Enrollment No. _____

Shree Manibhai Virani and Smt. Navalben Virani Science College (Autonomous)

Affiliated to Saurashtra University, Rajkot

SEMESTER END EXAMINATION APRIL – 2017

M. Sc. Chemistry

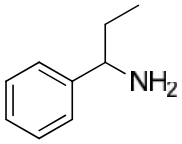
16PCECC08 – INTERPRETATIVE MOLECULAR SPECTROSCOPY (SSC)

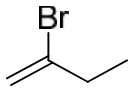
Duration of Exam – 3 hrs ***Semester – II*** ***Max. Marks – 70***

<u>Part A</u> (5x2= 10 marks)

Answer **<u>ALL</u>** questions

1. Enlist the IR absorption wavenumbers for C=O in acid, ketone, aldehyde, ester, anhydride and amide.
2. Differentiate 1-propanol and 2-propanol by CMR spectroscopy.
3. Identify the types of protons in the following compounds:

i) 

ii) 

4. Calculate the chemical shift value of C_1 and C_2 carbon of 1-hexene.
5. Indicate the number of signals and multiplicity off-resonance decoupled ^{13}C NMR spectra of the following compounds:
   i) 2-bromopropane
   ii) Ethylbenzene

<u>Part B</u> (5X5= 25 marks)

Answer **<u>ALL</u>** questions

6a. Calculate the chemical shift value of carbon of following compounds:
   i) 3-bromotoluene ii) p-xylene

OR

6b. Calculate the chemical shift value of carbon of following compounds:
   i) 1-hexene ii) 4-bromobenzaldehyde

7a. Differentiate 1-aminopropane and 2-aminopropane by PMR spectroscopy.

OR

7b. Differentiate 2-pentanone and 3-pentanone by PMR spectroscopy.

8a. How will you distinguish the following pairs of compounds on the basis of IR spectroscopy?
   i) o-nitrophenol, m-nitrophenol and p-nitrophenol
   ii) CH_3COOH and CH_3COCl

OR

8b. How will you distinguish the following pairs of compounds on the basis of IR spectroscopy?
   i) ortho, meta and pera-xylene
   ii) Benzyl alcohol and anisole

9a Deduce the structure of compound from the given analytical data.

MW: 264 g/mol
Elements: C-36.3%, H-3.1%, Br-60.6%,
NMR: a/singlet/20.0 square/7.4 δppm, b/triplet/20.5 square/3.6 δppm

OR

9b Deduce the structure of compound from the given analytical data.

MW: 102 g/mol
Elements: C-70.5%, H-13.72%.
NMR: a/triplet/6H/9.0 τppm, b/quintet/4H/8.5 τppm, c/multiplet/1H/7.8 τppm
d/doublet/2H/6.1 τppm, e/singlet/1H/5.5 τppm

10a Deduce the structure of compound from the given analytical data.

MW: 158 g/mol
Elements: C-60.8%, H-8.8%.
IR: 2910(m), 1830(s), 1750(s), 1410(m), 1385(s), 1365(s), 1225(s), 710(m) cm^{-1}
NMR: a/Septate/2H/2.73 δppm,
b/doublet/12H/1.20 δppm.

OR

10b Deduce the structure of compound from the given analytical data.

MF: $C_{12}H_{16}O_2$
IR: 3040, 2960, 2880, 1740, 1610, 1585, 1470, 1445, 1230,1030, 970, 760, 710 cm^{-1}
NMR: a/singlet/6H/1.0 δppm,
b/singlet/2H/2.8 δppm, c/singlet/3H/3.8 δppm, d/multiplet/5H/7.5 δppm

<u>Part C</u> (5X7= 35 marks)

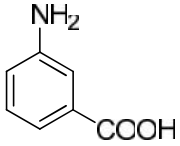
Answer **<u>ALL</u>** questions

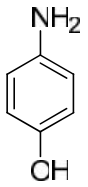
11a. Calculate the chemical shift value of carbon of following compounds:
i) 2-flouropentane ii) 3-bromopentane iii) 4-chloroaniline

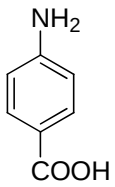
OR

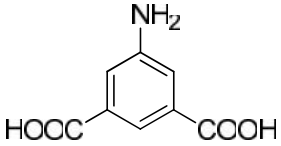
11b. Calculate the chemical shift value of carbon of following compounds:
i) 3-methylpentane ii) 3-nitrobenzoic acid iii) 2-chlorobenzaldehyde

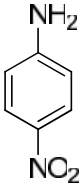
12a. Acetylation of following compounds were carried out with acetic anhydride in the presence of catalytic amount of Con. H_2SO_4.

