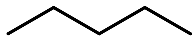
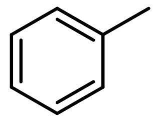
SPECTROSCOPY

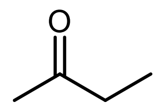
1. How many types of H and C are there and what it the index of hydrogen deficiency of each of the following molecules ?



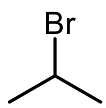
i



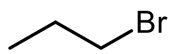
ii



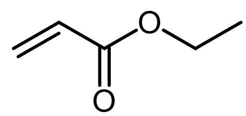
iii



iv

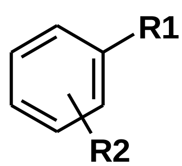


v



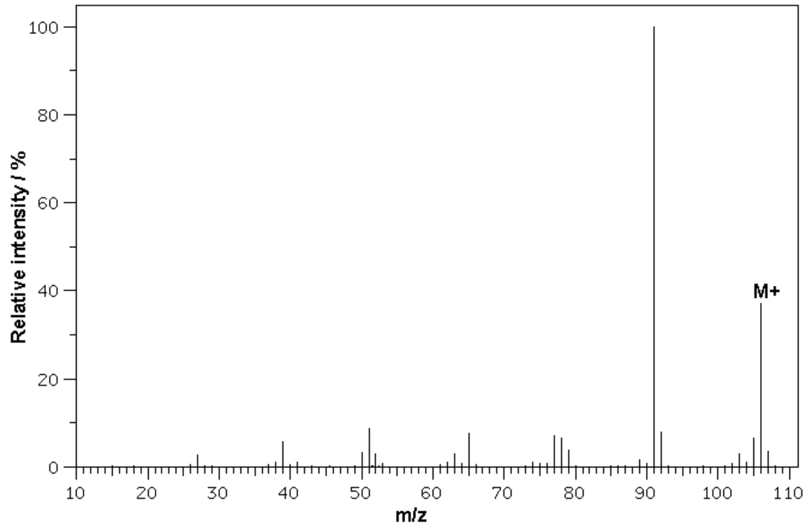
vi

2. Complete the table below working out how many types of aromatic C and aromatic H would be present (*assuming neither substituent R1 or R2 contains any aromatic groups*) for each of the *ortho*, *meta* and *para* isomers of disubstituted benzenes where the two substituents are either the same (R1 = R2) or different (R1 ≠ R2).



	types	**ortho**	**meta**	**para**
R1 = R2	#Ar H			
	#Ar C			
R1 ≠ R2	#Ar H			
	#Ar C			

3. The mass spectrum of "**A**" is shown below :



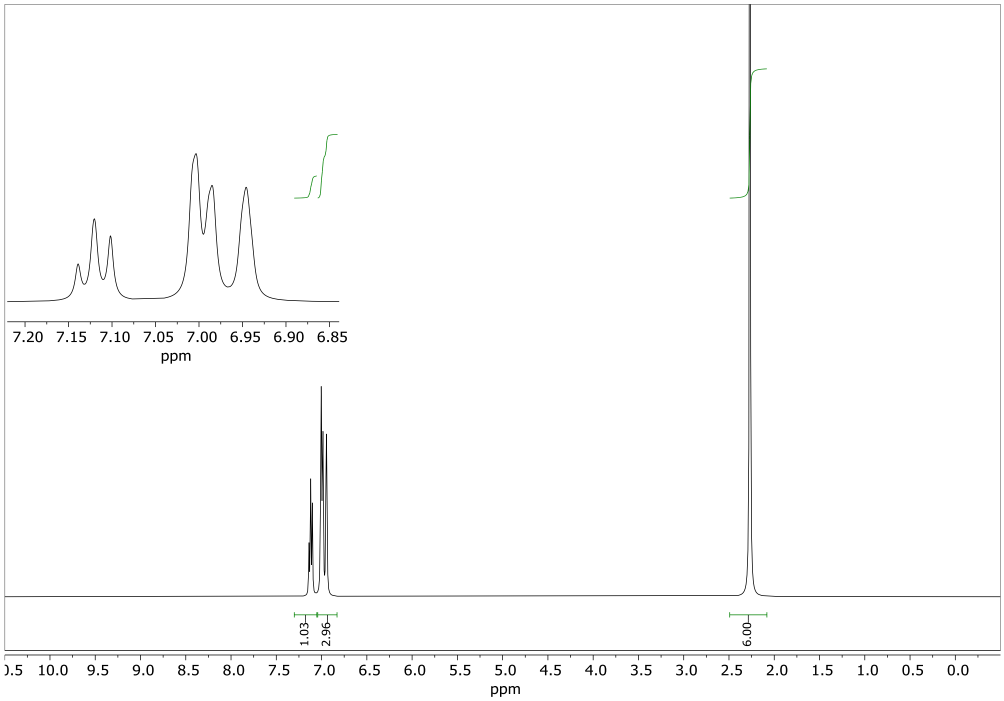
What is the molecular weight of the compound ?

