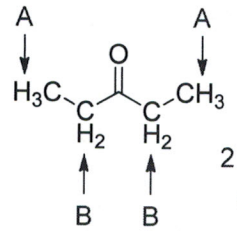
Chemistry 344: Spectroscopy Problem Set 1

Name (print): _____

TA Name (print): _____

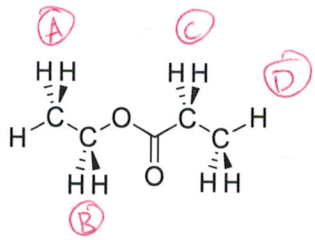
I. For each of the following molecules, determine how many signals you would expect to see in an ^{1}H-NMR spectrum of the molecule. Additionally, label each of the hydrogen atoms (A, B, C, ...) such that those in the same chemical environment are given the same designation. See the example below.

A.



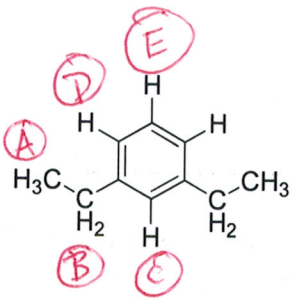
2 ^{1}H signals expected

B.



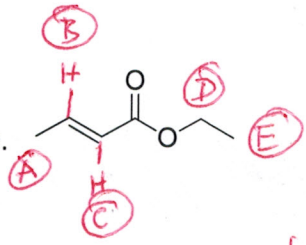
4 signals

C.



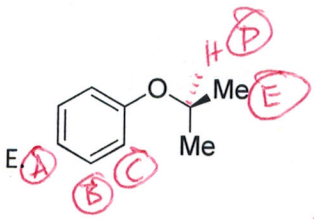
5 signals

D.



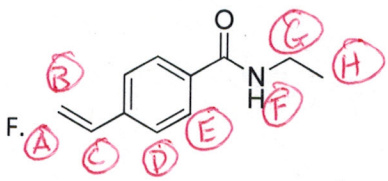
5 signals

E.



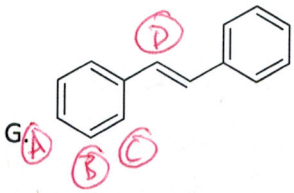
5 signals

F.



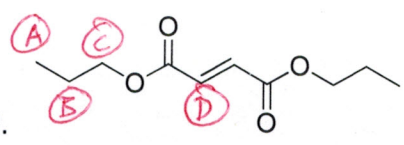
8 signals

G.



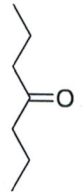
4 signals

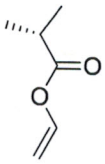
H.