i) 

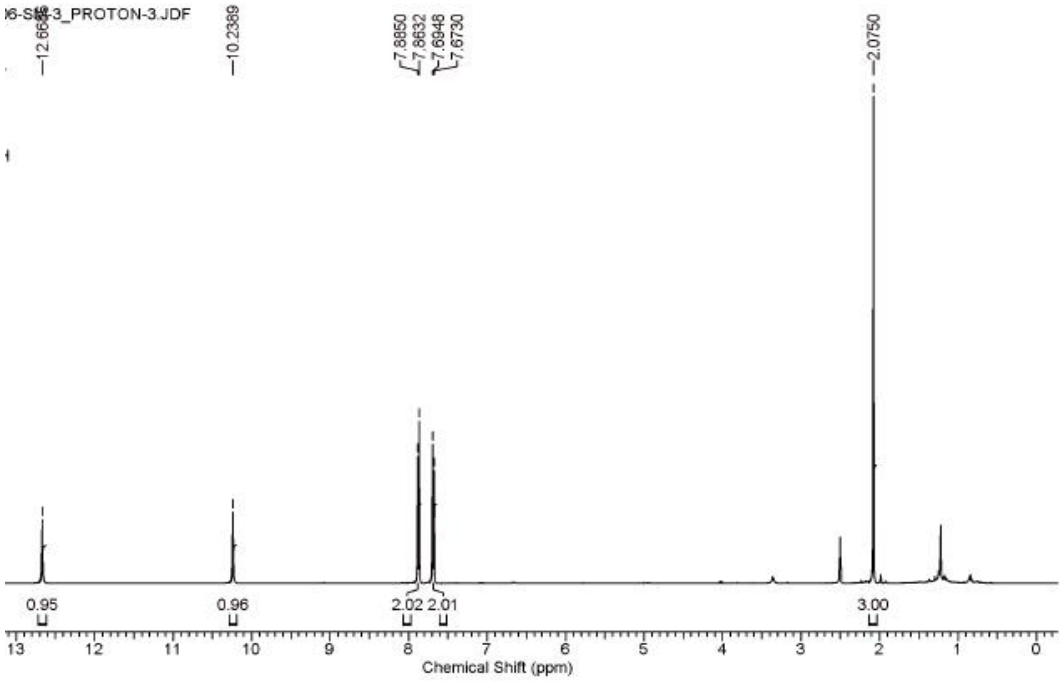
ii) 

iii) 

iv) 

v) 

Among them one of the product ^1H NMR spectrum is given below. Identify the product and interpret it.

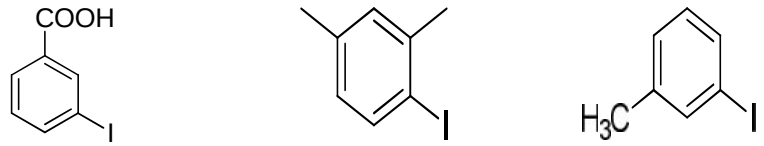


(^{1}H NMR 400 MHz)