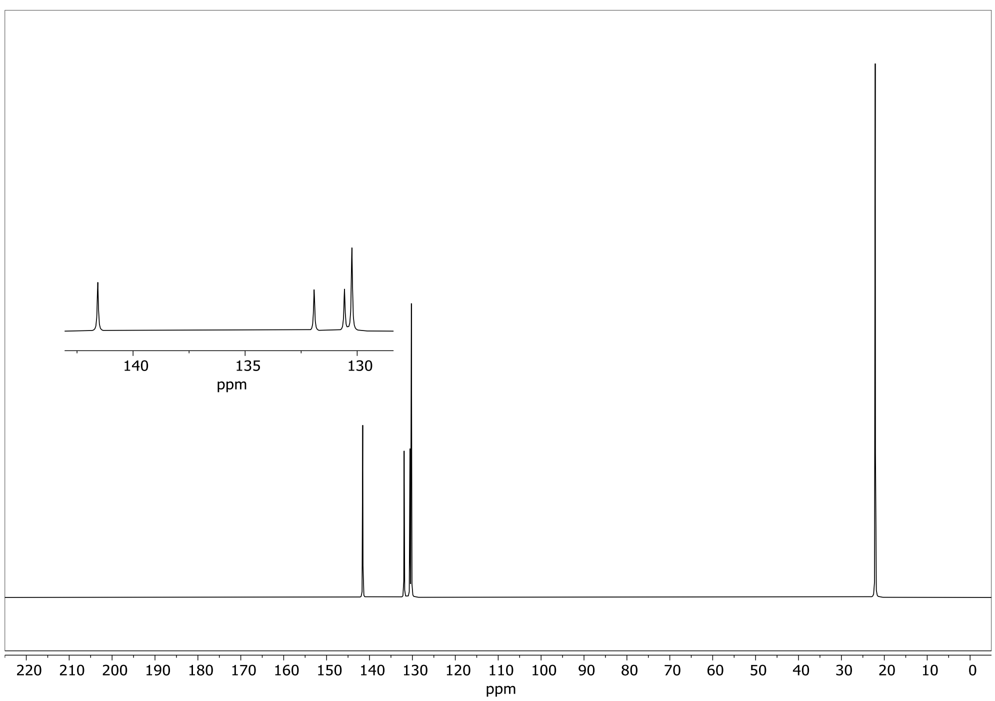
Standard elemental analysis (*i.e.* C,H and N) of compound "**A**" gave 90.50% C and 9.47% H.
Calculate the molecular formula of the compound.
What is the IHD (Index of Hydrogen Deficiency) ?

The H-NMR and 13-CNMR of 4 isomers of "**A**" are shown below.
What do the peaks in the H-NMR between 6.5-8.5 ppm and the 13-CNMR 100-160 ppm indicate is present in all of these isomers ?
In the H-NMR, check the integration for the 6.5-8.5 ppm region. What does this tell you ?
Based on the information you've gathered, so far, draw out the four possible constitutional isomers of "**A**"

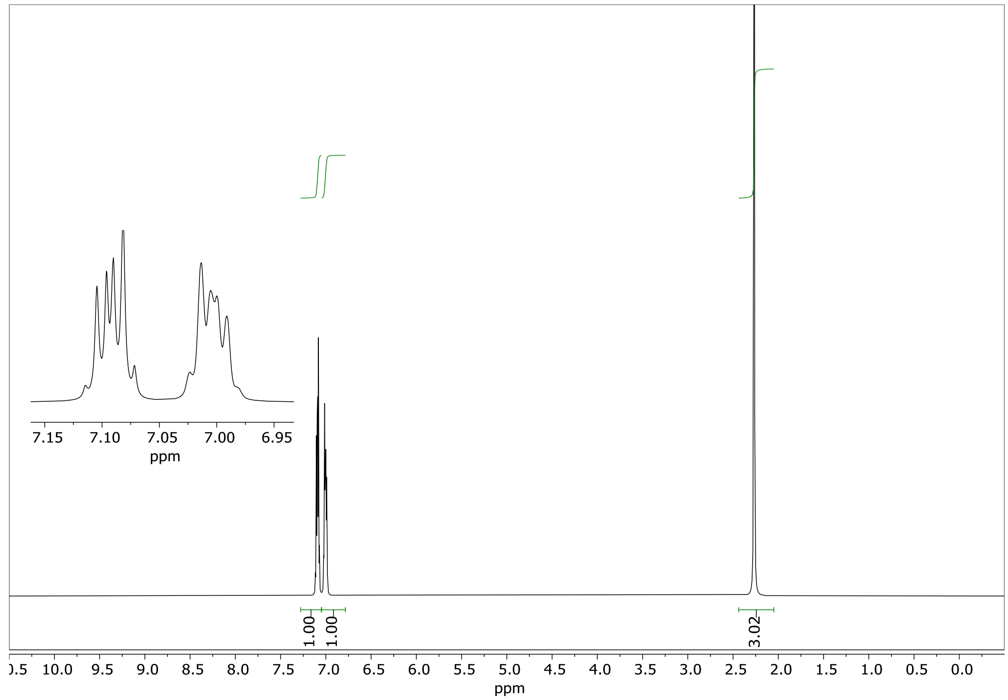
For each of the four isomers of "**A**", use the two NMR spectra to count the number of types of H and C in total AND the number of types of H in the H-NMR between 6.5-8.5 ppm and the number of types of H in the 13-CNMR between 100-160 ppm. Use this information and the table you develop in question 2 to match the structures of each of the isomers **A(i)**-**A(iv)** to the structure of the four possible constitutional isomers identified above.

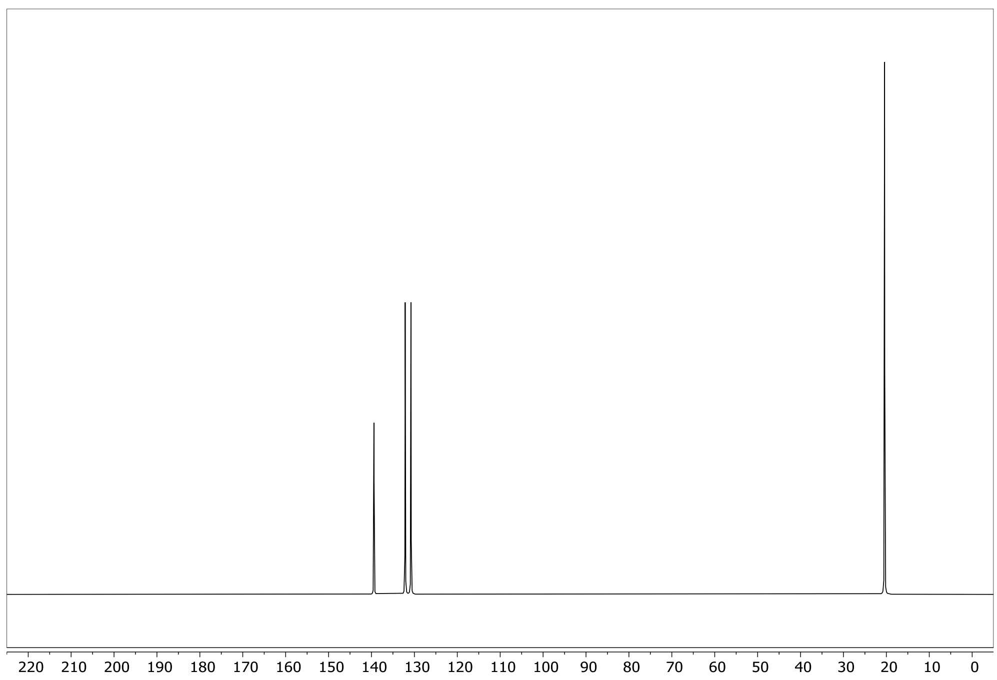
Ai


7.20 7.15 7.10 7.05 7.00 6.95 6.90 6.85
ppm
1.03
2.96
6.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm

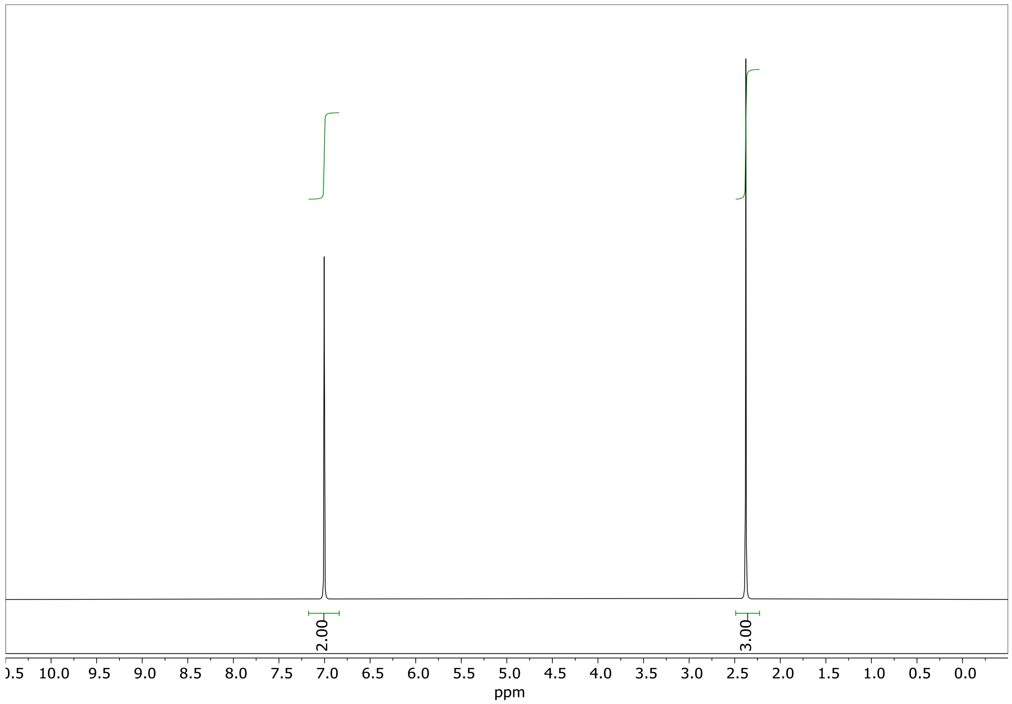

140 135 130
ppm
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

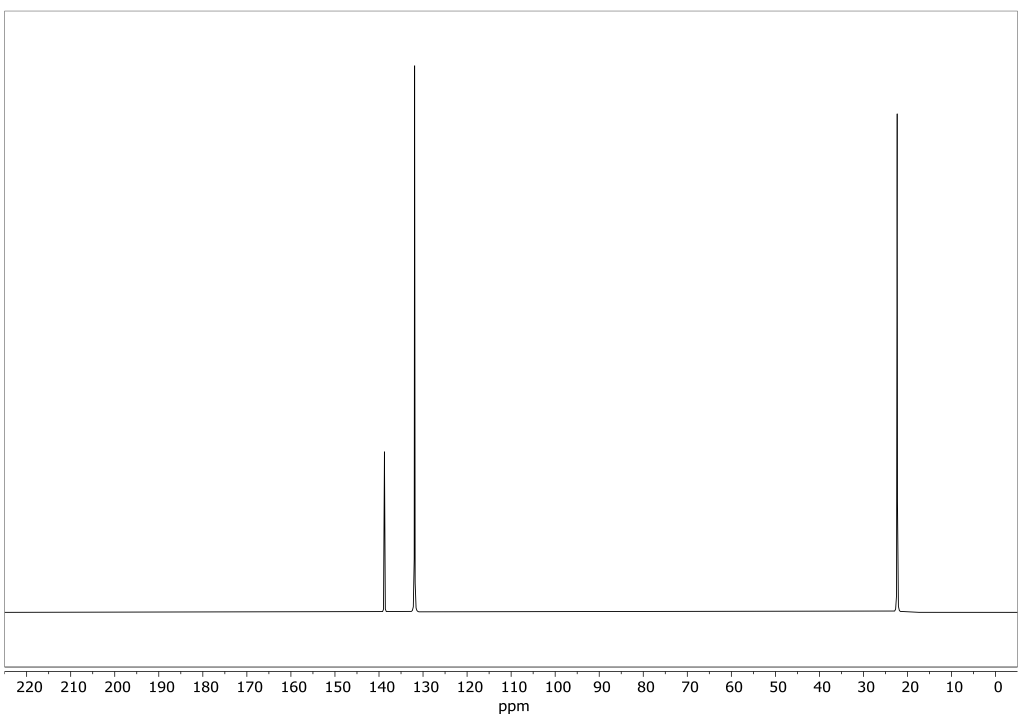
Aii


7.15
7.10
7.05
7.00
6.95
ppm
1.00
1.00
3.02
0.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm

