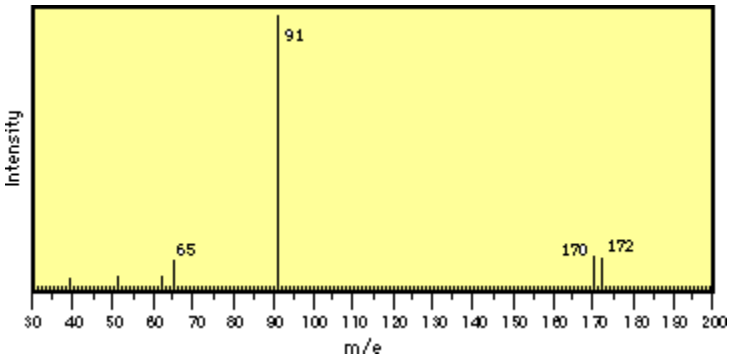
CHAPTER 12&13- (MS, IR, NMR -Practice Exercises) CHEM 2425

Dr. Pahlavan / Dr. Cherif / Dr. Dessens

1. The mass spectrum an benzylhalide (haloalkyl bezene) is given:



a) Identify the parent peak

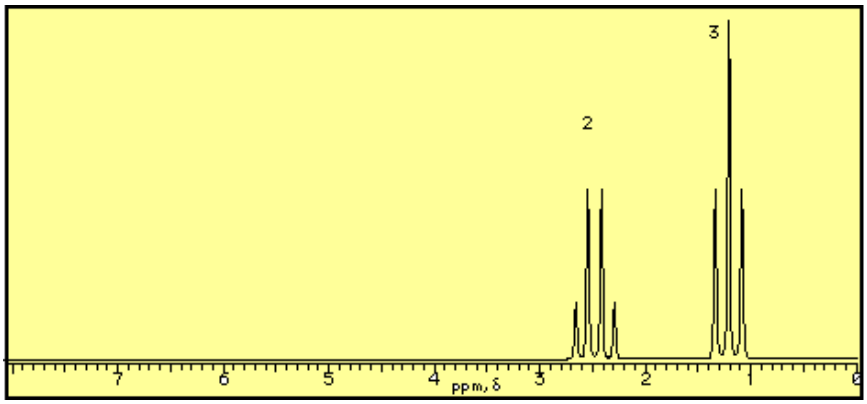
b) Identify the base peak

c) Determine the possible structure for the compound

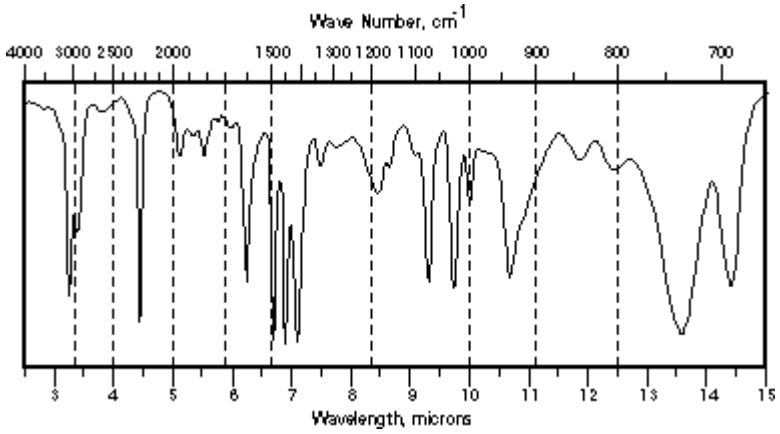
d) What is the molecular structure for the most stable cation fragment (most intense peak)

