Organic Chemistry II

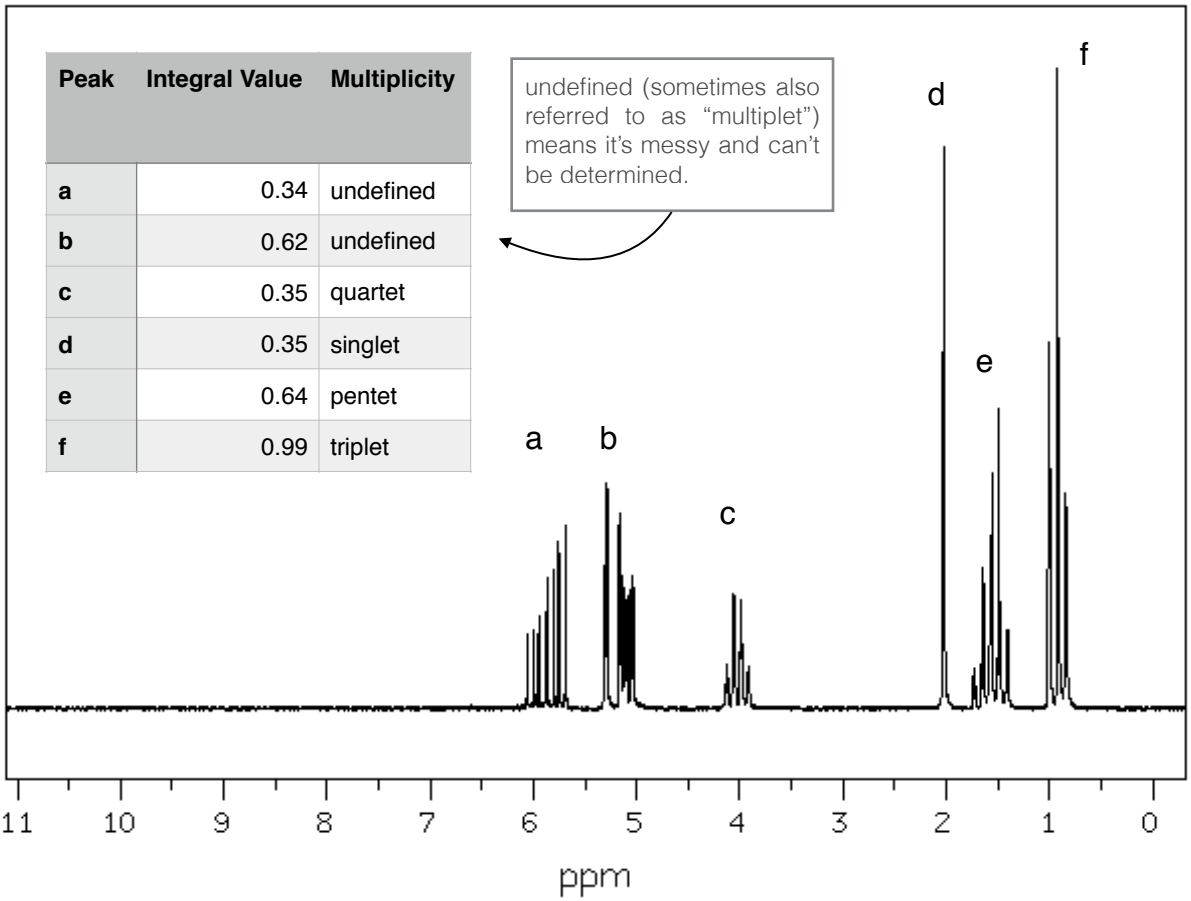
CHM 224

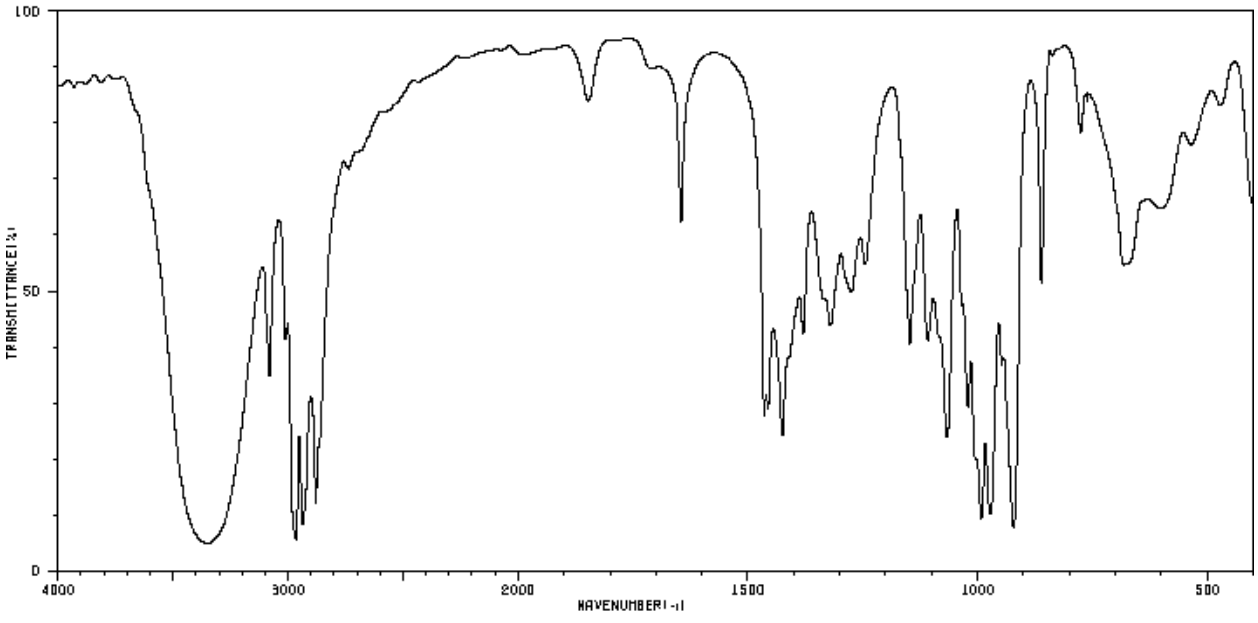
Homework

Name: _____ Due Date: 9/29/17

Peak	Integral Value	Multiplicity
a	0.34	undefined
b	0.62	undefined
c	0.35	quartet
d	0.35	singlet
e	0.64	pentet
f	0.99	triplet

undefined (sometimes also referred to as "multiplet") means it's messy and can't be determined.





1. The ^{1}H NMR and IR spectra for an unknown compound are on page 1. Propose a structure for this compound and assign all peaks on the ^{1}H NMR to the structure.

   Solving these questions is all about following the right strategy. Here's one:

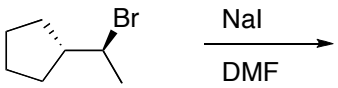
a. *Determine molecular formula.* Although no mass spectra is provided, you can easily count hydrogens using a 1H NMR. You can also determine the number of carbons from a ^{1}H NMR, however this is complicated if you have symmetry or carbons that have no hydrogens). Signals found in the ^{1}H NMR are generally from CH, CH_2 and CH_3 groups, however the integral values provided (in the table) are not whole number integers that match up to these expected groups. Divide the integral values by the lowest integral value in the list - if this gives you numbers close to 1, 2 and 3, then you may be able to count carbons and hydrogens (again, this is possible only if all carbons have hydrogens and there is no symmetry in the molecule). Look at the IR for functional groups you might recognize (especially those containing oxygen). You should now be able to determine a molecular formula for this molecule.

