Chemistry 344: Spectroscopy Problem Set 1

Name (print): _____

(Not for credit)

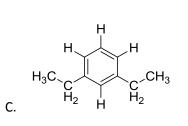
TA Name (print): _____

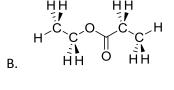
 $\begin{array}{c} A \\ H_{3}C \\ H_{2} \\ H_$

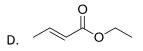
Α.

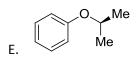
I. For each of the following molecules, determine how many signals you would expect to see in an ¹H-NMR spectrum of the molecule. Additionally, label each of the hydrogen atoms (A, B, C, ...) such that those in the same chemical environment are given the same designation. See the example below.

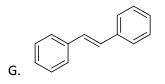
> 2 ¹H signals expected

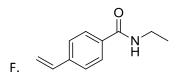


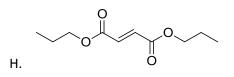




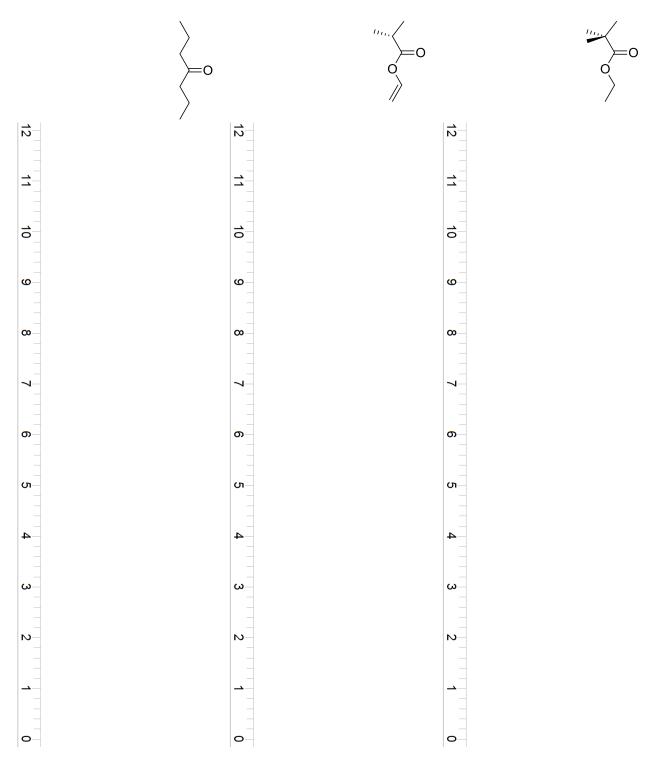


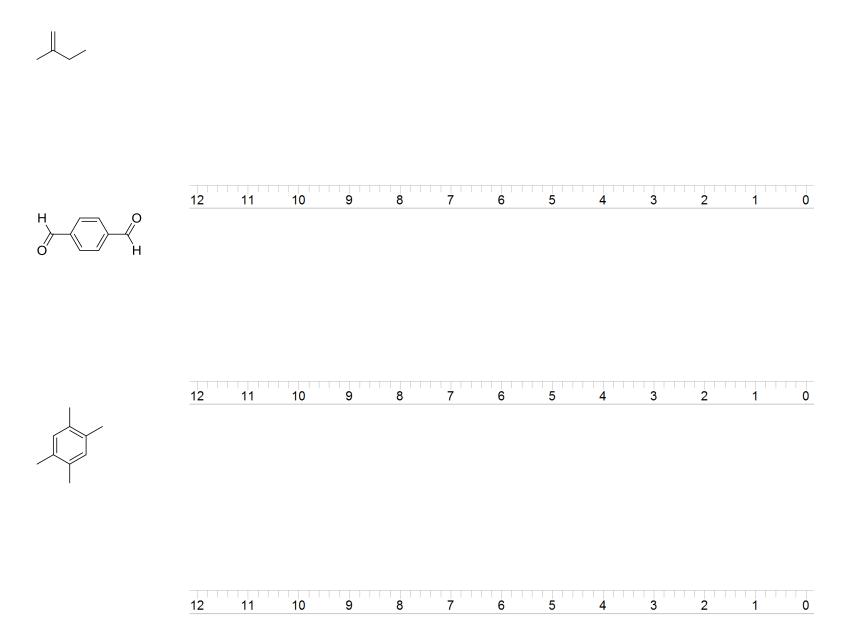


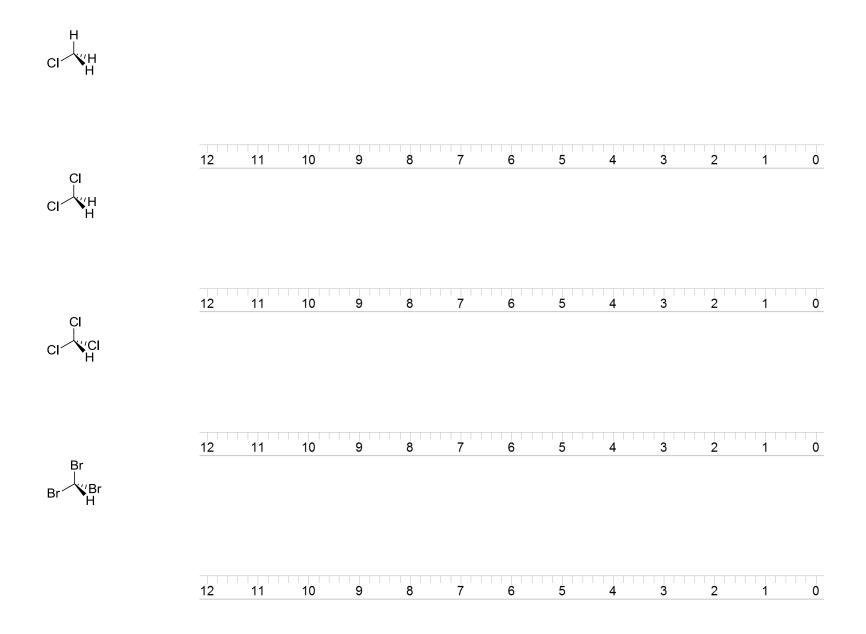


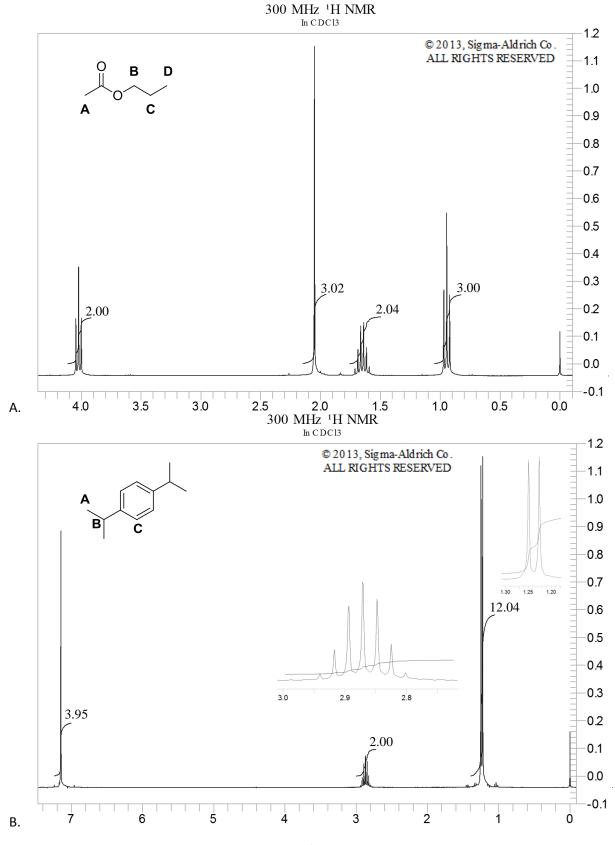