2. Give several types of spectroscopic data **IR, ^{1}H NMR**, and **MS** of particular compounds. What are they?

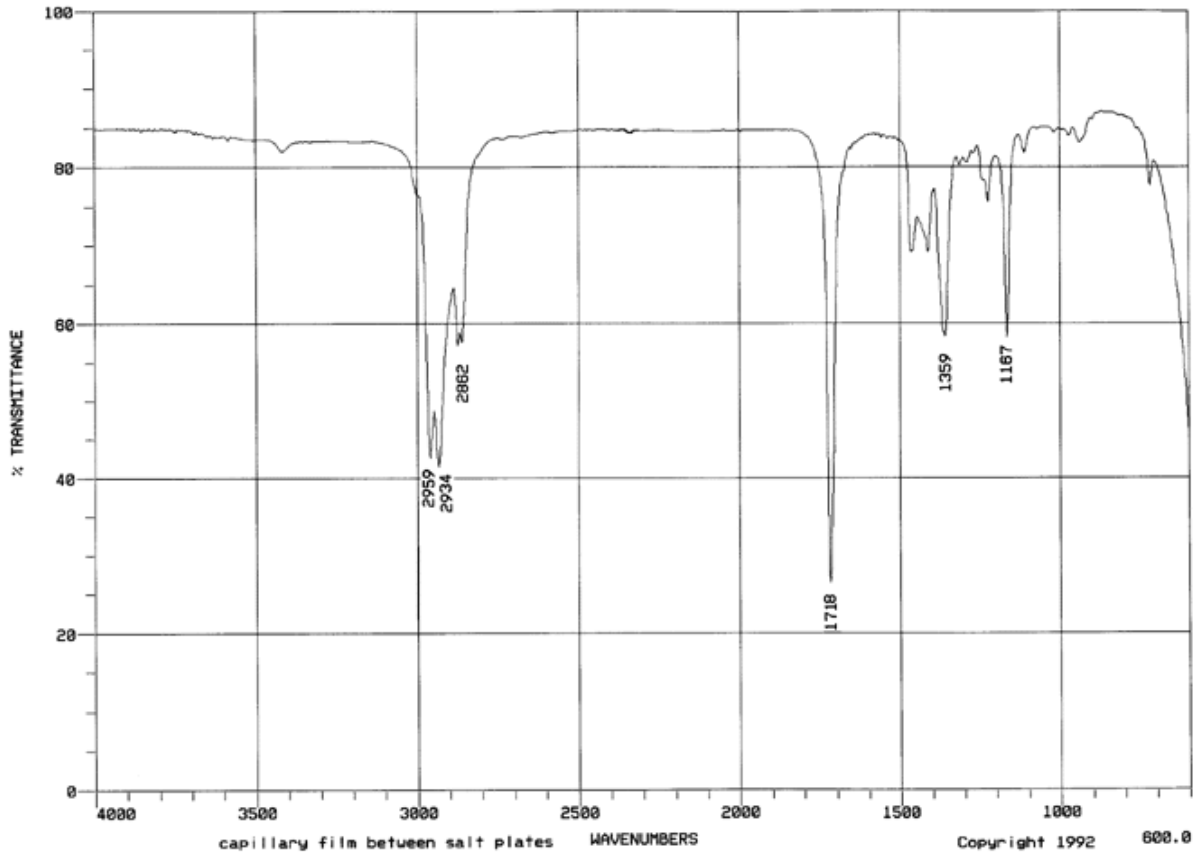
a) **$C_5H_{10}O$**

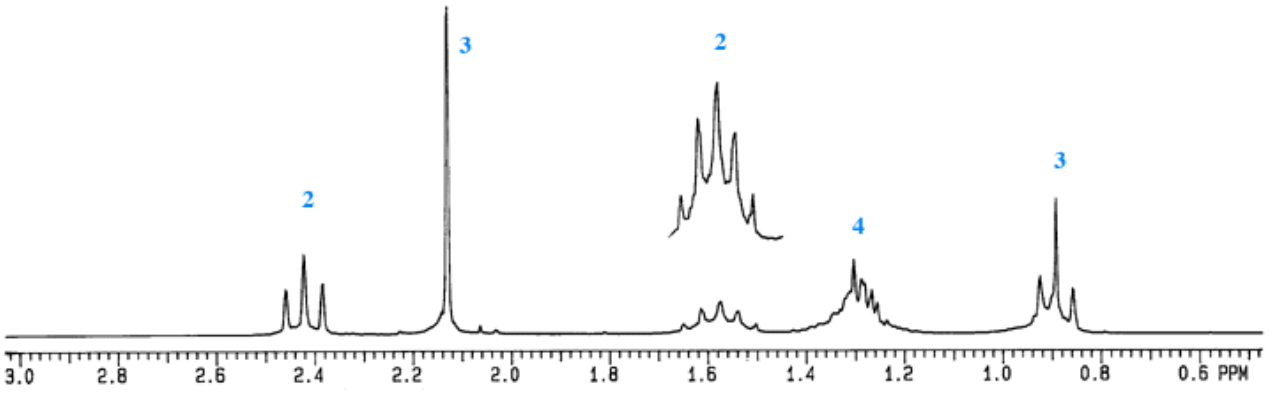


b) C_8H_7N



c) $C_7H_{14}O$





3 . Each of the following compounds is characterized by a single 1H NMR spectrum that consists of only a single peak having the chemical shift. Identify each compound.

a) **C_8H_{18}** ; δ 0.9 ppm b) **C_4H_9Br** ; δ 1.8 ppm

4. Each of the following compounds is characterized by a single ^{1}H NMR spectrum that consists of two peaks, both singlets, having the chemical shifts indicated. Identify each compound.

a) **C_6H_8** ; δ 2.7 ppm (4H) and 5.6 ppm (4H)

b) **$C_6H_{10}O_2$**; δ 2.2 ppm (6H) and 2.7 ppm (4H)

5. Deduce the structure of each of the following compounds in the basis of their ^{1}H NMR spectral and molecular formula.

a) **C_8H_{10}** δ 1.2 ppm (triplet, 3H)
δ 2.6 ppm (quarter, 2 H)
δ 7.1 ppm (broad singlet, 5H)

b) **$C_4H_6Cl_4$** δ 3.9 ppm (doublet, 4H)
δ 4.6 ppm (triplet. 2H)

6. How many different types of hydrogens (in different environments) are there in the following compounds?