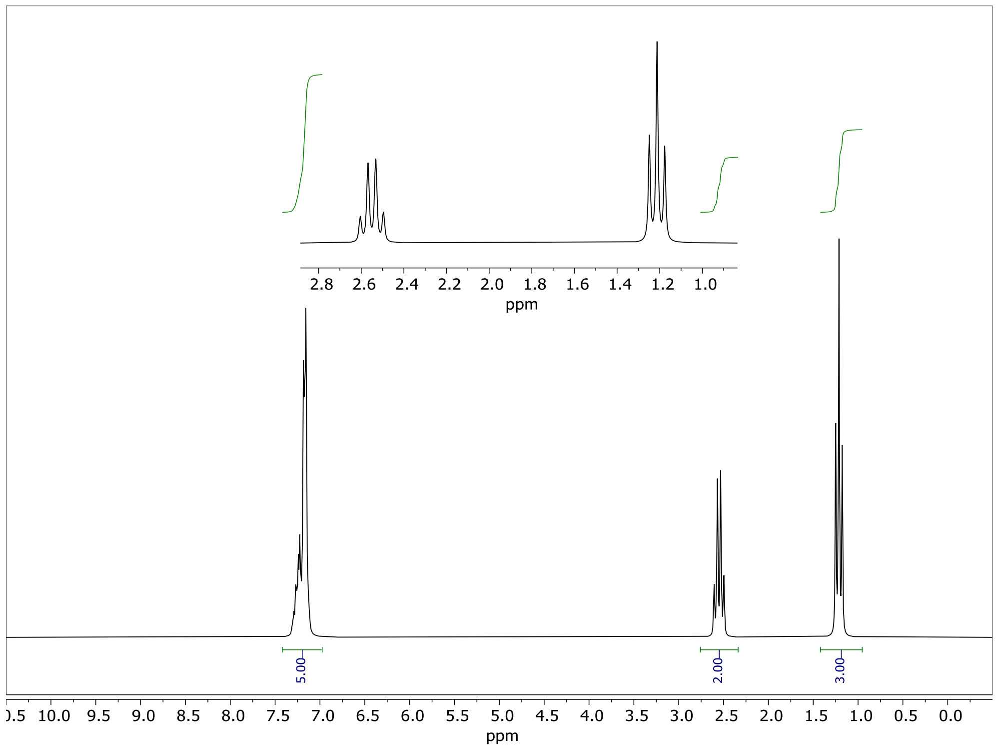

220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

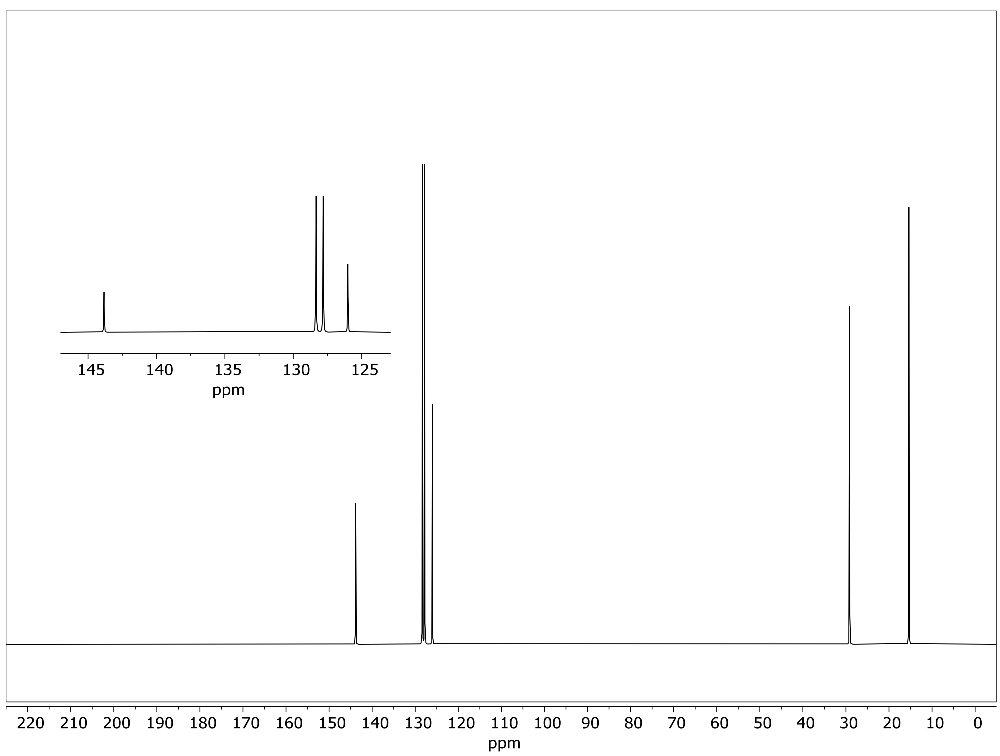
Aiii


2.00
3.00
).5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm

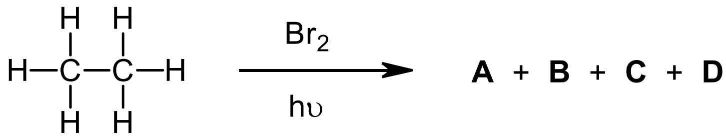

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

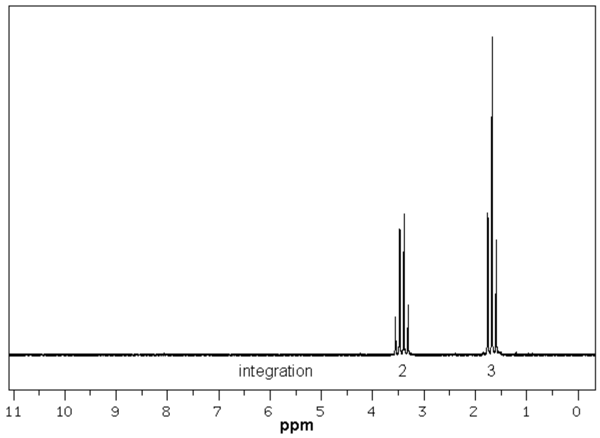
Aiv


2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0
ppm
5.00
2.00
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm

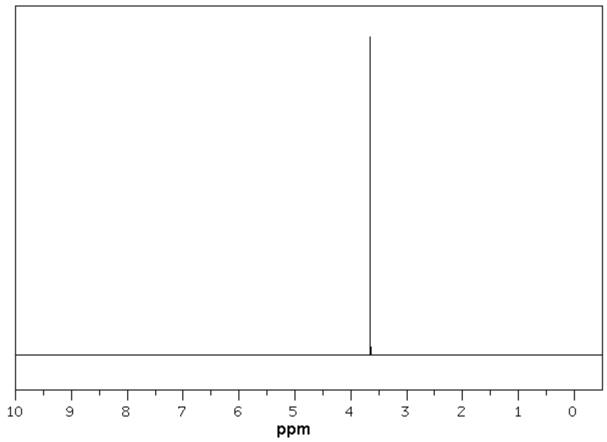

145 140 135 130 125
ppm
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

4. A chemist isolated a mixture of four products was obtained from the radical bromination of ethane. Identify the products from the H-NMR spectra.

