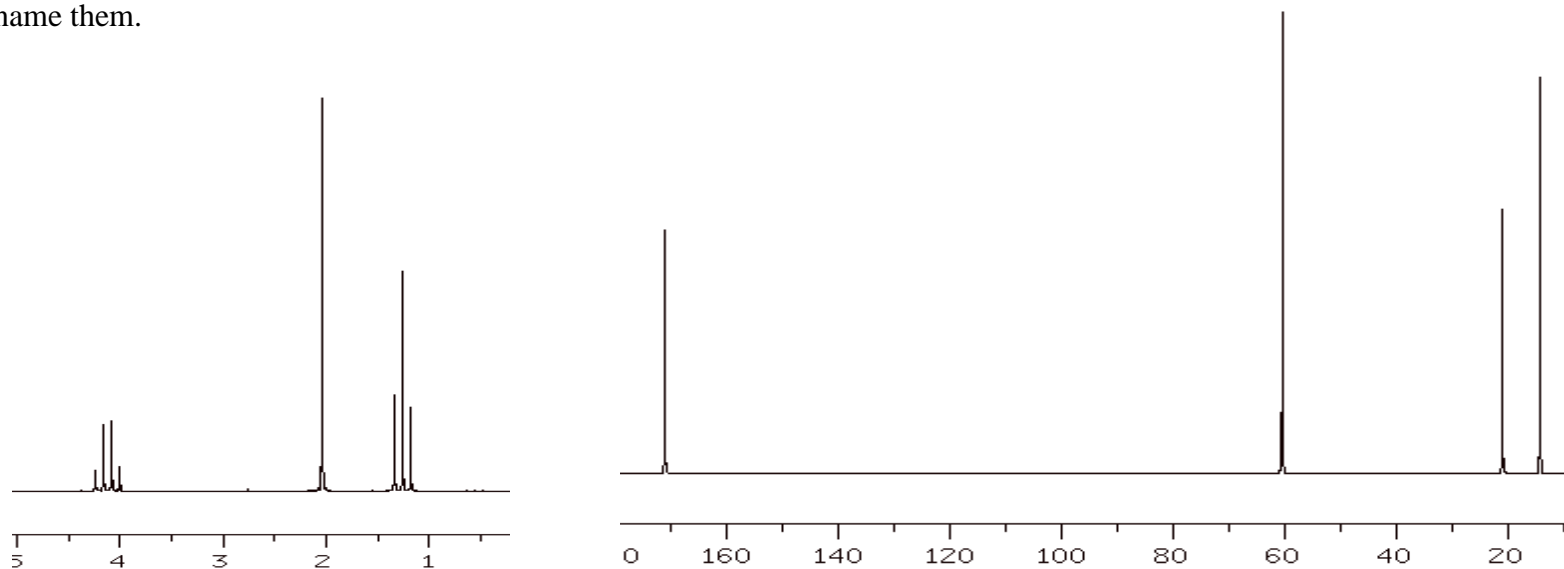


Homework 7

1. The following are the proton and carbon-13 spectra of 4 compounds with the molecular formula, $C_4H_8O_2$. Identify their structures and name them.

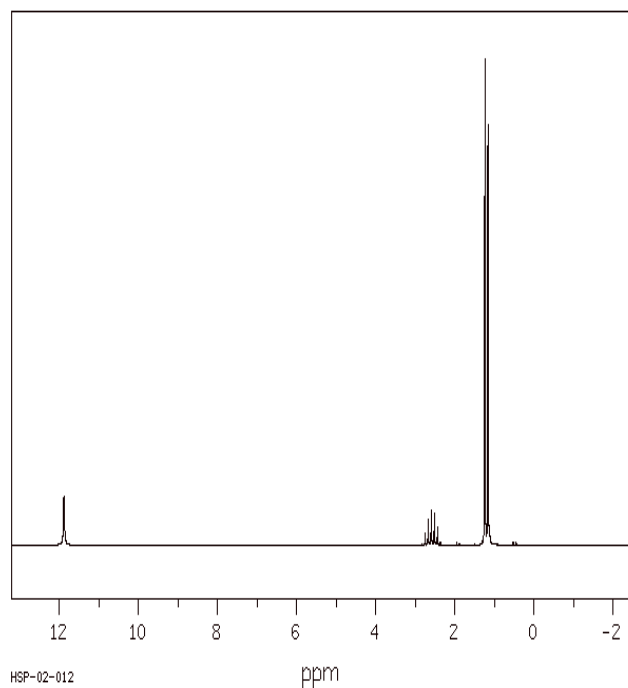
A.



