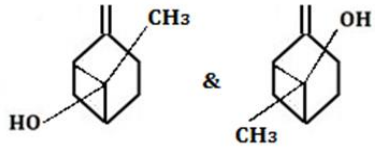
NMR: 2.74τ (singlet, 24.5 squares), 5.4τ (singlet, 9.5 squares), and 6.10τ (singlet, 4.8 squares).Predict the structure of the compound. (2+6)

(c) (i) Write a short note on McLafferty rearrangement.

(ii)How can you distinguish between 1-propanol and 2-propanol by mass spectrometry? (4+4)

(d) How will you differentiate the following pairs by NMR spectroscopy?

(i)  &

(ii) 

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

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Internal Assessment-10

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(Turn over)

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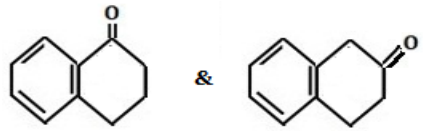
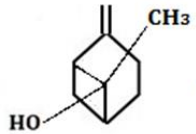
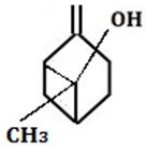
(i)  &

(ii)  &



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