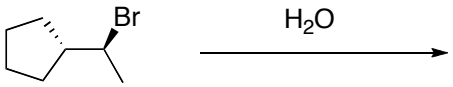
b. *Determine unsaturations.* I = (2C + 2 - H + N - X) / 2. A useful way to remember how to treat halogens (that's what X is in this equation) is that you treat halogens like hydrogens - you subtract them. For nitrogens, then, you do the opposite - you add them. Your value for I will give you number of pi bonds or rings. If your value is greater than 0, look in the ^{1}H NMR for pi bonds. If there are hydrogens on sp^2 carbons, they will appear downfield of 5. Depending on how many hydrogens are on the sp^2 carbons, you should be able to determine if the pi bond is in within a chain or if it is terminal (meaning you have a CH_2).

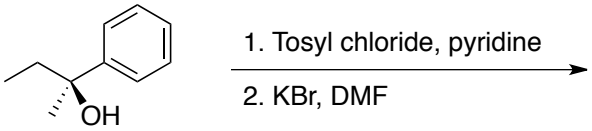
c. *Chemical shift.* Look where the peaks are on the x-axis. Downfield signals (either in the sp^2 region or sp^3 region) will be near an electron withdrawing group or atom.

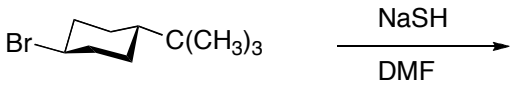
d. *Multiplicity.* The n + 1 rule is used to predict multiplicity. However if you already know the multiplicity, for example if a signal appears as a quartet, you can subtract 1 from the multiplicity to determine how many hydrogens the signal is coupled to (4 - 1 = 3).

2. Draw the structure of the major organic product(s) for each of the following reactions (no mechanism required). Indicate the stereochemistry for each reaction when appropriate. Write the name of the reaction mechanism to the right of each structure (these are all either S_N1 or S_N2 reactions).