a) 1- chloropropane b) 2,2-dimethylpropane c) phenol d) 2-chloropropane
d) 2- chloropropene e) cis-1, 3-dichloropropene f) (E)-1,3-dibromopropene.

7. An unknown compound having molecular formula **C_4H_8O** exhibits the following IR and H NMR data. Give the structure of this compound based on these spectra, indicating the salient features of each spectrum.

IR: 1710 cm^{-1} (strong, single band)

^{1}H NMR : δ 1.0 (broad, t , 3H), δ 2.1 (broad, s, 3H) , δ 2.5 (qt., 2H)

8. Propose a structure that is consistent with the following spectral data.

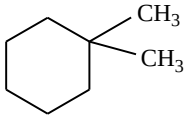
MS: M^+ at m/z = 73

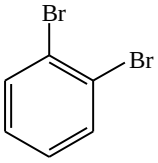
IR: 3350 cm^{-1} (weak, single band)

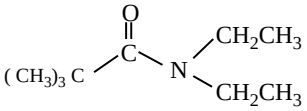
^{1}H NMR : δ 1.05 (broad, s , 1 H), δ 1.15 (t, 6 H) , δ 2.65 (qt., 4H)

9. The mass spectrum of a hydrocarbon shows a molecular ion at m/z =182, and the 1 H NMR spectrum has two signals. δ 2.9 (singlet, 4 H), δ 7.2 (singlet, 10 H). Propose a structure for this compound.

10. For each compound below, tell how many types of nonequivalent protons there are.

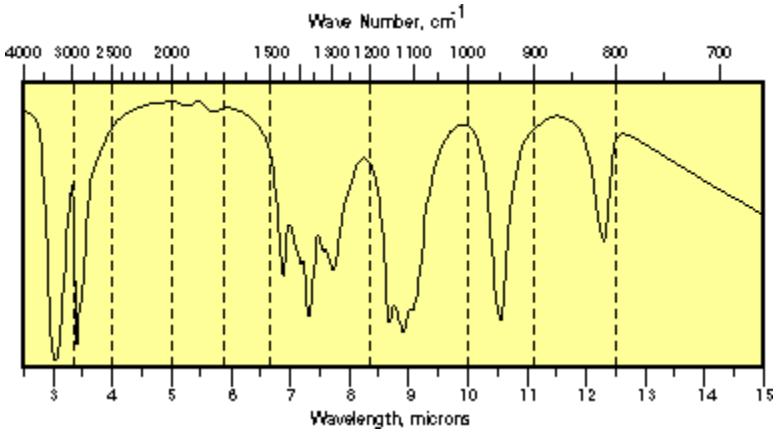
a) 

