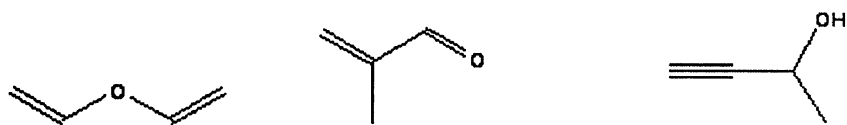


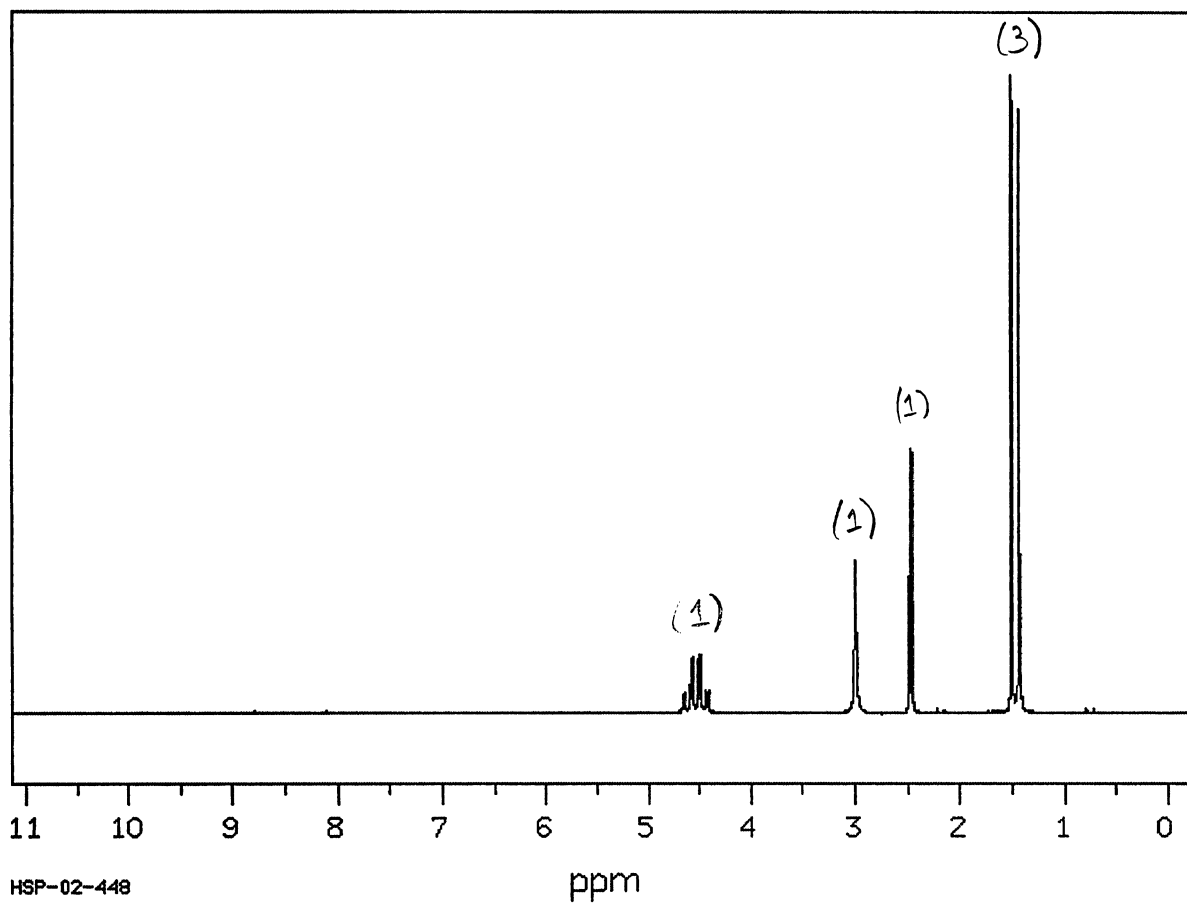
Chem332 Discussion Section 6

1. While in the lab, you decided to run three reactions using the following three compounds:

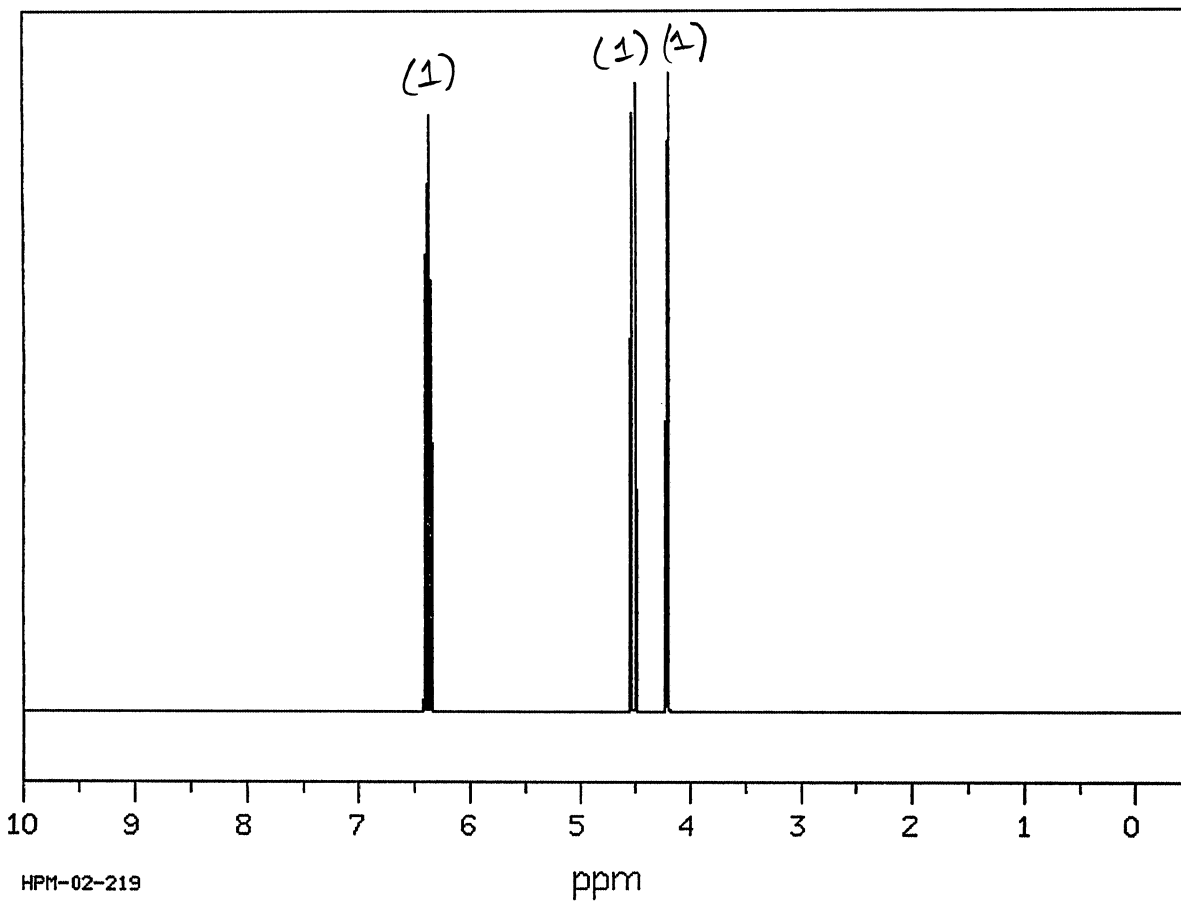


However, you forgot to label each flask and mixed up which flask had which compound. You decide to take some ¹H NMRs to fix your mistake.

Flask 1:



Flask 2:



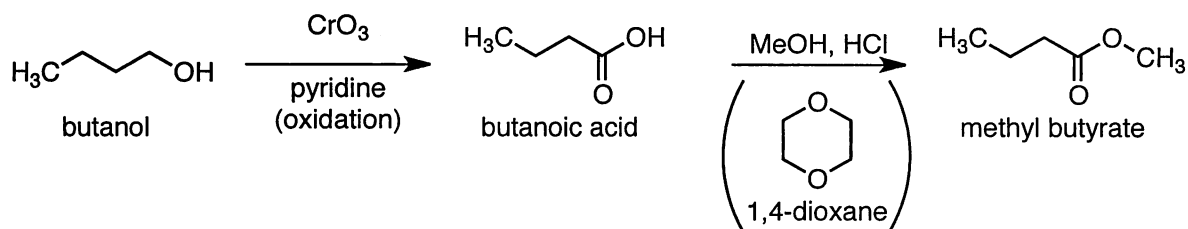
Which flask had which compound?