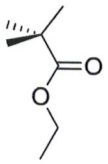


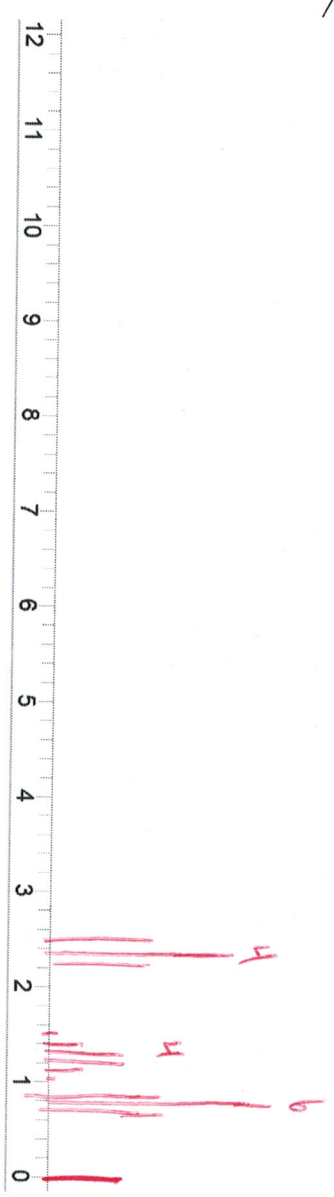
4 signals

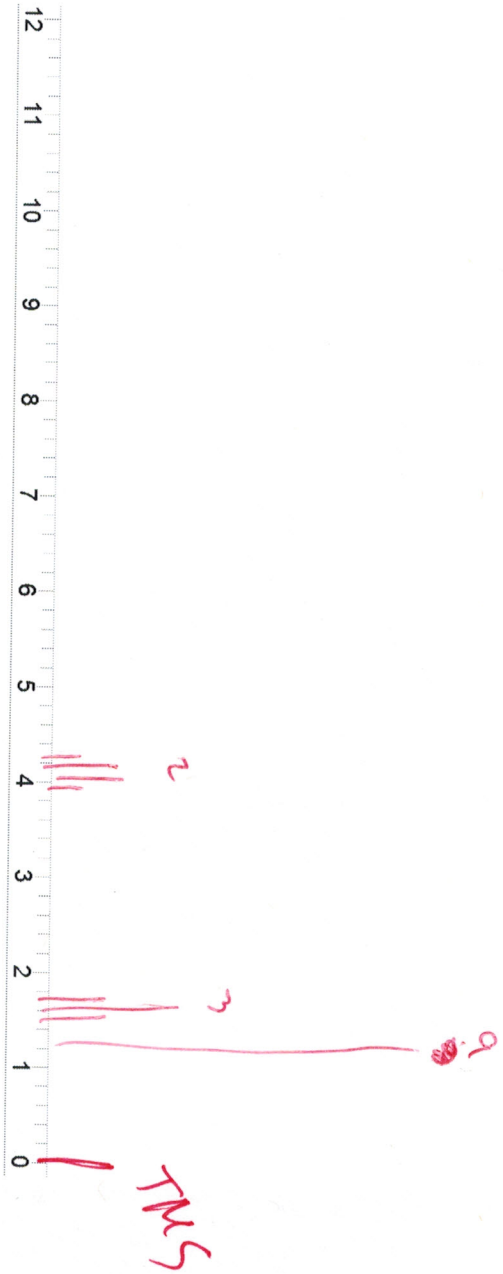
II. For each of the molecules below, predict the splitting and chemical shift of each of the signals in the ^{1}H-NMR spectrum and make a rough sketch on the horizontal ppm axis provided. Be sure to consider the relative intensity of each signal and label its integration. Draw a TMS peak and label it on each spectrum.