Ethyl acetate*

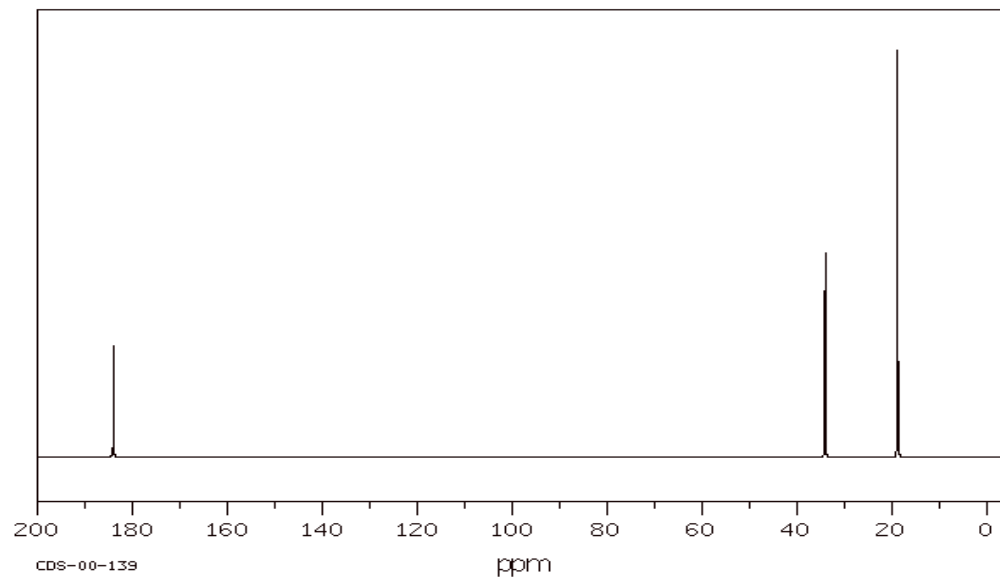
*It probably is not methyl propionate because the 1H singlet is at 2.0. If the methyl group were bound directly to the oxygen, it would probably be further downfield.

B



HSP-02-012

ppm

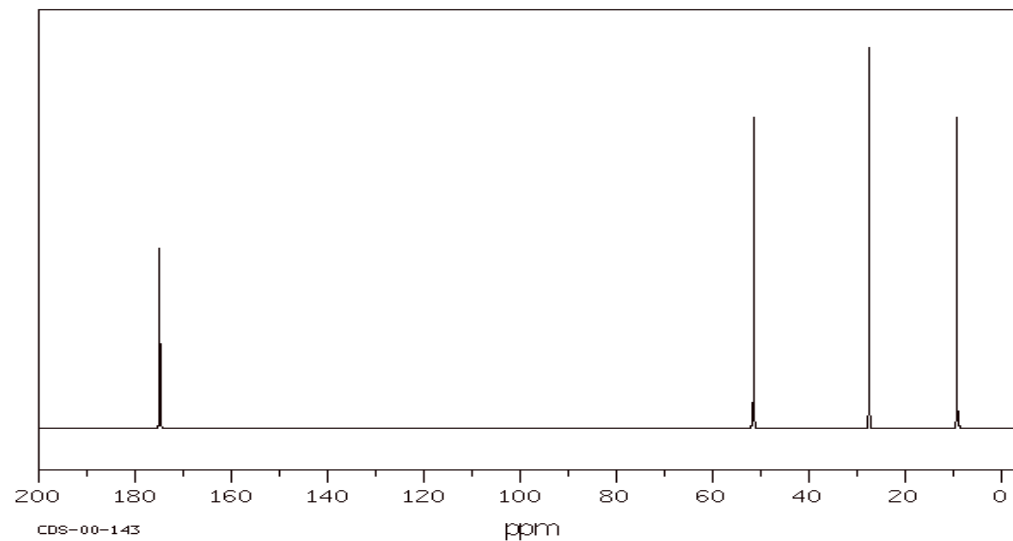
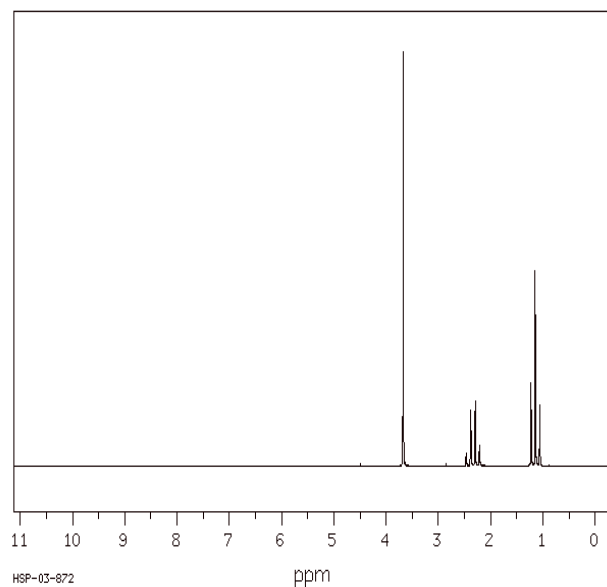