Out of curiosity, you wonder what the NMR would look like for the remaining compound. What are some features you would look for to distinguish that compound from the rest?

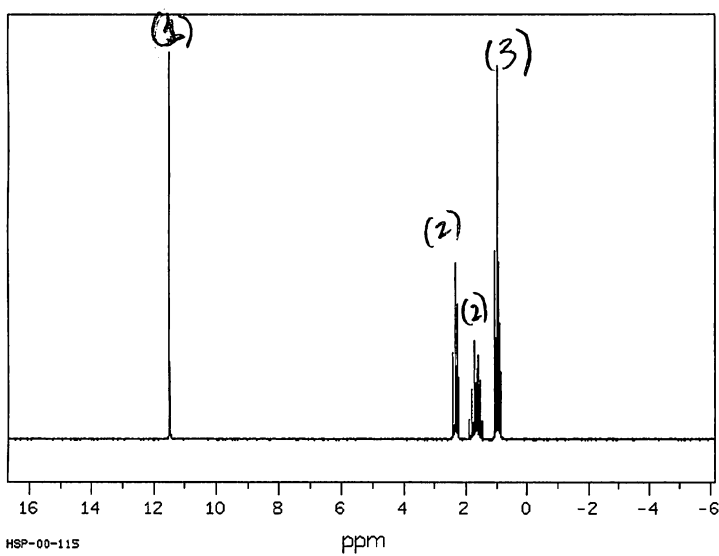
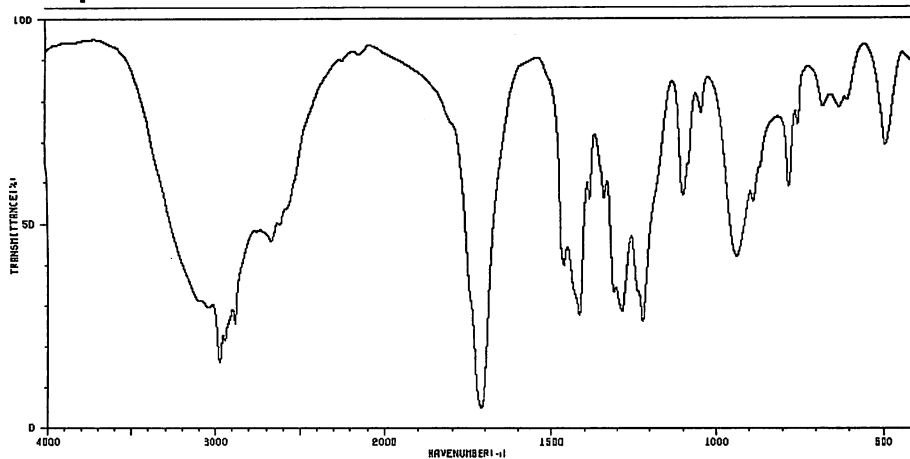
2. You want to prepare methyl butyrate and devise the following synthesis from butanol. However, you are a little short on reagents and time (you're about to go to Florida for Spring Break, after all). You manage to get through the synthesis, purify your products (for some reason, you isolated 5 compounds from this reaction), and stick them in the freezer before leaving town. When you come back, you determine their molecular formulas using MS and elemental analysis and collect IR, ^1H NMR and ^{13}C NMR data on the compounds you isolated to figure out what they are.

Note: The work-up conditions may be important. To purify your product, you added 1,4-dioxane (on accident, rushing to catch your plane) and then EtOAc and H_2O (on purpose). You separated the organic layer from the aqueous layer and then fractionally distilled to obtain the 5 compounds.