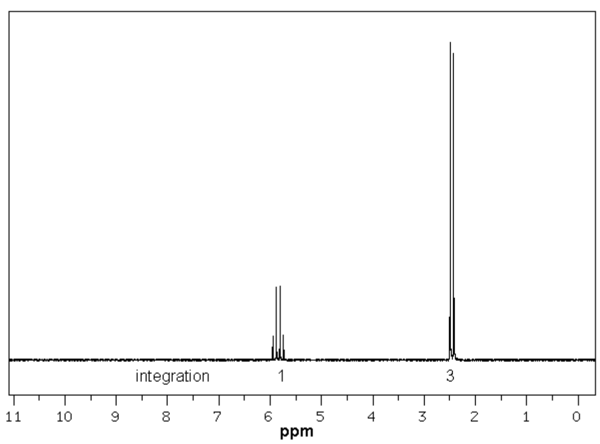




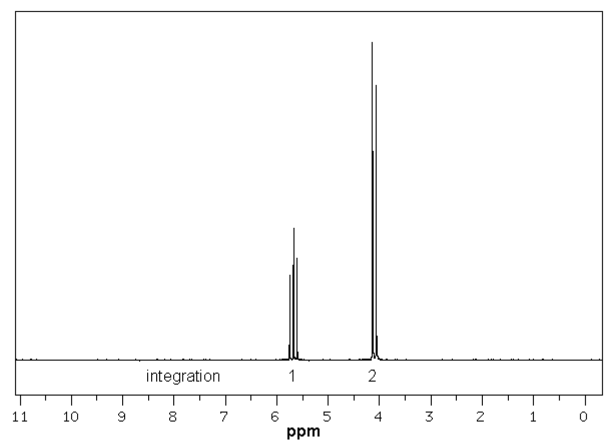
A



B



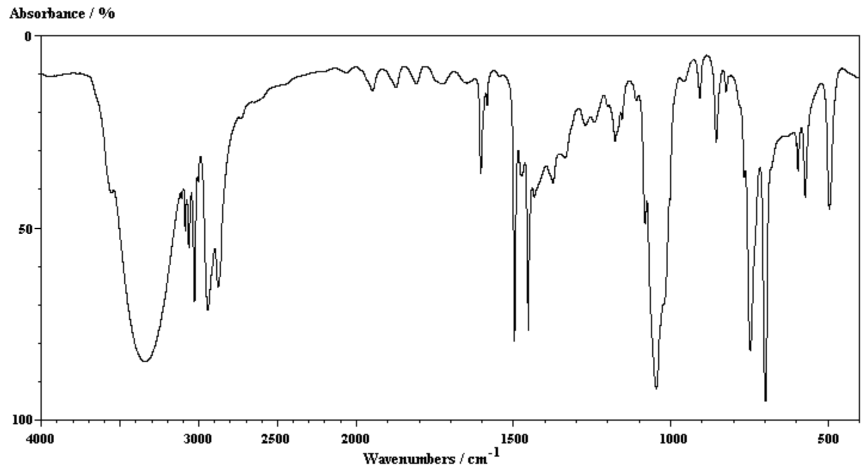
C

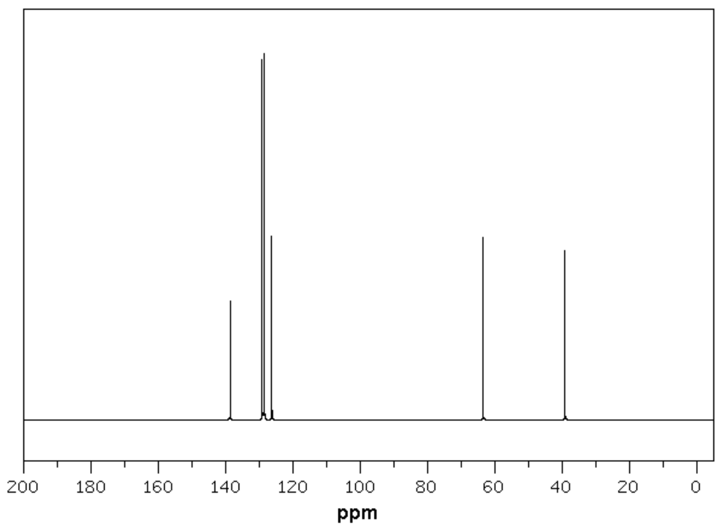


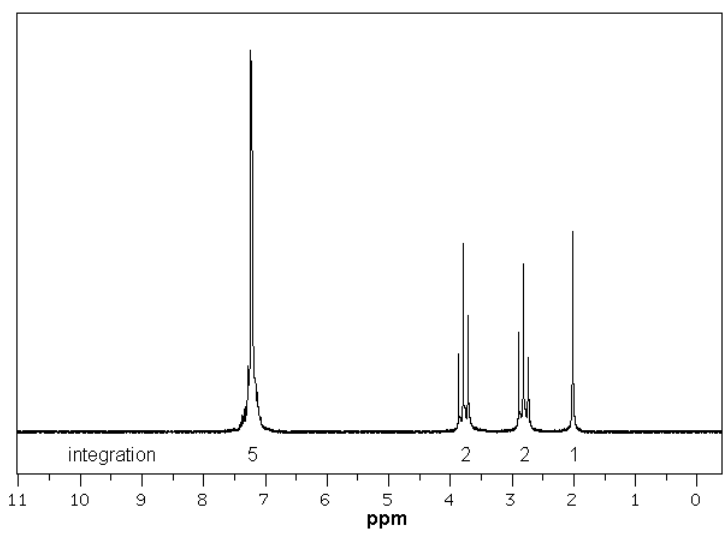
D

5. Identify **D** & **E,** two isomers of $C_8H_{10}O$ **D** given their IR, 13C and H-NMR spectra below.