II. For each of the molecules below, predict the splitting and chemical shift of each of the signals in the ¹H-NMR spectrum and make a rough sketch on the horizontal ppm axis provided. Be sure to consider the relative intensity of each signal and label its integration. Draw a TMS signal and label it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









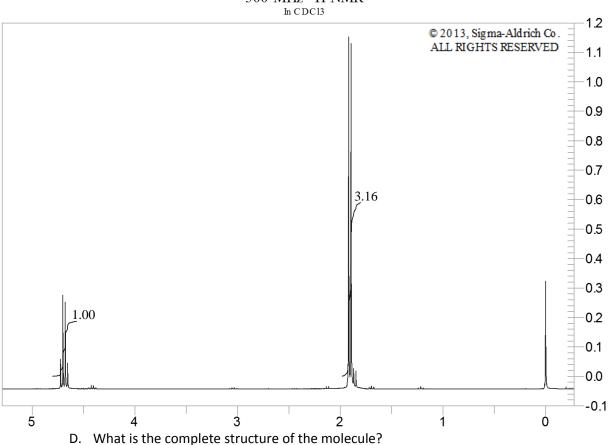
III. For the ¹H-NMR spectra shown below, assign each of the signals using labels provided on the structure.

- 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)?

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

B. What does this indicate about the molecule?

C. Using the ¹H-NMR spectrum below, draw part structures for the signals at δ 1.91 and δ 4.69 ppm.



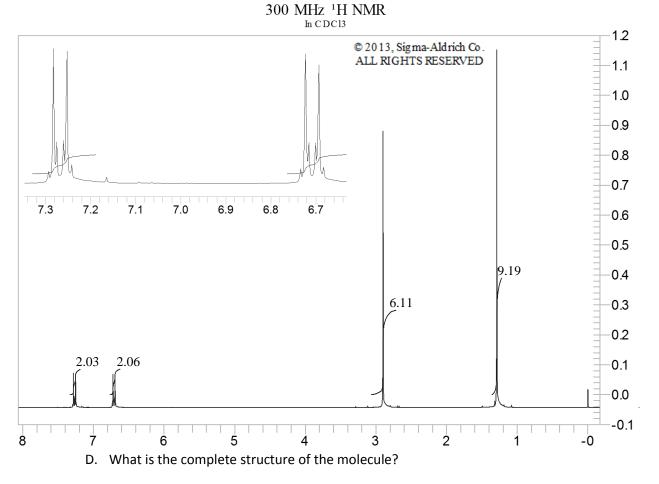
300 MHz ¹H NMR

- 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)?

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

B. What does this indicate about the molecule?

C. Using the ¹H-NMR spectrum below, draw part structures for the signals at δ 1.29, δ 2.90, δ 6.71 and δ 7.27 ppm.



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