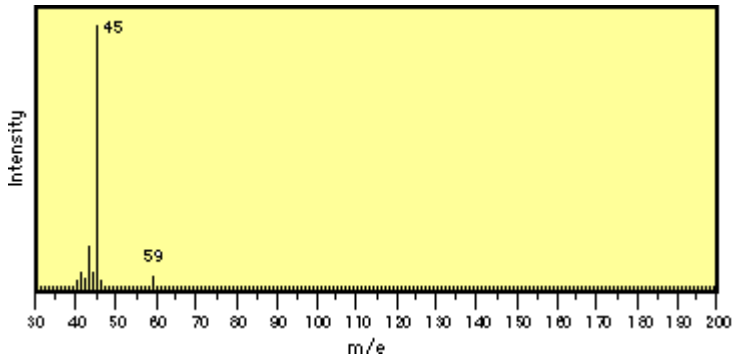
b) 

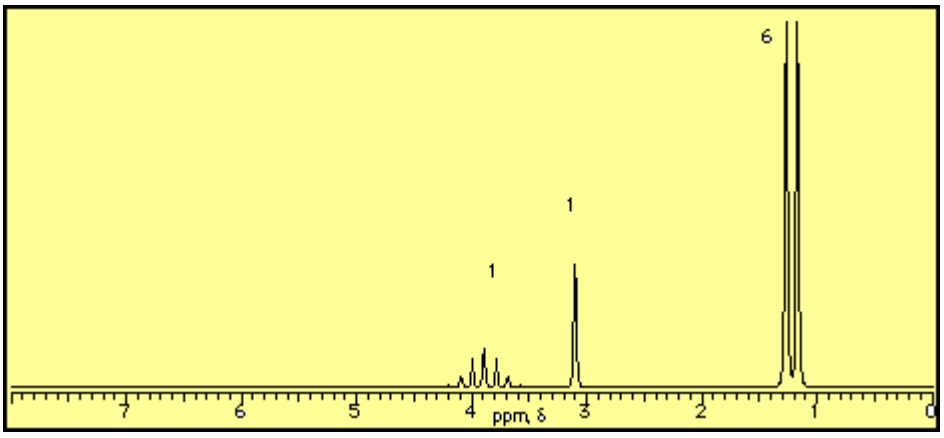
c) 

11. Cyclohexane and 2-hexene both have molecular formula **C_6H_{10}**. How would you use infrared spectroscopy to distinguish between the two compounds? Please explain your answer.

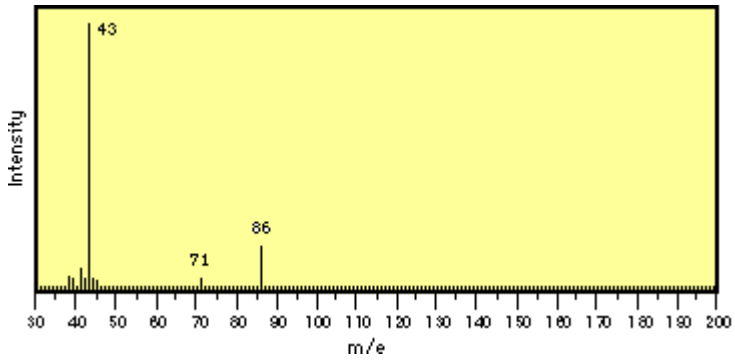
12.The molecular formula for an unknown compound is **C_xH_yO(MW = 60)**. Data for the ^{1}H NMR, infrared and mass spectra for this compound are shown below. Using the spectral and analytical information provided, determine the structure for this compound.