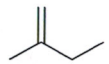


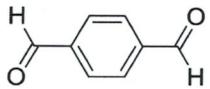


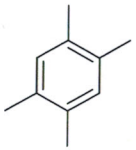


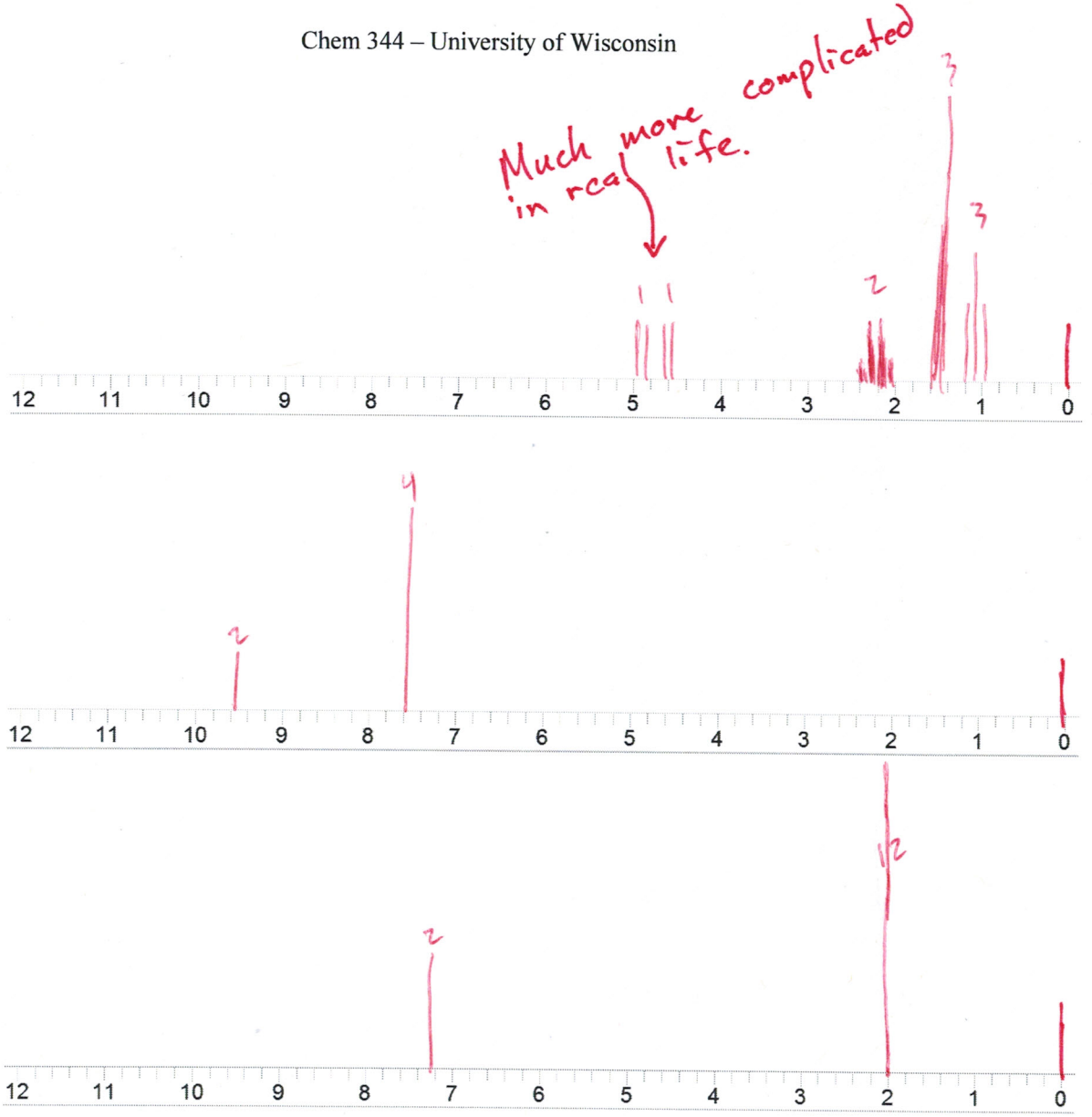


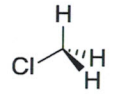


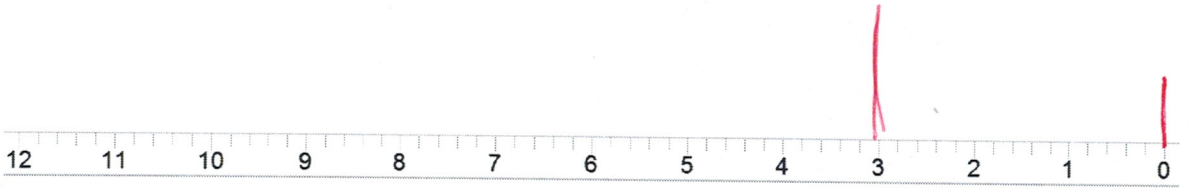


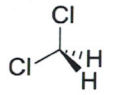

H
O
O
H

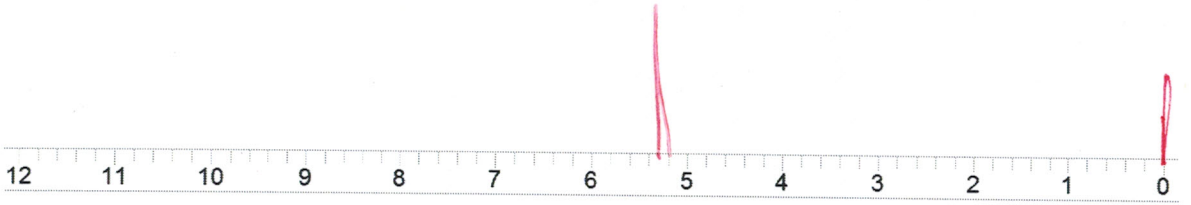


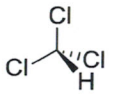

Much more complicated in real life.
1 1
2
3
3
12 11 10 9 8 7 6 5 4 3 2 1 0
2
4
12 11 10 9 8 7 6 5 4 3 2 1 0
2
1/2
12 11 10 9 8 7 6 5 4 3 2 1 0