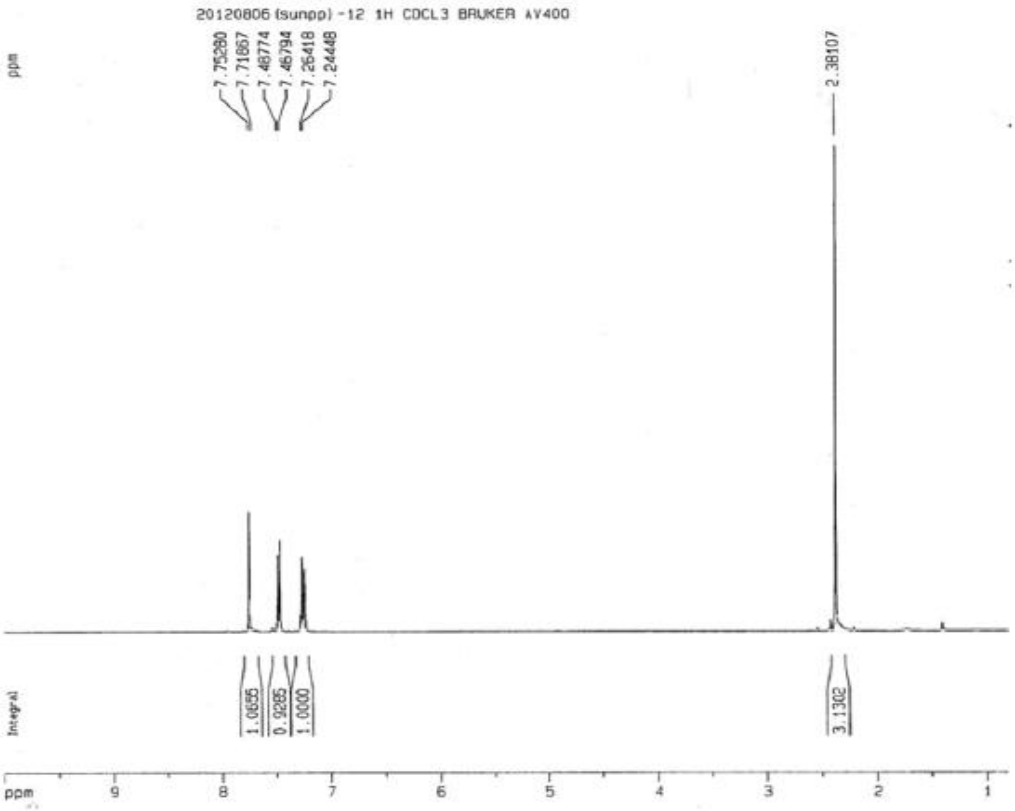
OR

12b. The Cyanation of following compounds were carried out with ethyl cyanoacetate in the presence of palladium catalyst.

i) ii) iii)



Among them one of the product ^{1}H NMR (400 MHz) spectrum is given below. Identify the product and interpret it.



13a. Deduce the structure of compound from the given spectral data.

MF: $C_{10}H_{10}O$
IR: 3030, 2950, 1710, 1480, 1380, 750 and 700 cm^{-1}
PMR: (a/singlet/3H/7.8 τppm), (b/doublet/1H/3.8 τppm/*J* = 16.5 *Hz),* (c/doublet/1H/3.2 τppm/*J* =16.5 *Hz*), (d/multiplet/5H/2.2-2.8 τppm),
CMR (Proton noise decoupled): 8 signals

OR

13b. An organic compound with MF: $C_{10}H_{14}O$ furnished the following spectral data:

UV: 277 nm.
IR: 3520, 3020, 2960, 2875, 1622, 1458, 1383, 1385, 1222, 852 and 804 cm^{-1}
PMR: δ 1.2 (6H, d), 2.2 (3H, s), 3.2 (1H, m), 4.2 (1H, s), 6.6 (1H, dd, *J* = 8 Hz), 6.9 (1H, dd, *J* = 8 Hz) and 7.2 (1H, dd, *J* = 2Hz).
CMR (Off-resonance decoupled): Three singlet, four doublet and two quartet.
Deduce the structure of the compound and explain the spectral data.

14a. Deduce the structure of compound from the given spectral data.

MF: $C_9H_{11}NO$
IR: 3430, 3030, 2975, 1700, 1612, 1550, 1422, 1325, 1380 and 830 cm^{-1}
PMR: (a/singlet/3H/2.8 δ ppm), (b/singlet/3H/3.0 δ ppm), (c/multiplet/4H/6.7-7.7 δ ppm/*J* = 8 *Hz*), (d/singlet/1H/9.7 δppm),
CMR (Proton noise decoupled): 7 signals

OR

14b. An organic compound having molecular weight 174 g/mol gave following spectral data:

MF: $C_{11}H_{13}NO$
IR: 3010, 2950, 2920, 2850, 2750, 1690, 1380, 1140 and 810 cm^{-1}
NMR: δ 2.9 (6H, s), 6.4 (1H, dd, *J* = 16 Hz), 6.8 (1H, d, *J* = 16 Hz), 7.2-7.4 (2H, d, *J* = 9 Hz), 7.7-7.9 (2H, d, *J* = 9 Hz) and 9.3 (1H, d).
Deduce the structure of the compound and explain the spectral data.

15a. Deduce the structure of compound from the given spectral data.

MF: C_4H_6O
IR: 3010, 2950, 2860, 1790, 1690, 1550, 1440, 1380, 1010, 970 and 930 cm^{-1}
PMR: (a/doublet/3H/1.5 δ ppm), (b/multiplet/1H/6.0-6.2 δ ppm/ *J* = 9 Hz),
(c/double doublet/1H/6.7-6.9 δ ppm/*J* = 9 *Hz*), (d/doublet/1H/9.5 δppm),
CMR (Off-resonance decoupled): one quartet and three doublet.
MS: Prominent peaks at m/e 70, 69, 44, 41 and 29

OR

15b. A compound containing C, H, O and Cl shows a strong IR absorption band near 1720 cm^{-1} and a near 3200 cm^{-1}. Its PMR spectrum displays two triplets at δ 2.8 and 3.8 and a singlet at δ 12 in the intensity ratio 2: 2: 1, respectively. Deduce the structure of the compound.