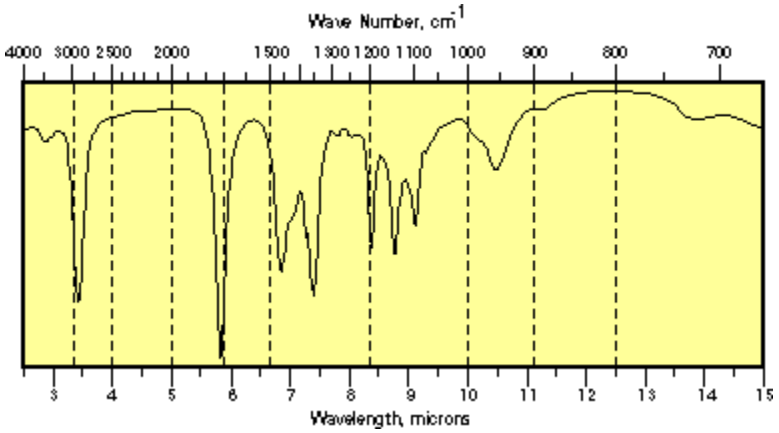


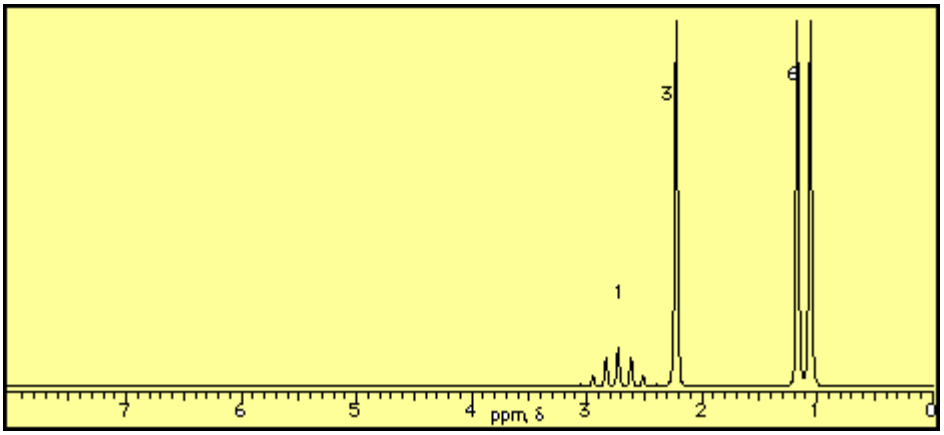




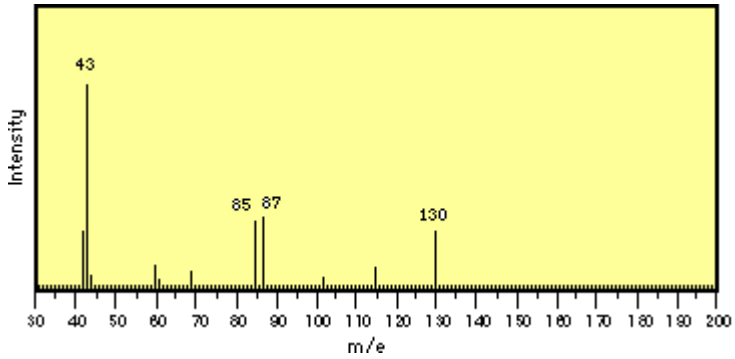
13. The molecular formula for an unknown compound is **C_xH_yO**. Data for the ^{1}H NMR, infrared and mass spectra for this compound are shown below. Using the spectral and analytical information provided, determine the structure for this compound.