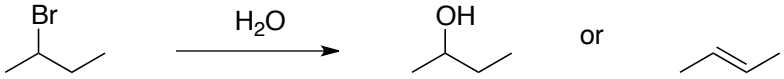


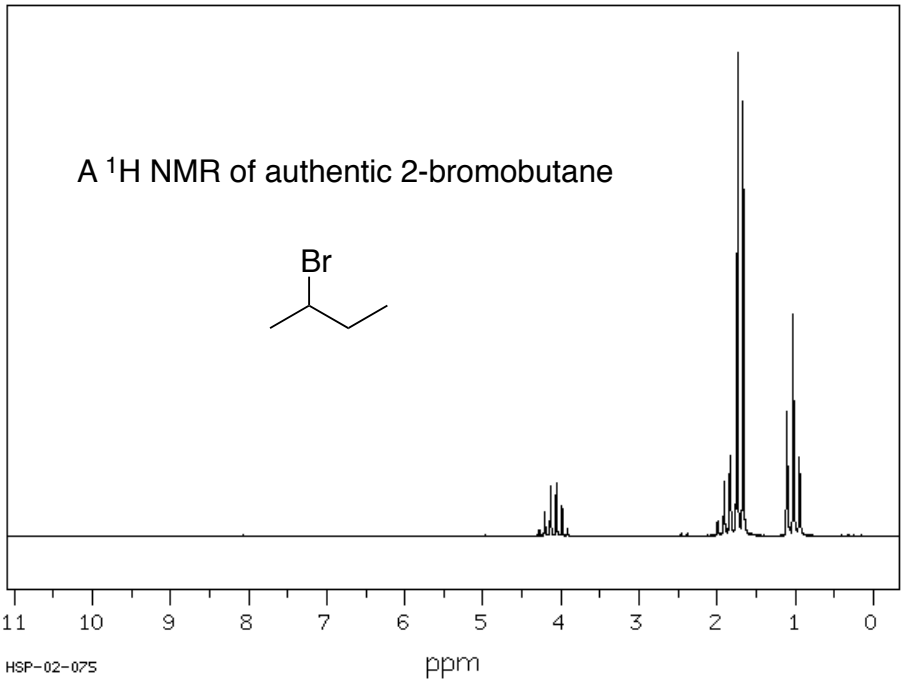


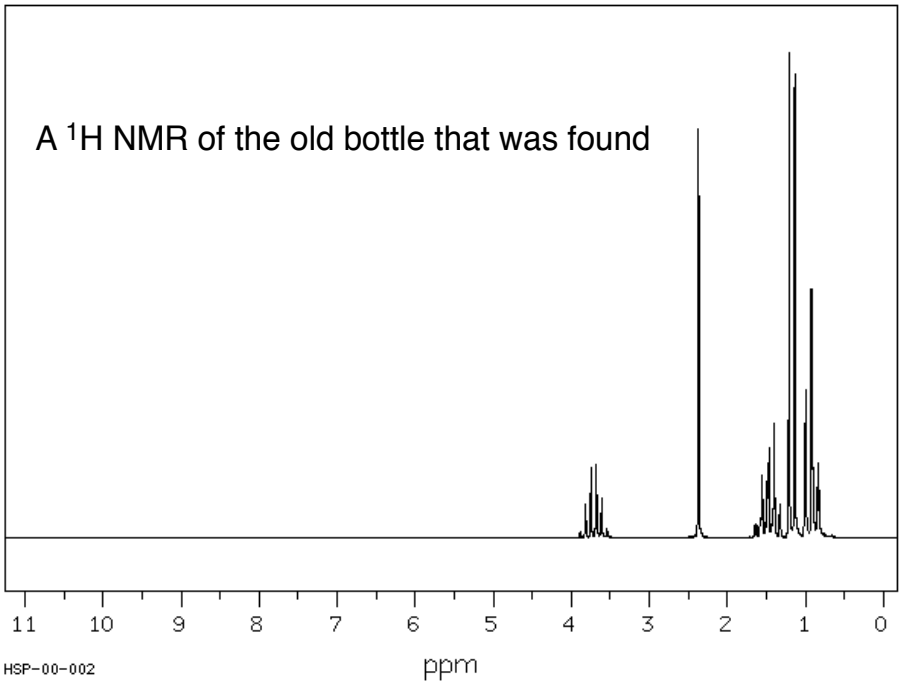




3. An old bottle 2-bromobutane was found in a lab; the bottle cap was missing and thus the chemical was exposed to water (from the atmosphere) at room temperature for an extended period of time. There are several possible products of the reaction between 2-bromobutane and water; the most common are shown in the reaction scheme below. Using the spectra on the following page, which is the most likely material in the bottle? Circle the chemical (on the scheme below) that you think the bottle contains.




A 1H NMR of authentic 2-bromobutane
Br
11 10 9 8 7 6 5 4 3 2 1 0
HSP-02-075
ppm


A 1H NMR of the old bottle that was found
11 10 9 8 7 6 5 4 3 2 1 0
HSP-00-002
ppm