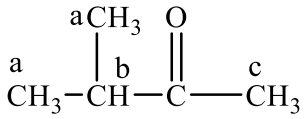
Homework 9

1. On a 400 MHz instrument, 0.2 ppm in the proton spectrum corresponds to 80 Hz. On the same instrument, 0.2 ppm on the C-13 corresponds to 25 Hz.

   ^{13}C has a spin of ½ and 2 orientations, whereas ^{2}H has a spin of 1 and 3 orientations.

2. Consider the NMR of 3-methyl-2-butanone.

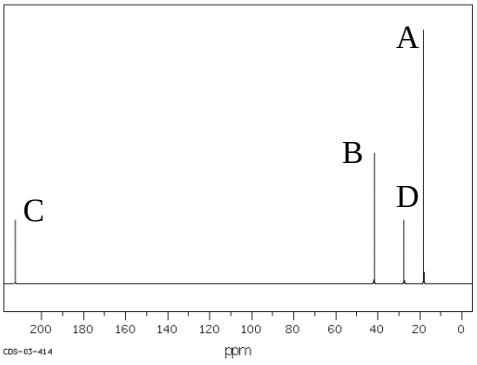
   Draw the structure of the compound and label the different H's in the compound using lower case letters starting with 'a.'

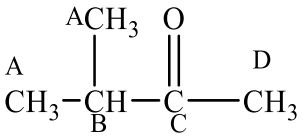


   Fill in the following table of these labeled protons with both the multiplicities of each and the integration. Leave blank any unneeded row. Fill in the integration of for each of these protons.

proton	Multiplicity Doublet, singlet, etc	Relative integration
a	doublet	6
b	septet	1
c	singlet	3
d		
e		

3. Sketch and label the expected decoupled C-13 spectrum of 3-methyl-2- butanone. This includes the number of peaks, approximate position of the peaks, rough intensity of the peaks, assignment of the peaks, and the labeling of the y-axis.



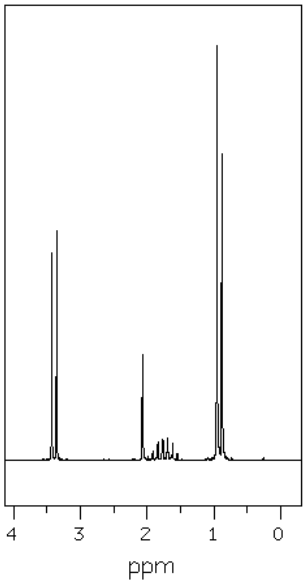


   The placement of B & D are somewhat arbitrary.

4. Sketch and label the expected DEPT spectra (the kind you would get using the EFT-60 instrument) of 3-methyl-2-butanone.

   A: unu
   B: uuu
   C: nnn
   D: unu

5. Report as much as you can about the compound that gave the following proton spectrum. The relative integration of the peaks (from left to right) were experimental determined to be 49, 25, 26, and 146.



The integration is 2:1:1:6, when simplified.
The peaks appear to be: doublet, singlet, hextet/septet, doublet.
It seems like the 0.9 ppm doublet & multiplet are a coupled group, i.e. isopropyl.
Next, it seems that the 3.4 doublet would be a methylene (CH2) coupled to the methyne (CH) of the isopropyl, making this an isobutyl group.
This leaves a singlet at around 2. This is too far upfield to be an acid or aldehyde proton, which suggests that it is an alcohol.
So, isobutyl alcohol? SDBS says: yes!