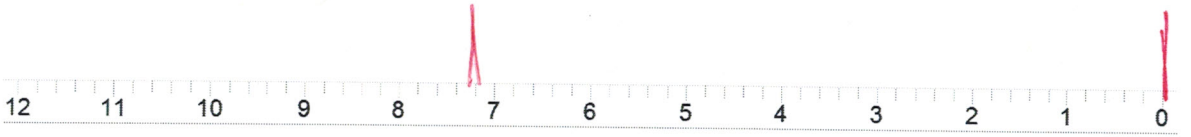

H
Cl
H
H

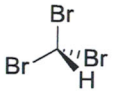

12 11 10 9 8 7 6 5 4 3 2 1 0

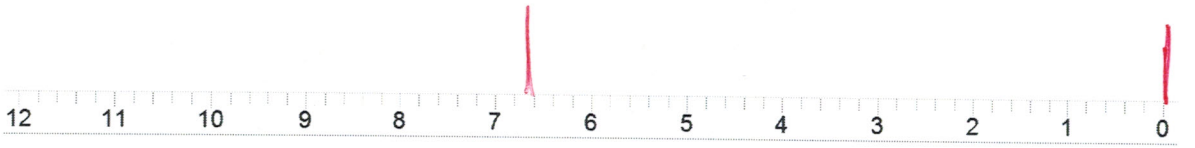

Cl
Cl
H
H


12 11 10 9 8 7 6 5 4 3 2 1 0


Cl
Cl
Cl
H

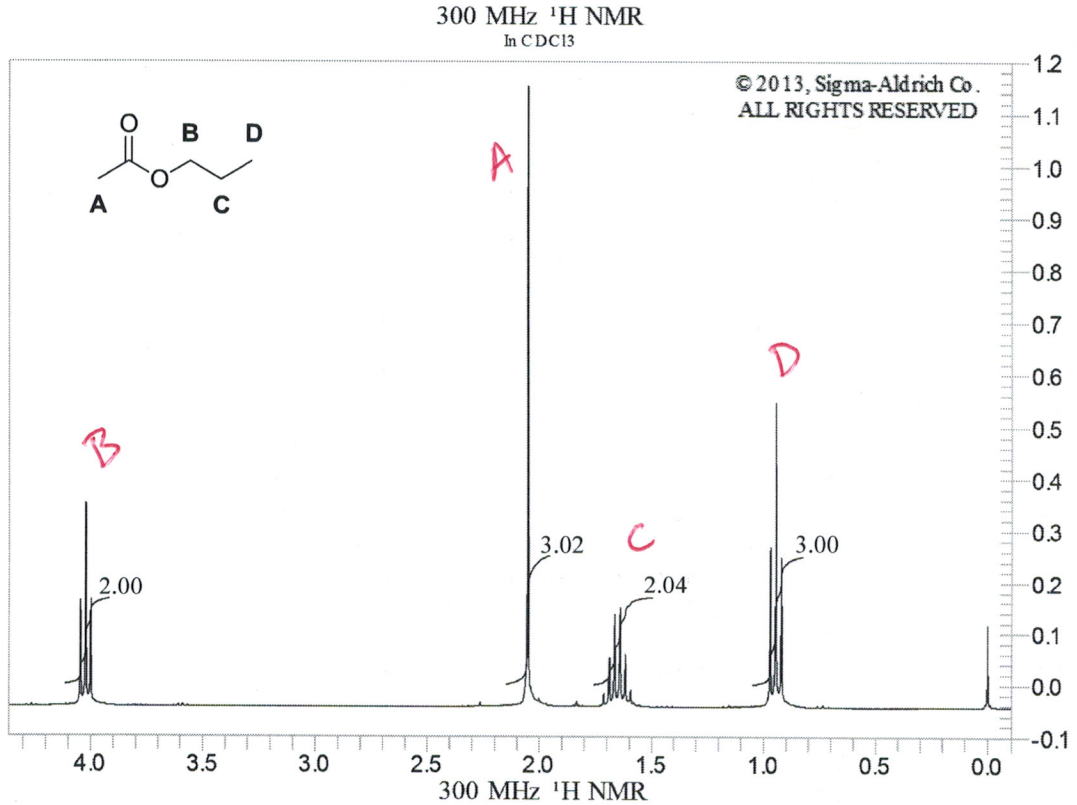

