Chem 22 **Homework set 2**

End-of-chapter problems from Hornback: **Ch 14**: 15-30. Note, however, that our emphasis will be on ^{1}H NMR and determining structures of molecules from combinations of ^{1}H NMR and IR spectra. You will (probably) not be asked to determine structures based on a ^{13}C NMR spectrum alone. Although the book has many clever problems of this type that you can certainly do, this is not the way anyone determines molecular structures in the Real World.

1. Draw the compounds responsible for the ^{1}H NMR data given, and indicate which NMR signals correspond to which Hs in your structures. The ratios of the numbers of Hs contributing to each NMR absorption are given. (This information comes from integration of the spectrum.)

If you understand how to identify equivalent vs different sets of Hs, and you understand the effects of electronegative atoms, this problem is just a matter of systematic reasoning. Identify the molecule pieces, and then think about how to connect them. Don't just guess until you stumble across something that "kind-of-sort-of seems to work".

(a) Formula $\mathbf{C_5H_{12}O}$, δ 3.3 and δ 1.2 in a 1:3 ratio.

(b) Formula $\mathbf{C_4H_{10}O_2}$, δ 3.3 and δ 3.4 in a 3:2 ratio.

(c) Formula $\mathbf{C_3H_8O_2}$, δ 4.4 and δ 3.3 in a 1:3 ratio.

(d) Formula $\mathbf{C_5H_{12}O_2}$, δ 3.1 and δ 1.2 in a 1:1 ratio.

2. The ^{1}H NMR spectra of seven isomeric compounds having the formula $\mathbf{C_4H_{10}O}$ are summarized below. Identify each compound, and indicate which Hs in your structure correspond to each absorption. All *J* values are ≈ 7 Hz. Standard abbreviations for splittings — s = singlet; d = doublet; t = triplet; q = quartet; br = broad.

(a) δ 2.87 (br s, 1H); δ 1.28 (s, 9H).

(b) δ 1.20 (t); δ 3.45 (q); ratio 3:2.

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

(d) δ 0.92 (t, 3H); δ 1.18 (d, 3H); δ 1.45 (quintet, 2H); δ 1.80 (br s, 1H); δ 3.75 (sextet, 1H).

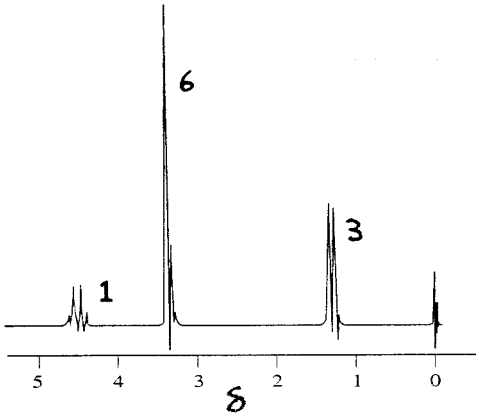
(e) δ 0.90 (d, 6H); δ 1.78 (nonet, 1H); δ 2.45 (br s, 1H); δ 3.30 (d, 2H).

(f) δ 0.95 (t, 3H); δ 1.52 (sextet, 2H); δ 3.30 (s, 3H); δ 3.40 (t, 2H).

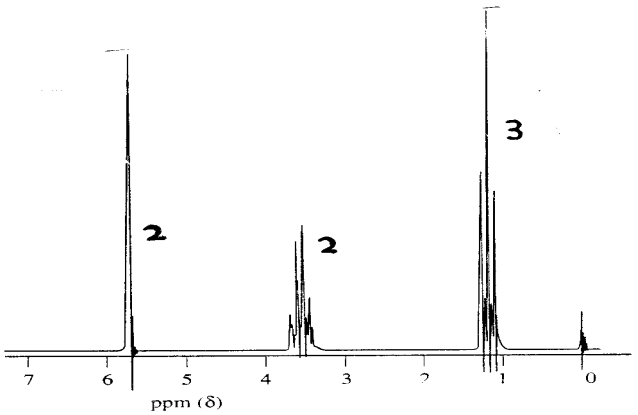
(g) δ 0.95 (t, 3H); δ 1.50 (complex abs, 4H); δ 2.20 (br s, 1H); δ 3.70 (t, 2H). ("Complex" is a polite way of saying "uninterpretable blob" — that's life in the Real World. Just work around it.)