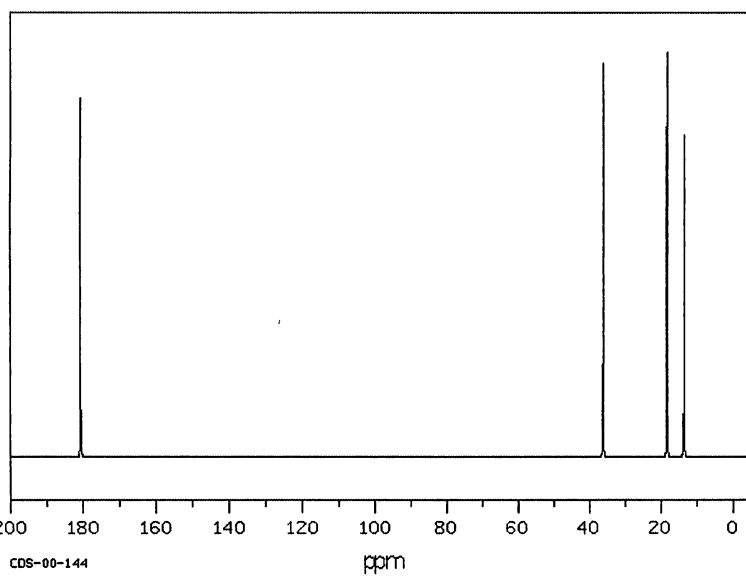
What are the 5 compounds??? (And what could you have done differently to avoid these problems? Think about your options for work-up...)



Compound 1 Molecular Formula: $C_4H_8O_2$



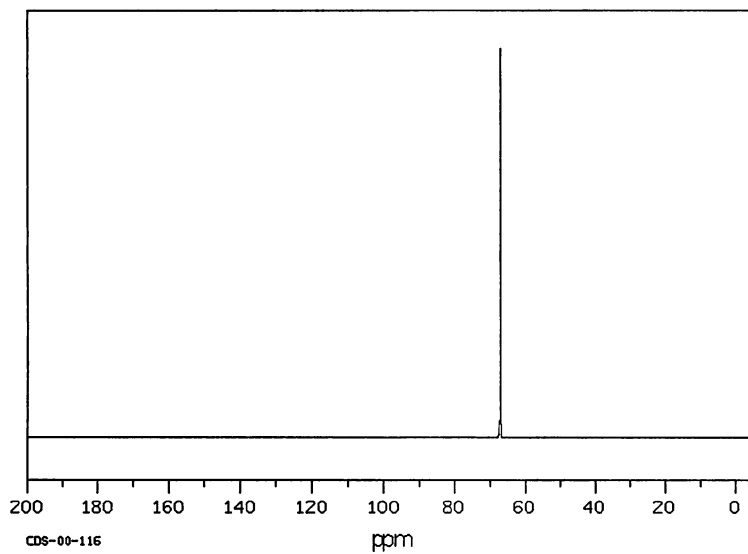
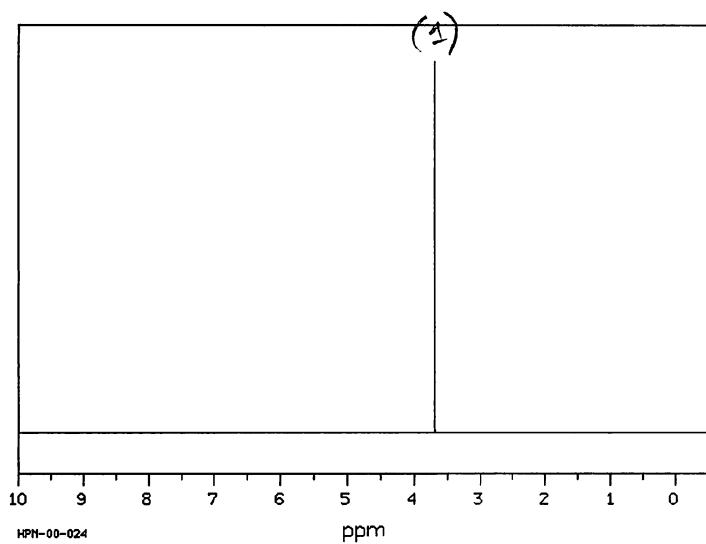
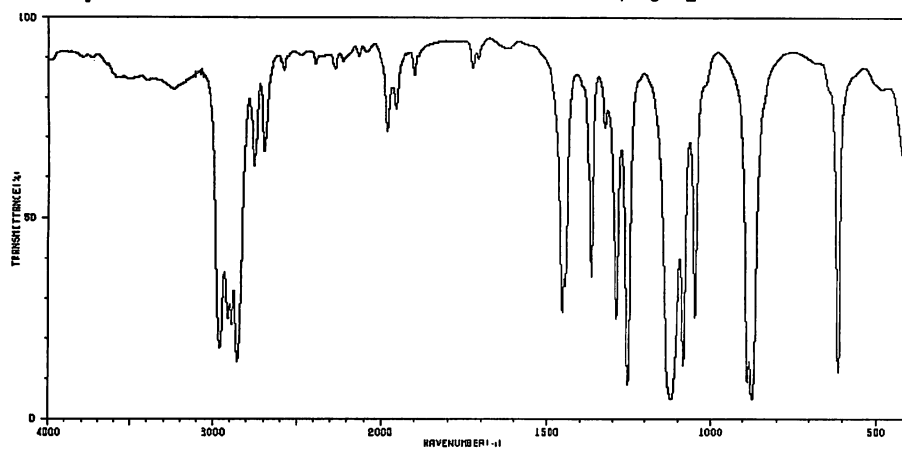
HSP-00-115