12 11 10 9 8 7 6 5 4 3 2 1 0


Br
Br
Br
H

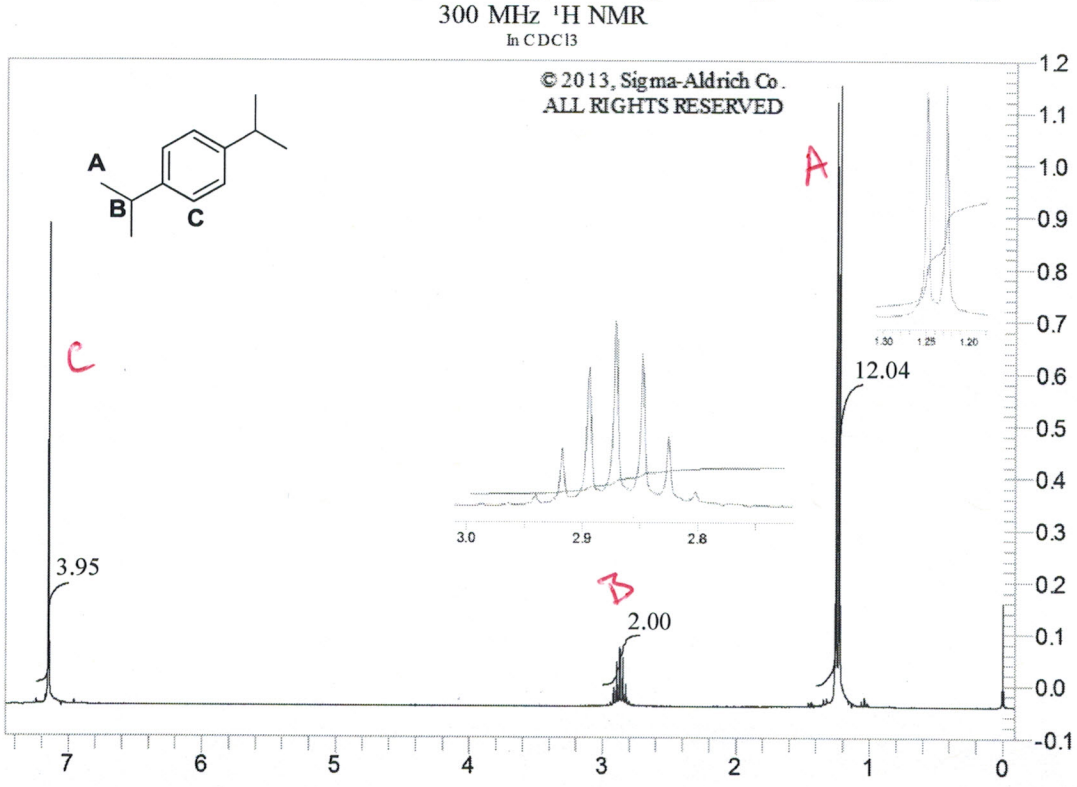

12 11 10 9 8 7 6 5 4 3 2 1 0

III. For the ^{1}H-NMR spectra of shown below, assign each of the signals using labels provided on the structure.

A.



B.