3. Draw the compounds responsible for the following 60 MHz NMR spectra and indicate which Hs in your structure are responsible for each absorption. (In some, the numbers of Hs contributing to each signal are given; for the others, you will have to measure the integration curves to figure it out.)

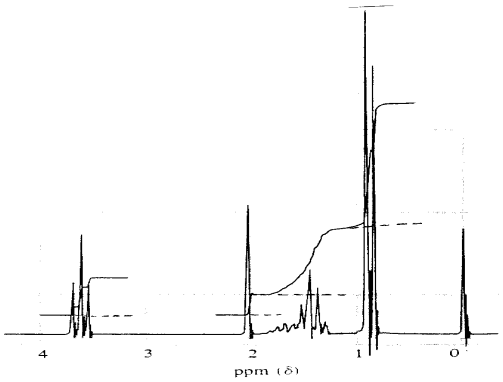
(a) **$C_4H_{10}O_2$**



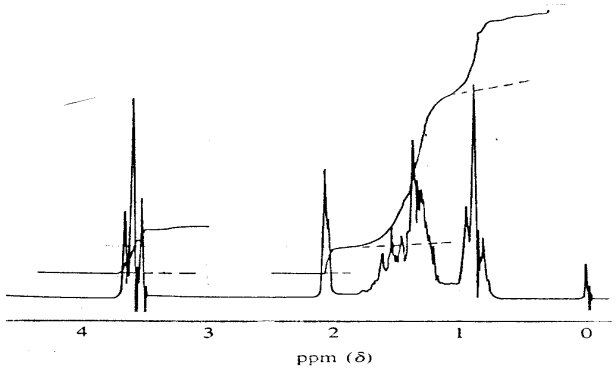
(b) **C_3H_7BrO**



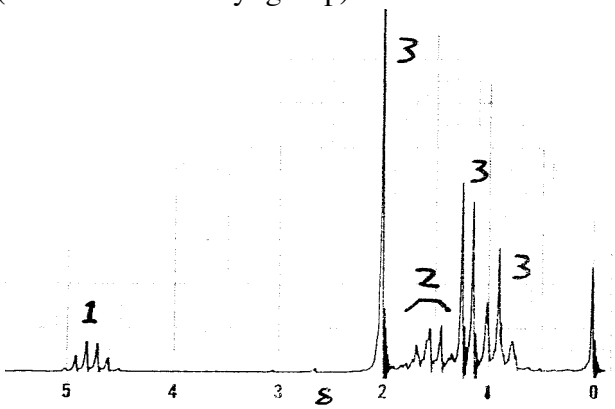
(c) **$C_5H_{12}O$**



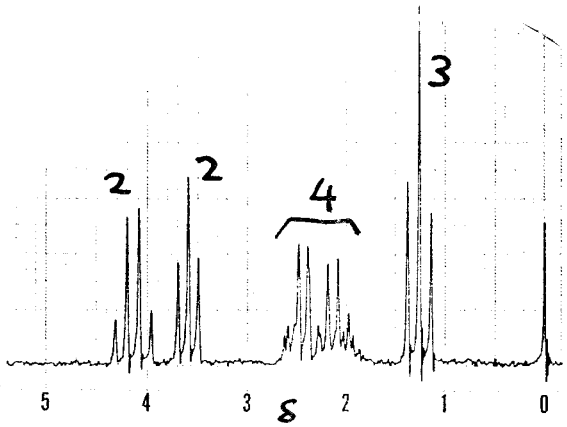
(d) **$C_5H_{12}O$**



(e) **$C_6H_{12}O_2$**
(hint: has a carbonyl group)