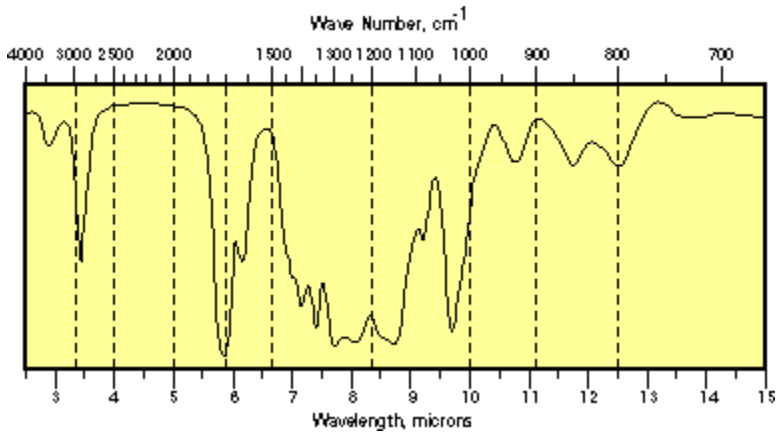


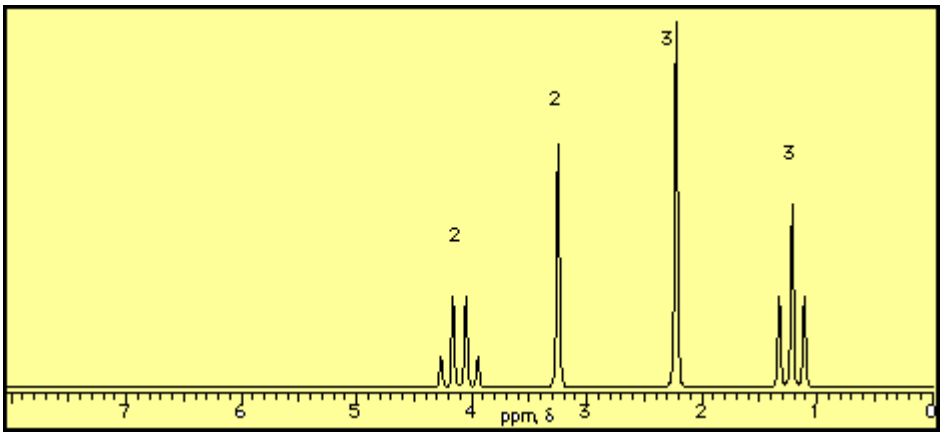




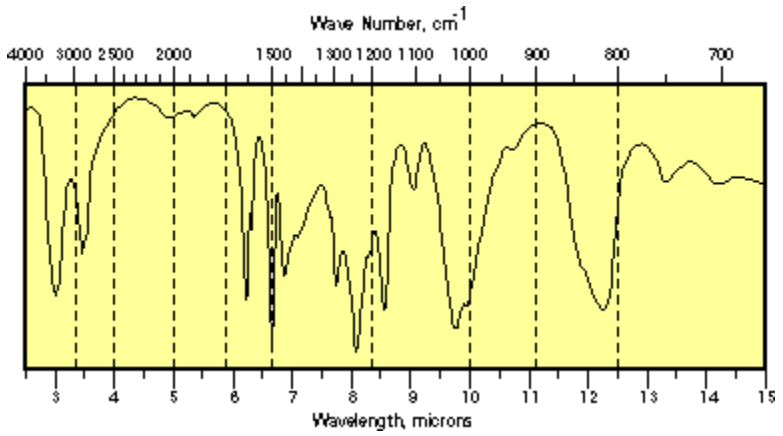
14. The molecular formula for an unknown compound is $\mathbf{C_xH_yO_3}$. Data for the ^{1}H NMR, infrared and mass spectra for this compound are shown below. Using the spectral and analytical information provided, determine the structure for this compound.