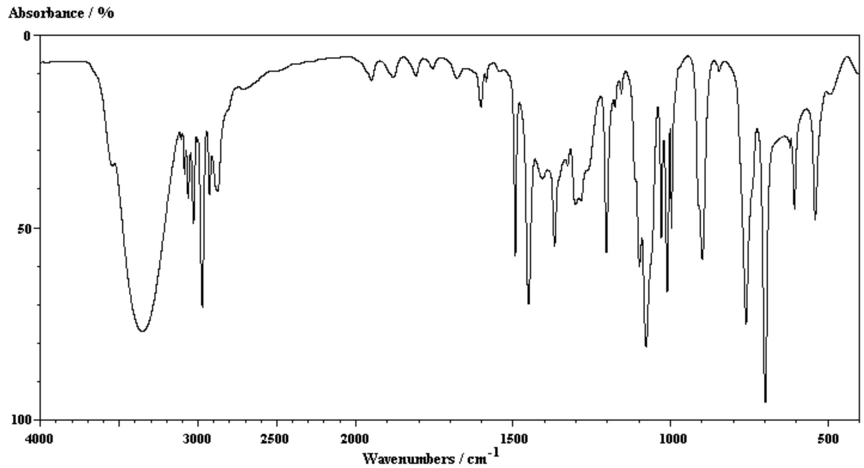
D

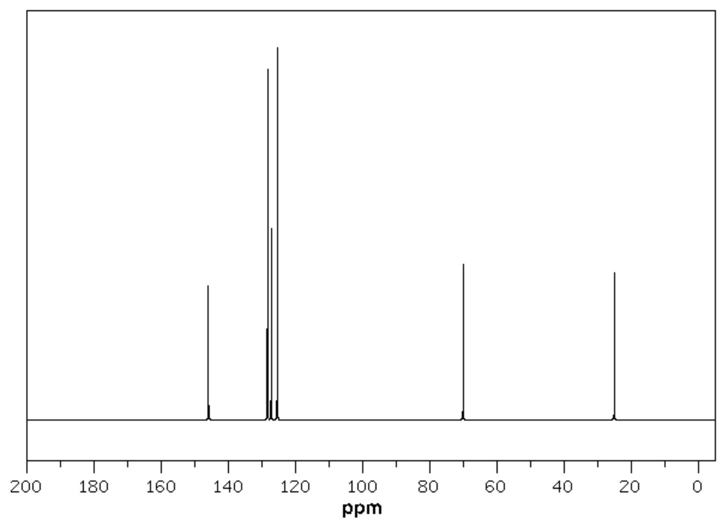


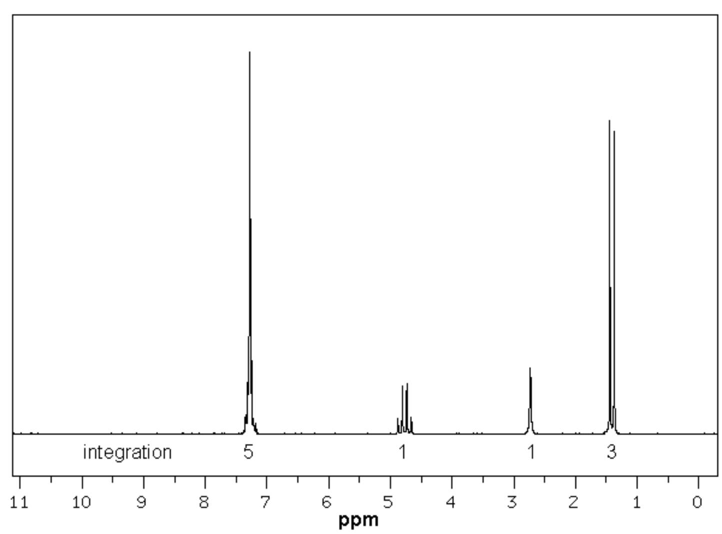




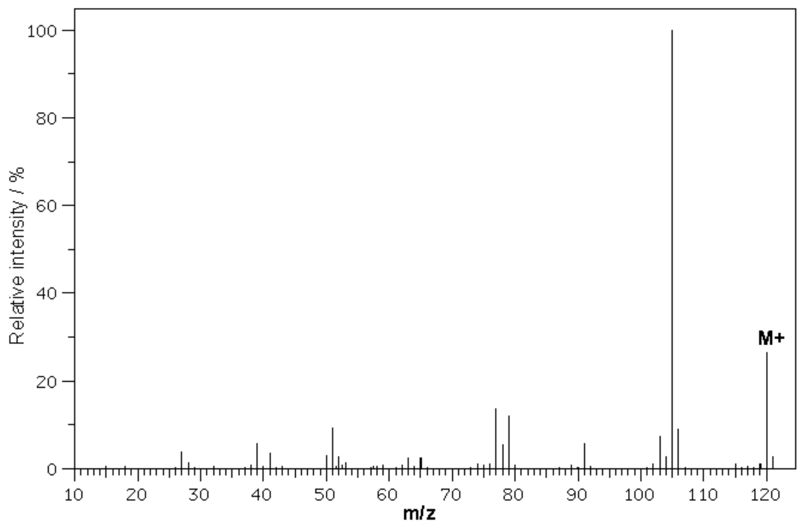
E

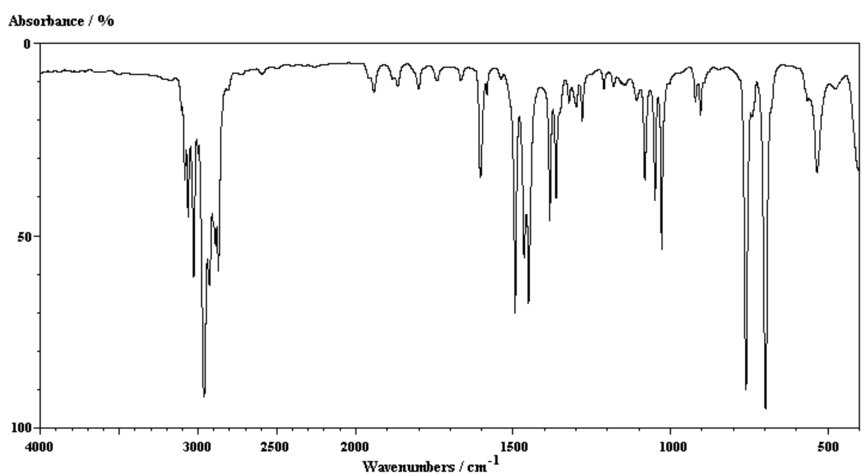

Absorbance / %
0
50
100
4000
3000
2500
2000
1500
1000
500
Wavenumbers / cm^{-1}