CDS-00-144

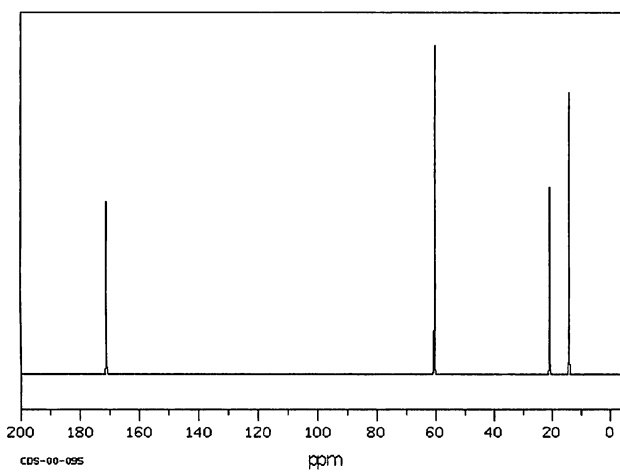
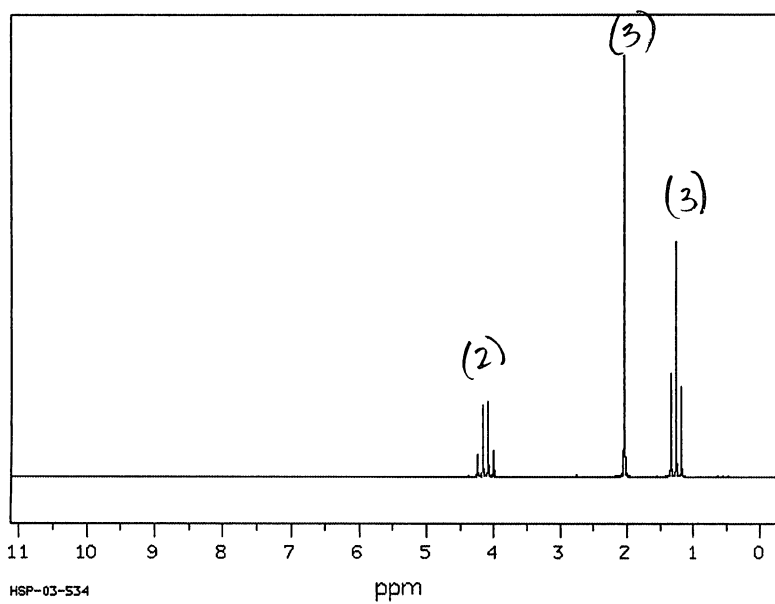
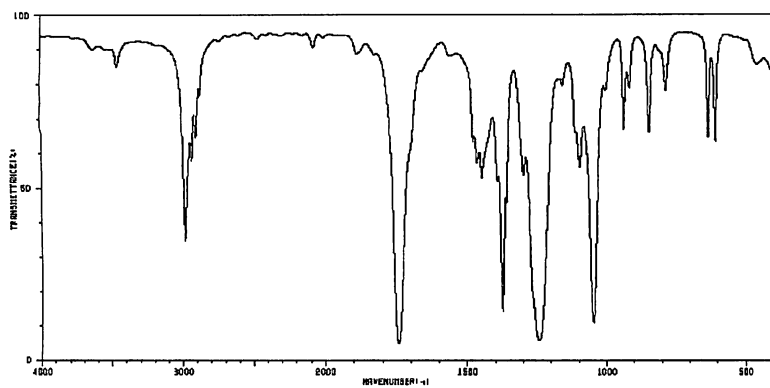
Compound 2