IV. For a molecule with a chemical formula of $C_3H_4Br_2O$, answer the following questions.

A. What is the unsaturation number (**U**) or index of hydrogen deficiency (**IHD**)?

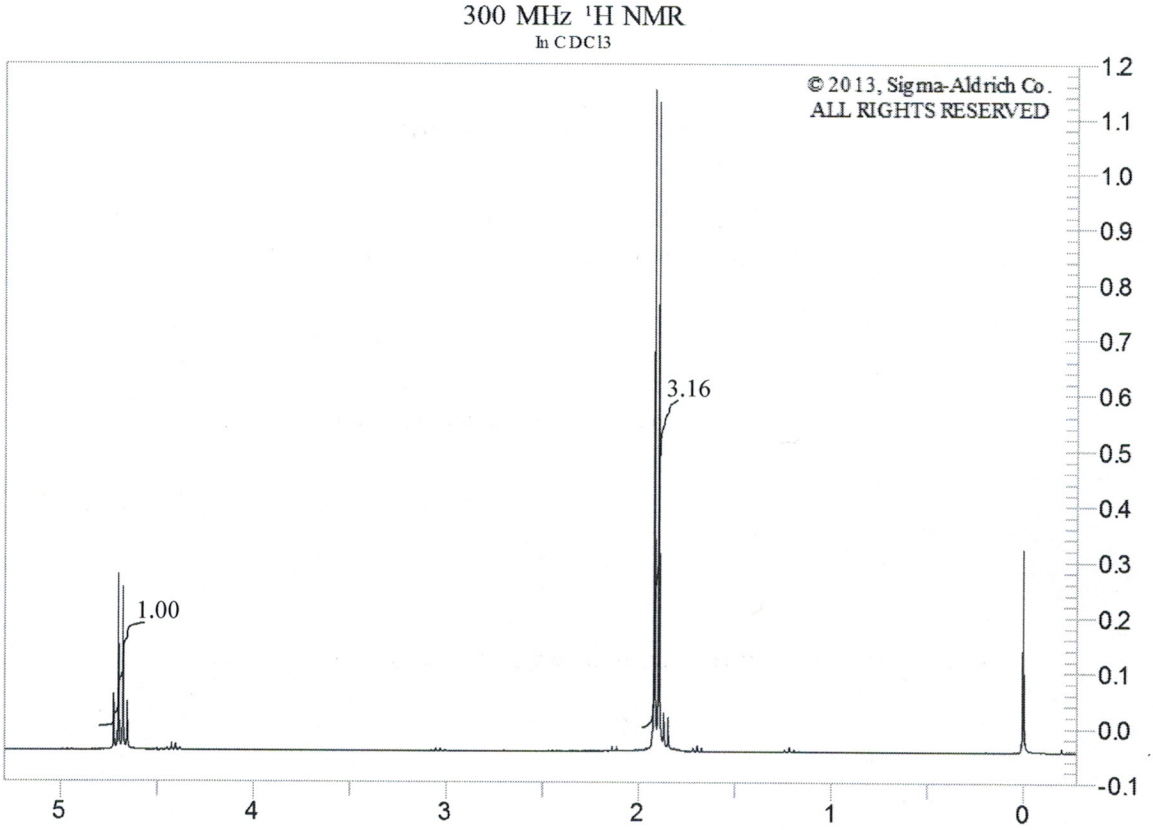
1

$$U = IHD = \frac{2C + 2 + N - H - X}{2}$$

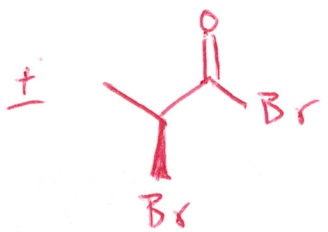
B. What does this indicate about the molecule?