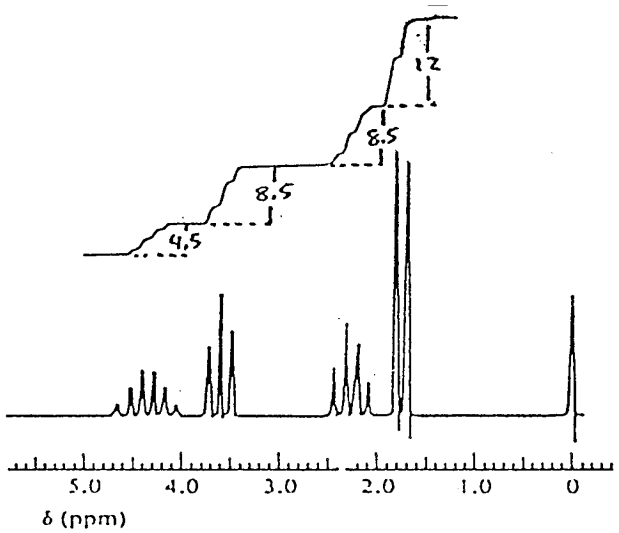
(f) **$C_6H_{11}ClO_2$**
(an ester)



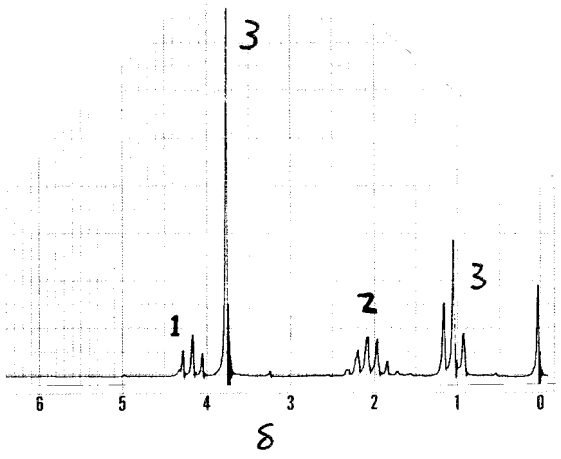
Chem 22
Spring 2010 *Name* _____
HW set 2
25 points; due Wed, Feb 3 at the beginning of class.

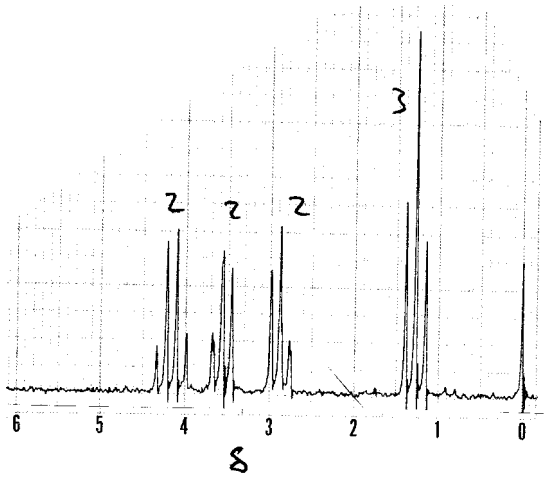
1. Same instructions as for #3 on the non-graded part.

(a) **$C_4H_8Br_2$**

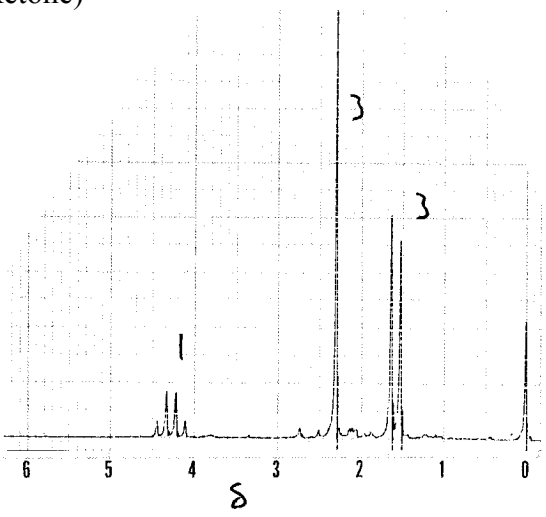


(b, c) both are esters with formula **$C_5H_9BrO_2$**





(d) **C_4H_7ClO**
(ketone)



(e) **$C_7H_{14}O_2$**
(ester)