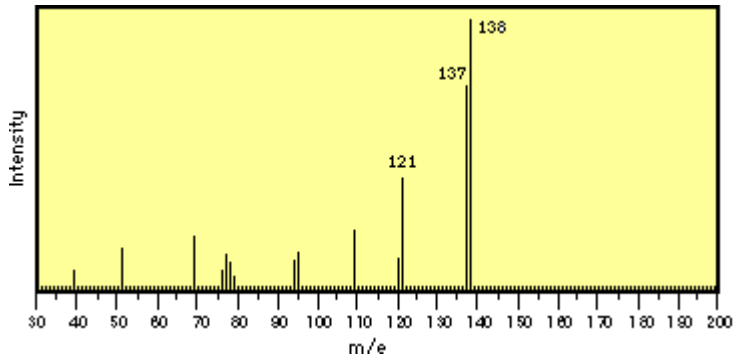


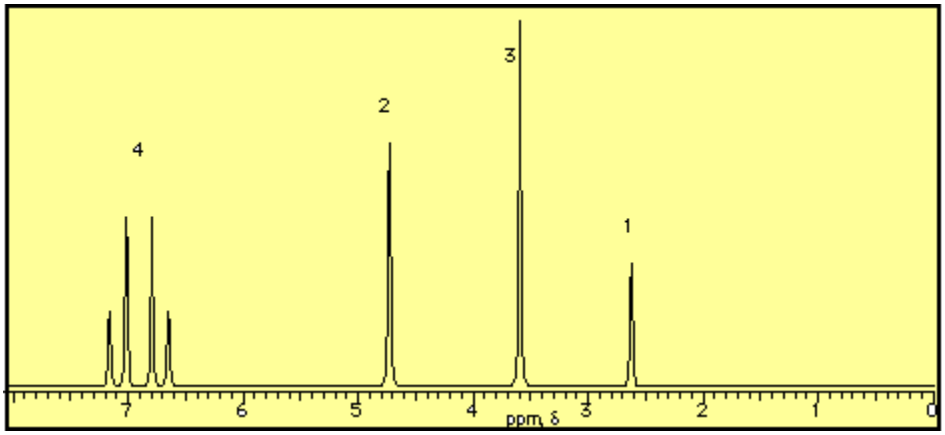




15. The molecular formula for an unknown compound is $\mathbf{C_xH_yO_2}$. Data for the ^{1}H NMR, infrared and mass spectra for this compound are shown below. Using the spectral and analytical information provided, determine the structure for this compound.







ANSWERS

CHAPTER 12&13- (MS, IR, NMR -Practice Exercises) CHEM 2425

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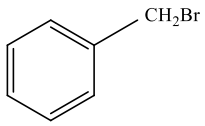
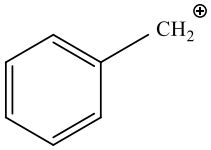
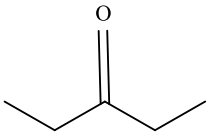
1. a) m/e = 172 b) m/e = 91 c) d)



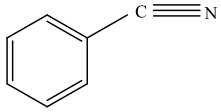


2. a) $C_5H_{10}O$ ➔ D.U. = 5 – 10/2 +1 = 1 (db) carbonyl group (C = O)



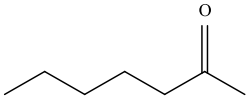
3-Pentanone or Diethylpentane

b) C_8H_7N ➔ D.U. = 7 – 7/2 + 1/2 + 1 = 6 (1 benzene ring , 1 tb)



Benzylhydride

c) $C_7H_{14}O$ ➔ D.U. = 7 – 14/2 +1 = (carbonyl group C = O)

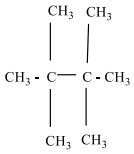


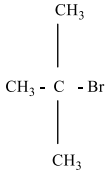
2- Heptanone or pentylmethyl ketone

3. a) C_8H_{18} D.U. = 8 – 18/2 + 1 = 0 (single bond) ➔ $(CH_3)_3$ C – C $(CH_3)_3$

b) C_4H_9Br D.U. = 4 – 9/2 - 1 /2 + 1 = 0 (single bond) ➔ $(CH_3)_3$ C – Br

a) 2,2,3,3 - Tetramethyl butane b) t – Butyl bromide

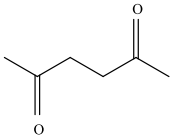




4. a) C_6H_8 D.U. = 6 – 8/2 + 1 = 3 (two types protons)