Molecular Formula: $C_4H_8O_2$



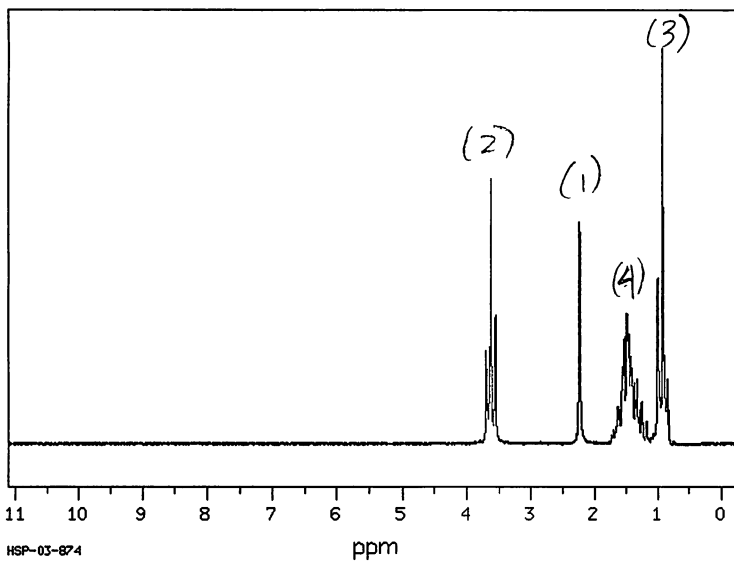
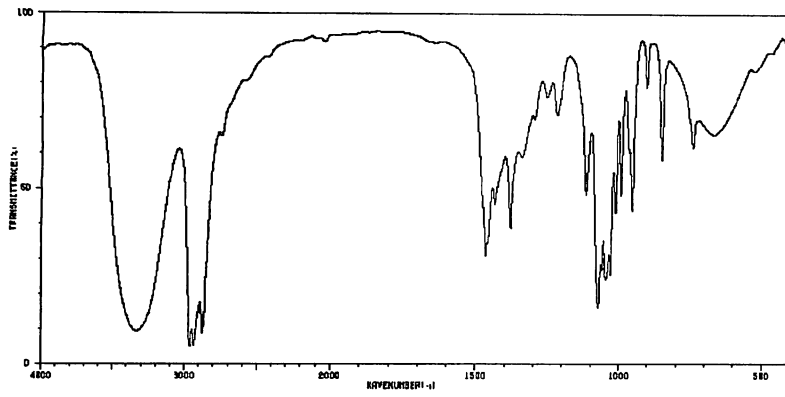
Compound 3