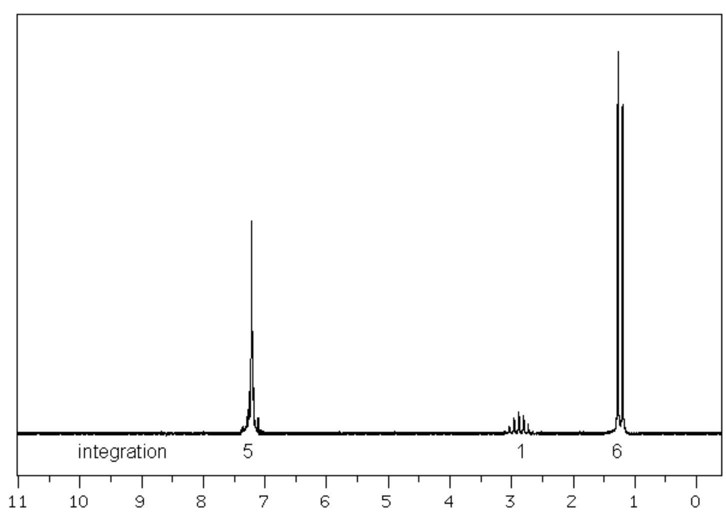

200 180 160 140 120 100 80 60 40 20 0
ppm


integration 5 1 1 3
11 10 9 8 7 6 5 4 3 2 1 0
ppm

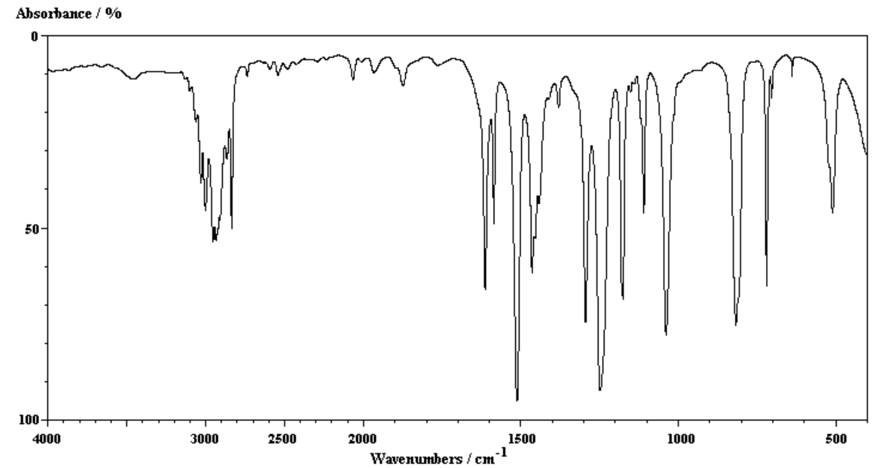
6. Molecule **F** was found to contain 90.0 % carbon and 10.0 % hydrogen by weight. Given the following MS, IR and H-NMR spectra, deduce the structure of **F**.