one C=C
or
one C=O
or
one ring

C. Using the ^{1}H-NMR spectrum below, draw part structures for the signals at δ1.91 and δ4.69.



D. What is the complete structure of the molecule?



V. For a molecule with a chemical formula of $C_{12}H_{19}N$, answer the following questions.

A. What is the unsaturation number (**U**) or index of hydrogen deficiency (**IHD**)?

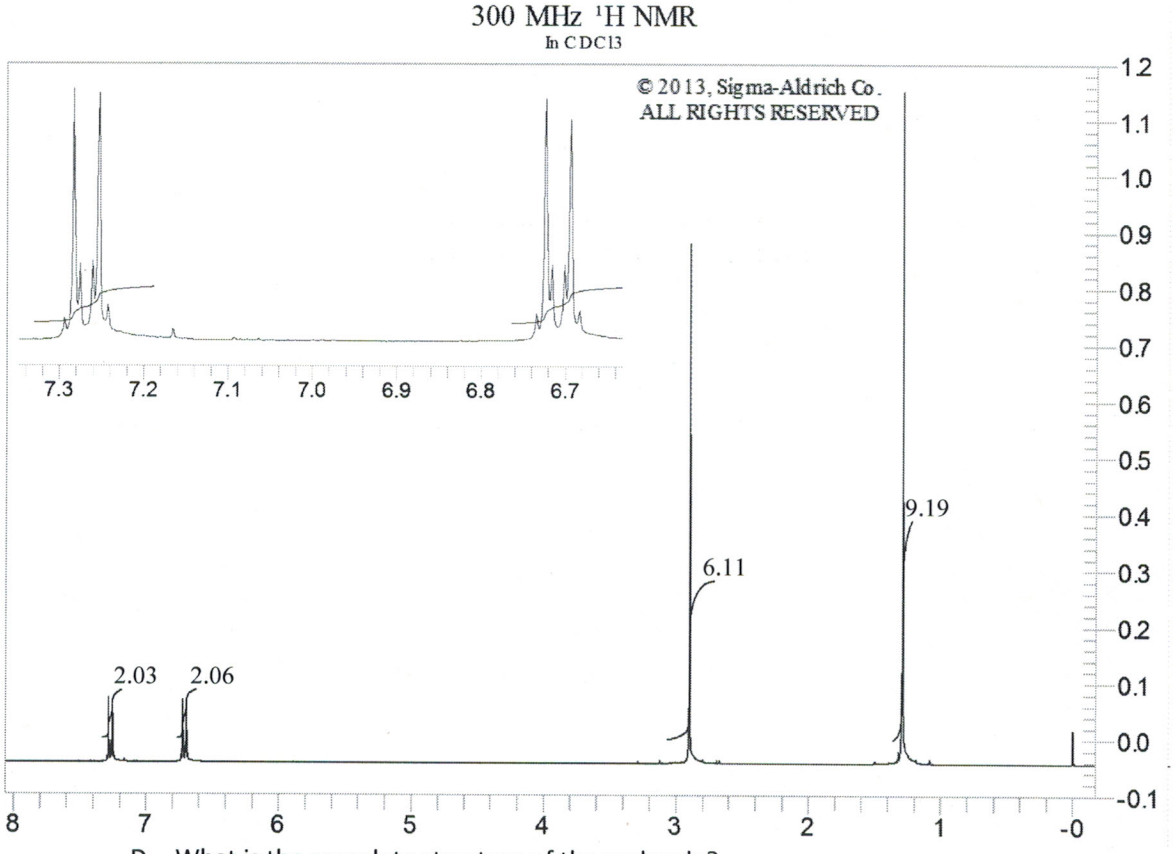
4

$$U = IHD = \frac{2C + 2 + N - H - X}{2}$$

B. What does this indicate about the molecule?

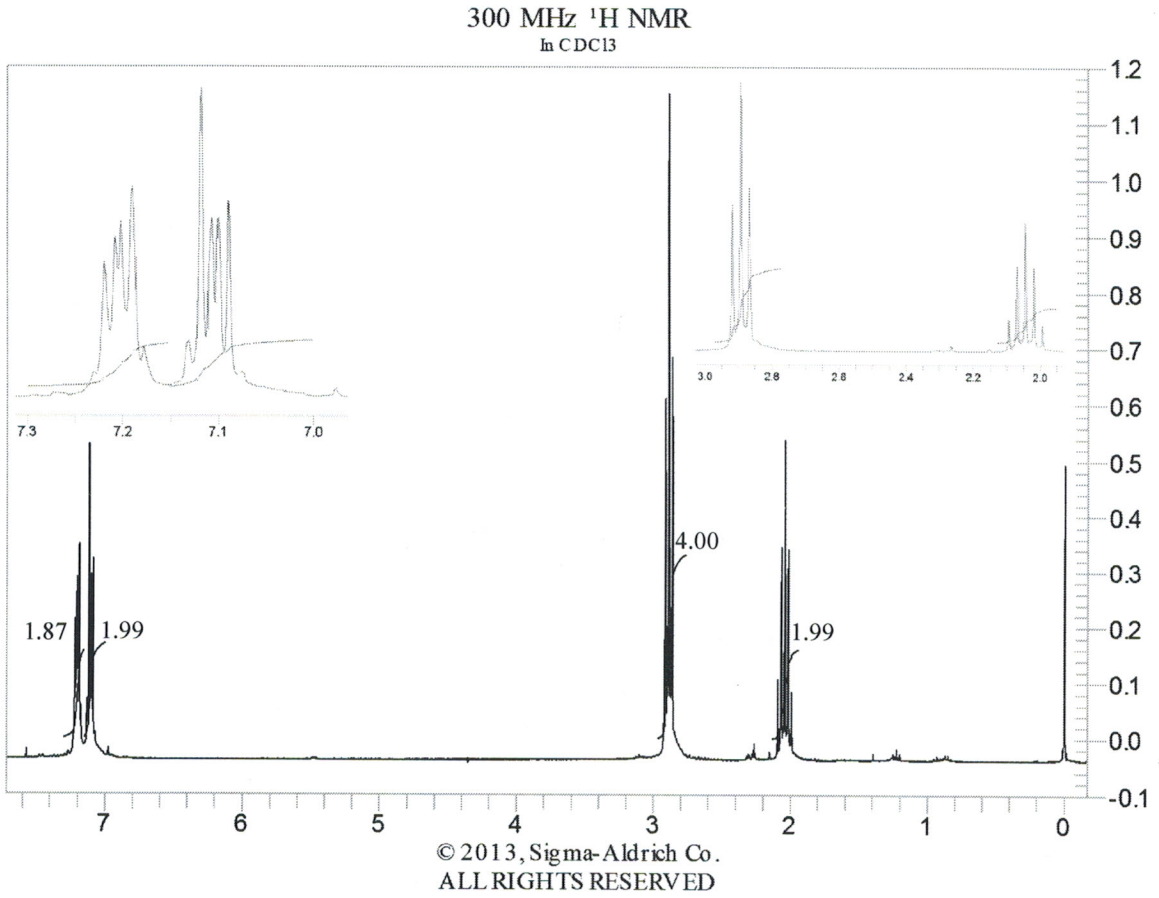
- lots of double bonds or rings
- often 4 leads to benzene

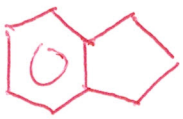
C. Using the ^{1}H-NMR spectrum below, draw part structures for the signals at δ1.29, δ2.90, δ6.71 and δ7.27



D. What is the complete structure of the molecule?

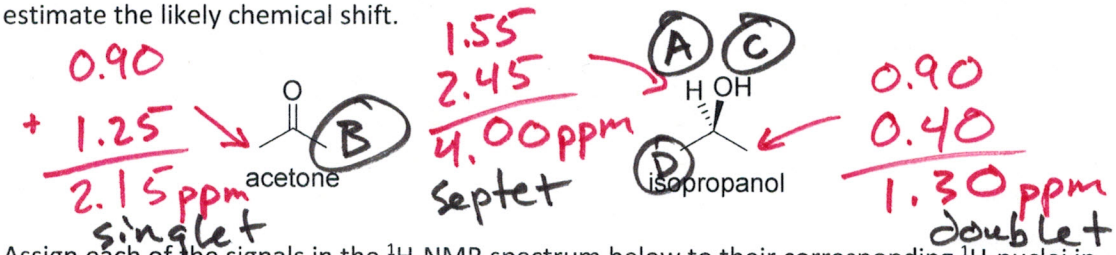
VI. Determine the structure of the molecule with formula C_9H_{10} that corresponds to the ^{1}H-NMR spectrum shown below.





VII. Using the ^{1}H-NMR spectrum and questions below, determine the relative amount of acetone and isopropyl alcohol in a mixture of the two molecules. For more information on determining ratios by ^{1}H-NMR. *(https://www.chem.wisc.edu/content/experiment-6-elimination-reactions-e1e2#Q1)*

A. For each of the molecules shown below, identify the likely observed coupling pattern and estimate the likely chemical shift.



B. Assign each of the signals in the ^{1}H-NMR spectrum below to their corresponding ^{1}H-nuclei in the molecules above using the letter designations A-D.

C. Using the spectrum below, determine the relative amount of acetone and isopropyl alcohol in the spectrum of a mixture relative to the least abundant molecule. Report the ratio with the lowest abundance species set to a value of 1.00.

$\frac{6.64/6}{1.00}$ = 1.10 acetone : 1 isopropanol

$\frac{6.64}{6.25}$ = 1.06 : 1