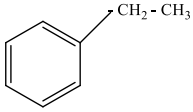
b) $C_6H_{10}Br_2$ D.U. = 6 – 10/2 + 1 = 2 (two double bonds)

a) 1,4- Cyclohexadiene b) 2,5 – Heptadiene



5. a) C_8H_{10} D.U. = 8 – 10/2 + 1 = 4 (Benzene ring)

b) $C_4H_6Cl_4$ D.U. = 4 – 6/2 - 4/2 + 1 = 0 (single bond)

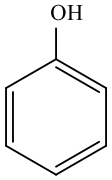


$CH_2Cl – CHCl – CH Cl – CH_2Cl$

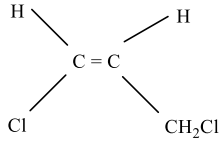
6.

a) $CH_3 – CH_2 - CH_2 – Cl$ (3 types H's) b) $CH_3 – C (CH_3)_2 – CH_3$ (1 types H's)

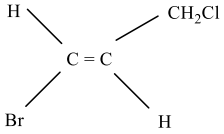
c) (4 types H's) d) $CH_3 – CHCl- CH_3$ (2 types H's) e) $CH_3 – CCl = CH_2$ (2 types H's)



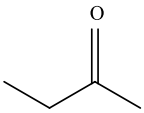
f) (3 types H,s)



g) (3 types H,s)

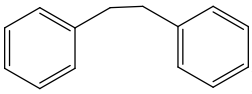


7. C_4H_8O D.U. = 4 – 8/2 + 1 = 1 (db bond , carbonyl group, C=O, 1710 cm^{-1})

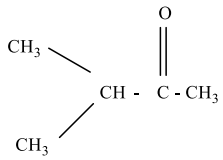


2 – Butanone or Ethylmethyl ketone

8. MS: m/z = 77 ➔ 77 -14 = 59 ➔ 59/12 = 6 C , 10 H , 1 N ➔ $C_4H_{10}N$
   D.U. = 4 – 10/2 +1 = 0
   IR : 3350 cm-1 ➔ amine C – N ➔ $CH_3 – CH_2 – NH – CH_2 – CH_3$ Diethylamine
9. m/e = 182 ➔ 182/12 = 14 C , 14 H ➔ $C_{14}H_{14}$ ➔ D.U. = 14 – 14/2 + 1 = 8 (2 benzene ring)

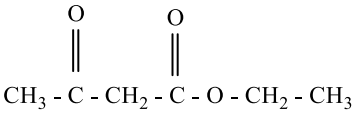

Diethylbenzene

10. a) 2 b) 2 c)
11. Use IR ➔ IR : cyclohexane 3000 – 3100 cm^{-1} and IR: 2 – Hexene 1640 – 1680 cm^{-1}
12. CxHyO (MW = 60) ➔ 60 – 16 = 44 ➔ 44/12 = 3 C , 8H , 1 O ➔ C_3H_8O
    D.U. = 3 – 8/2 +1 = 0 (single bond)
    IR 3100 cm^{-1} ➔ -OH group, ➔ $CH_3 – CHOH – CH_3$ 2 – propanol , isopropyl alcohol , isopropanol
13. CxHyO (MW = 86) ➔ 86 – 16 = 70 ➔ 70/12 = 5 C , 10H , 1 O ➔ $C_5H_{10}O$
    D.U. = 5 - 10/2 +1 = 1 (db, carbonyl group C=O, 1710 cm^{-1})



3-Methyl-2-butanone or isopropylmethyl ketone

14. $C_xH_yO_3$ (MW = 130) ➔ 130 – 48 = 82 ➔ 82/12 = 6 C , 10H , 3 O ➔ $C_3H_8O_3$
    D.U. = 6 – 10/2 +1 = 2 (2 dbs , 2 C=O)



15. $C_xH_yO_2$ (MW = 138) ➔ 138 – 32 = 106 ➔ 106/12 = 8 C , 10H , 2 O ➔ $C_8H_{10}O_2$
    D.U. = 8 – 10/2 +1 = 4 (Benzene ring)