বিদ্যাসাগর বিশ্ববিদ্যালয়

VIDYASAGAR UNIVERSITY

M.Sc. Examinations 2020
Semester IV
Subject: CHEMISTRY
Paper: CEM – 401
(Organic, Inorganic and Physical Special)

(Theory)

Full Marks:40 **Time: 2hrs.**

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

The questions are of equal value. Candidates are requested to give their answer in their own words (limit: 250 words) as far as practicable.

Answer any one of the following questions :

1. (a) What is Karplus equation?

   (b) (i) Two lines of a doublet in 400 MHz ^{1}H-NMR spectrum appear at 2.32 and 2.36 ppm. Calculate the coupling constant. (ii) What will be the separation (in ppm) between the two lines in 200 MHz and 800 MHz ^{1}H-NMR?

   (c) Show qualitatively how a complex NMR spectrum recorded in a lower magnetic field can be simplified in a higher magnetic field.

2. Write the basic principle of of NMR. Show the schematic diagram of a NMR spectrometer.

3. (a) What is the difference between a base peak and a molecular ion peak in Mass spectroscopy?

   (b) What is NMR shift reagent? Give an example and explain the mechanism of its activity.

   (c) Which reference compound is used for NMR in D_2O.? Write its structure.

(d) What is spin-spin coupling?

4. (a) An organic compound having molecular formula $C_9H_8O_2$ shows following spectral data ^{1}H nmr- δ (12.7, 1H, brs); δ (7.8, 1H, d, J=18 Hz); δ (7.56, 5H, m); δ (6.45, 1H, d, J=18 Hz), IR- 1680 cm^{-1}, 2520-3070 cm^{-1} (broad). Draw the structure of the compound.

   (b) An organic compound having molecular formula $C_{10}H_{12}O_2$ shows following spectral data ^{1}H nmr- δ (8.0, 2H, m); δ (7.2, 3H, m); δ (5.2, 1H, m); δ (1.3, 6H, d), IR- 1730 cm^{-1}, 3050 cm^{-1} and 2950 cm^{-1}. Draw the structure of the compound.

5. (a) An organic compound having molecular formula C_5H_8O shows following spectral data ^{1}H nmr- δ (6.2, 1H, d, J = 18 Hz); δ (5.4, 1H, m, J = 17 Hz); δ (2.3, 3H, s); δ (1.9, 3H, d), IR- 1685 cm^{-1}, 3020 cm^{-1}, UV-VIS- λ_{max}(ETOH)= 277 nm, ε_{max}= 4600. Draw the structure of the compound.

   (b) 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 ^{1}H nmr spectra. Draw the structure of the compound.

6. (a) An organic compound having molecular formula $C_6H_{12}O$ shows a very strong IR band at 1705 cm^{-1} and two singlet signal in its ^{1}H nmr spectra at δ (2.1, 3H, s); δ (1.2, 9H, s); Draw the structure of the compound.

   (b) An organic compound having molecular formula $C_5H_{12}O$ shows ^{1}H nmr spectra at δ (2.1, 3H, s); δ (1.1, 9H, s). Draw the structure of the compound.

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

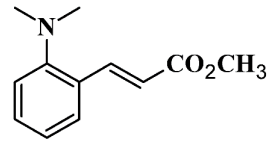
   For **isomer A** FTIR: 1680 cm^{-1} ^{1}HNMR(δ): 7.6(2H,d), 6.9(2H,d), 3.9(3H,s), 2.0(3H,s).

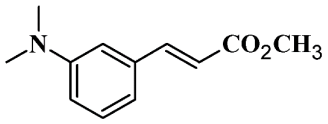
   For **isomer B** FTIR: 1740 cm^{-1} ^{1}HNMR(δ): 7.2(5H,m), 5.0(2H,s), 1.98(3H,s).

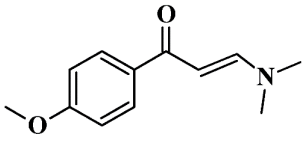
   (b) Deduce the structures of the compounds exhibiting the following data :

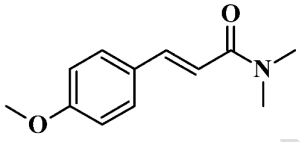
   Molecular formula: $C_{12}H_{15}O_2N$

   1H NMR: 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

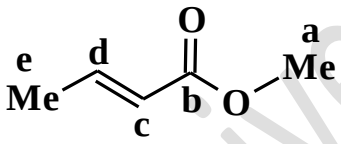
1 

2 

3 

4 

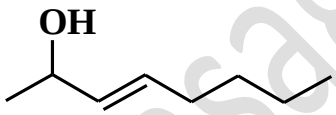
8. (i) Which of the following option is correct regarding the δ value in ^{13}C NMR of the marked carbon-

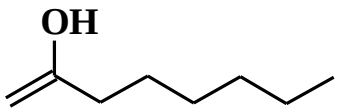


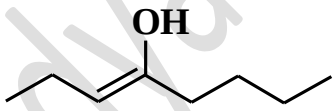
(a) a = 19, b = 143, c = 167, d = 125, e = 52 (b) a = 52, b = 143, c = 167, d = 125, e = 19

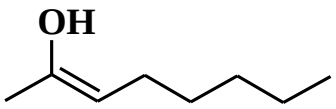
(c) a = 52, b = 167, c = 143, d = 125, e = 19 (d) a = 52, b = 167, c = 125, d = 143, e = 19

(ii) A compound show DEPT 135 show 3 negative peak at δ value 30.12, 29.1, 32.1, and show 5 positive peak at δ value 128, 122, 60.1, 19.2, 18.1

(a) 

(b) 

(c) 

(d) 

9. Write the basic principle Electron Ionization Mass Spectrometer. Show a schematic diagram of a Mass Spectrometer.

10. Compare and contrast CD and ORD.

11. Write notes on spin-spin and spin-lattice relaxation. How do these relaxations affect the intensity and shape of a NMR peak?

12. Write short notes on CD spectroscopy.