CDS-00-133

ppm

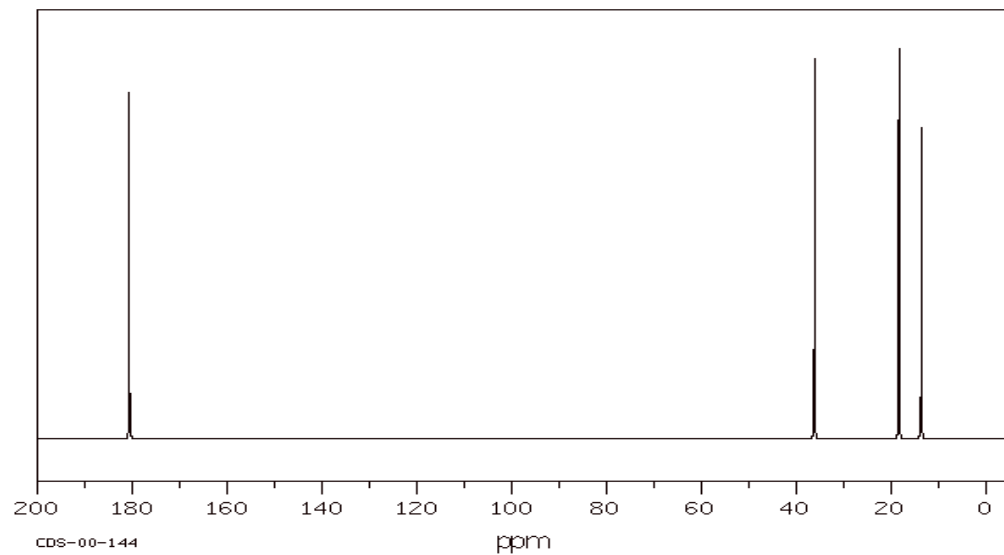
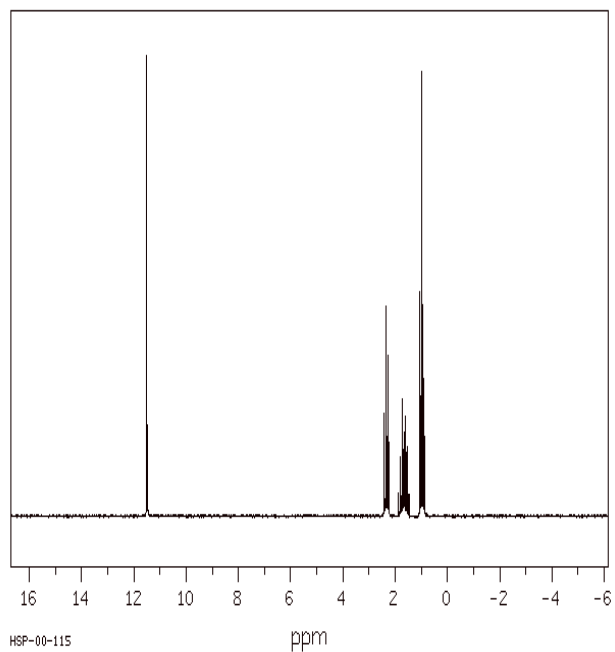
The ^1H peak at just under 12 ppm is a strong indicator that the compound is a carboxylic acid. The ^{13}C peak at just over 180 ppm is consistent with a CO group being present. The ^{13}C NMR furthermore displays two additional carbon resonances in a 1:2 ratio for a total of 4 carbons, consistent with the formula. This suggests an isopropyl group and the ^1H spectrum has a doublet and what could well be a small septet. Thus, the compound is likely to be 2,2-dimethylpropanoic acid.

C.



In the ¹H spectrum you have a triple and quartet, so begin by assuming an ethyl (CH₃CH₂-) group somewhere. That leaves C₂H₃O₂. The ¹³C peak at 175 or so, suggests a CO. So now you're left with CH₃O. Back to the ¹H spectrum where there is a single, so CH₃ isolated from the ethyl, leaving an oxygen atom. So you probably have an ester: methyl propionate (CH₃CH₂CO₂CH₃) or ethyl acetate (CH₃CO₂CH₂CH₃). While you can't know for certain which it is, the CH₃ single is far down field of the ethyl quartet. Thus, it's a good bet that the compound is methyl propionate.

D.



In the ¹H spectrum, there is a peak at almost 12 ppm, usually the location of a carboxylic acid proton. If so, the compound has to be either butanoic acid or 2-methylpropionic acid. Since all of the carbon resonances are the same height and there are 3 different proton resonances, you can rule out the propionic acid. It's a little hard to see, but the splitting looks reasonable for butanoic acid.

2. A compound is 69.6% C, 7.24% H, and 23.2% O. When 0.3 grams of the compound is dissolved in 10 g of t-butyl alcohol ($K_f=8.2\text{ }^\circ\text{C/m}$) the freezing point of the solution is $23.1\text{ }^\circ\text{C}$ compared to $24.9\text{ }^\circ\text{C}$ for the pure solvent. The compound has the following C-13 and proton NMR spectra. a) What is the empirical formula of the compound? b) What is the molecular formula of the compound? c) What is the structure and name of the compound?

