2018

M.Sc. 4th Semester Examination

CHEMISTRY

PAPER-CEM-403

Subject Code-24

Full Marks: 40

Time: 2 Hours

The figures in the margin indicate full marks.

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

Illustrate the answers wherever necessary.

(Organic)

Group-A

Answer any four questions.

2×4

- A compound of molecular formula C₆H₈ show only two types of signals in the ¹H NMR spectra. Identify the compound.
- 2. Compound of molecular formula $C_7H_7NO_2$ shows the following absorption in the ¹H NMR spectra. Identify the compound. δ 8.1 (d, J = 5.8 Hz, 2H), 7.3 (d, J = 5.8 Hz, 2H), 2.45 (s, 3H).

(Turn Over)

3. Isomeric esters D and E have the composition C₁₁H₁₂O₄. Spectral data are summarized below: Deduce the structure of D and E and rationalized your answer.

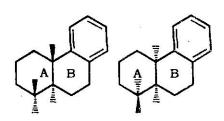
Compound D: δ 8.49 (t, J = 2 Hz, 1H), 8.05 (d, J = 2 Hz, 2H), 3.94 (s, 6H), 2.46 (s, 3H);

Compound E: δ 8.52 (d, J = 2 Hz, 1H), 8.00 (dd, J_1 = 8 Hz, J_2 = 2 Hz, 1H), 7.28 (d, J = 8 Hz, 1H), 3.91 (s, 6H), 2.63 (s, 3H).

4. A organic compound having molecular formula $(C_7H_{12}O_2)$ exhibit 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).

5. A organic compound having molecular formula $(C_9H_{10}O_2)$ exhibit following spectral data- FTIR (cm^{-1}) = 1690; ¹H MMR $-\delta$ (ppm); 7.8 (d, J = 8 Hz, 2H); 6.9 (d, J = 8 Hz, 2H), 3.8 (s, 3H), 2.5 (s, 3H); 13C MMR $-\delta$ (ppm): 197, 165, 130, 129, 114, 56, 26.

6. Distinguish the following pairs of compound by ¹H NMR spectroscopy



- 7. Distinguish the following compound by Mass spectroscopy:
 Cyclopropane and n-propane.
- 8. Deduce the structures of the compounds exhibiting the following data:

Molecular formula:

 $C_{12}H_{15}O_2N$, ¹H NMR d (ppm) : 8.0 (d, J = 12.3 Hz, 1H), 7.7 (d, J = 8.0 Hz, 2H) 6.8 (d, J = 8.0 Hz, 2H), 5.8 (d, J = 12.3 Hz, 1H), 3.8 (s, 3H), 3.0 (s, 6H) ppm.

Group-B

Answer any four questions.

4×4

9. A and B are two isomer having molecular formula C₉H₁₀O₂, deduced the structure of the isomers (A & B) with the help of given FTIR and ¹H NMR data:

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

For isomer B: FTIR: 1740 cm^{-1} , ¹H NMR δ (ppm): 7.2 (s, 5H), 5.0 (s, 2H), 1,98 (s, 3H).

10. Deduce the structures of the compounds exhibiting the following data:

Molecular formula: C9H10O

FTIR: 1710 cm⁻¹

¹H NMR & (ppm): 2.1 (s, 3H), 3,6 (s, 2H), 7.3 (s, 5H)

- 11. Calculate the Doppler velocity corresponding to the natural line width of γ -ray emission from 14,400 ev excited state of 57 Fe nucleus having a half-life of 9.78×10^{-8} s.
- 12. What are the essential characteristics which a nuclide must possess in order to exhibit Mössbauer effect?
- 13. Explain recoilles emission and absorption of γ -rays.
- 14. Discuss the differences between CD and ORD.
- Explain the nature of the absorption and CD spectra of adenine and guanine.
- Distinguish Z-DNA and B-DNA conformations applying CD-spectroscopic study.

Group-C

Answer any two questions.

2×8

17. (a) An organic compound having molecular formula (C₁₀H₁₂O₂) exhibit following spectral data:

FTIR (cm⁻¹) = 3400, 1600; ¹H NMR δ (ppm) 6.90 (d, J = 8 Hz, 1H), 6.8 (s, 1H), 6.75 (s, 1H), 2.5 (d, J = 8 Hz, 3H), 6.28 (d, J = 18 Hz, 1H), 6.0 (dq, 1H, J₁ = 18 Hz J₂ = 6 Hz), 5.0 (s, 1H, show D₂O expt.), 3.8 (s, 3H), 1.85 (d, J = 6 Hz, 3H); ¹³C NMR - d (ppm): 146.5, 144.0, 131, 130.5, 123, 119, 114, 108, 55, 18.

(b) In the following compound marked carbon atom shows 13°C NMR data given below:

(ii)
$$a = 52$$
, $b = 143$, $c = 167$, $d = 125$, $e = 19$

(iii)
$$a = 52$$
, $b = 167$, $c = 143$, $d = 125$, $e = 19$

(iv)
$$a = 52$$
, $b = 167$, $c = 125$, $d = 143$, $e = 19$

18. (a) Identify the correct structure of the compound, which shows the following 13 C NMR data DEPT 135-Negative peaks at δ = 30.2, 31.9, 61.9, 114.7 ppm and positive peak at δ 130.4 ppm.

(b) A C₉H₁₀O₂ compound shows two strong band infrared absorption bands at 1690 and 1100 cm⁻¹. It's ¹H NMR spectra shows sharp singlet peaks at δ 2.8 and 3.8 ppm (3H each) and two doublets at δ 6.9 and 7.8 ppm (2H each). The ¹³C NMR spectrum shows seven lines. Suggest a structure for this compound.

19. Explain the Mössbauer spectra of

- (i) FeSO₄ . 7H₂O
- (ii) K₄[Fe(CN)₆].

4+4

- (a) Write down the expression for specific and molar ellipticity.
 - (b) How can you determine the the a and b sheet of a protein by CD spectrometry.
 - (c) What do you mean by left handed circularly polarize light and right handed circulary polarize light.

2+3+3