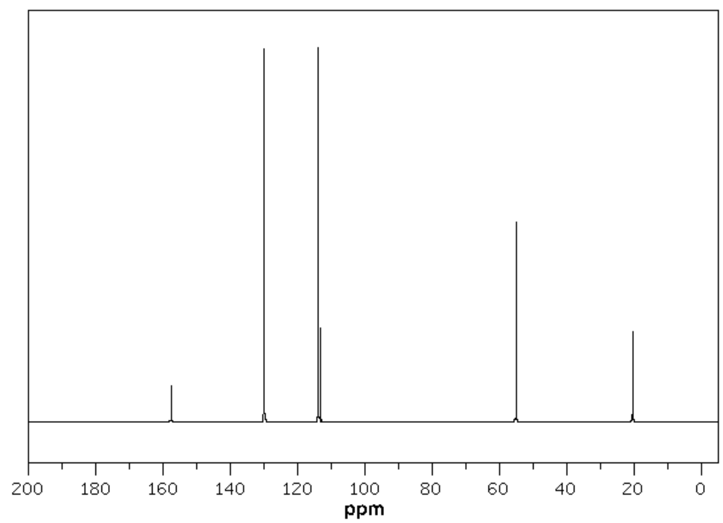


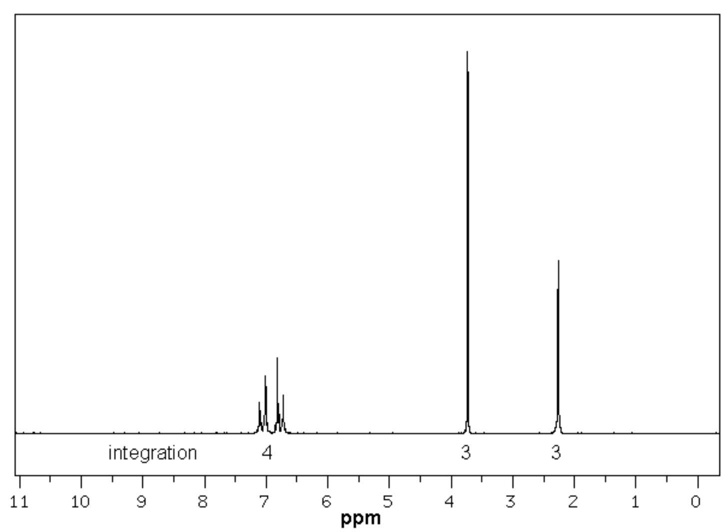




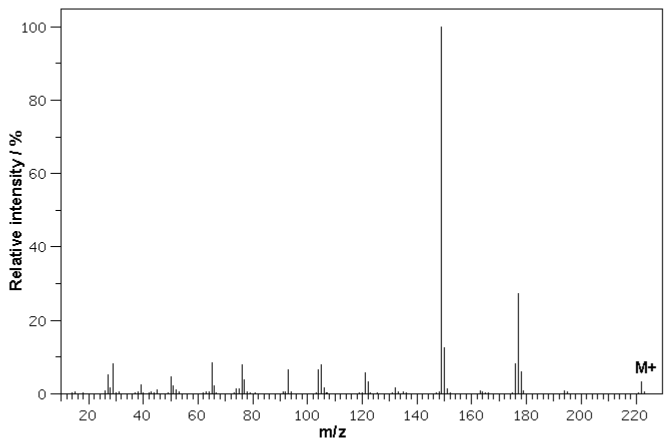
7. From the IR, 13C and H-NMR spectra shown below, propose a structure for compound **G**, which has a molecular formula of $C_8H_{10}O$.

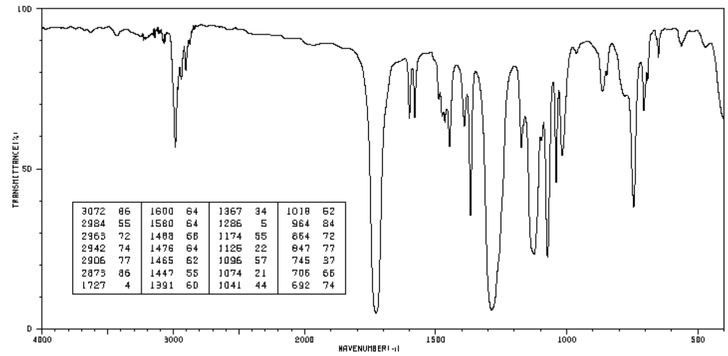


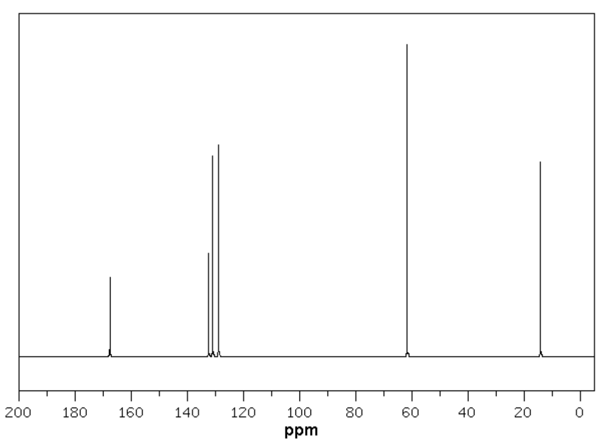


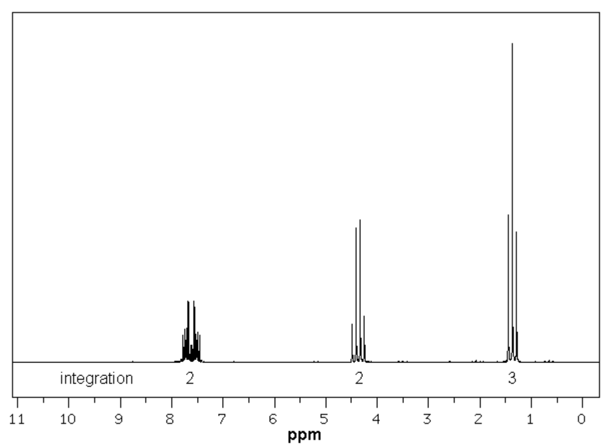


8. Elemental analysis of an unknown sample indicated that it contained 64.86% C and 6.31% H (by weight). Using this data along with the IR, MS, 13C, and H-NMR spectra provided below, determine structure of the unknown sample.









Extra Practice Problems

1. There are seven isomers of $C_4H_{10}O$. Draw line diagrams of the seven isomers and then match each isomer with the following H-NMR data.

   NOTE: s = singlet, d = doublet, t = triplet, m = multiplet

   i δ, 0.95 (t, 3H); 1.52 (m, 2H); 3.30 (s, 3H); 3.40 (t, 2H)

   ii δ, 1.15 (s, 1H); 1.29 (s, 9H)

   iii. δ, 1.20 (t, 3H); 3.45 (quartet, 2H)

   iv. δ, 0.90 (d, 6H); 1.78 (m, 1H); 2.45 (s, 1H); 3.30 (d, 2H)

   v δ, 1.13 (d, 6H); 3.30 (s, 3H); 3.65 (septet, 1H)

   vi δ, 0.95 (t, 3H); 1.50 (m, 4H); 2.20 (s, 1H); 3.70 (t, 2H)

   vii δ, 0.92 (t, 3H); 1.18 (d, 3H); 1.45 (m, 2H); 1.80 (s, 1H); 3.75 (m, 1H)

2. Using the following H-NMR data, propose structures for the following $C_5H_{10}O_2$ isomers:

   NOTE: s = singlet, d = doublet, t = triplet, m = multiplet

   i δ, 1.14 (t, 3H); 1.26 (t, 3H); 2.32 (q, 2H); 4.13 (q, 2H)

   ii δ, 1.17 (d, 6H); 2.56 (septet, 1H); 3.67 (s, 3H)

   iii δ, 0.95 (t, 3H); 1.65 (sextet, 2H); 2.05 (s, 3H), 4.02 (t, 2H)

   iv δ, 2.19 (s, 3H); 2.69 (t, 2H); 3.33 (s, 3H); 3.64 (t, 2H)

   v δ, 1.23 (d, 6H); 2.02 (s, 3H); 5.00 (septet, 1H)

   vi δ, 1.39 (s, 6H); 2.24 (s, 3H); 3.80 (broad s, 1H)