Molecular Formula: $C_4H_8O_2$

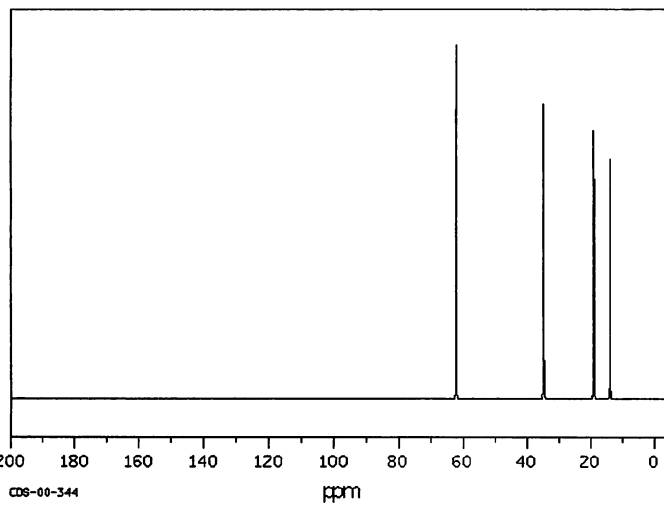


Compound 4

Molecular Formula: $C_4H_{10}O$



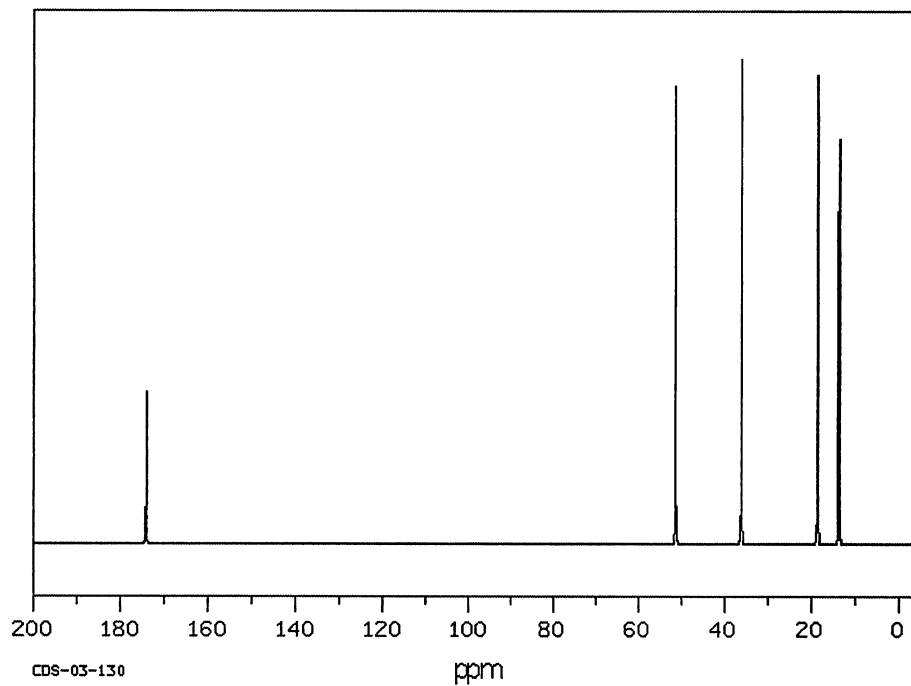
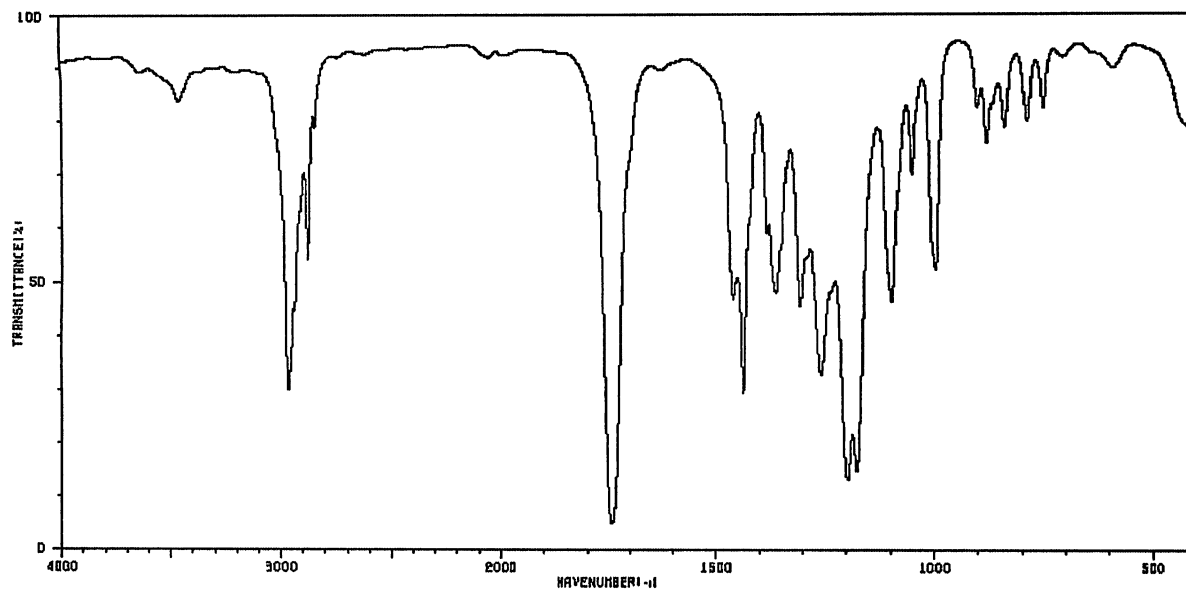
HSP-03-874



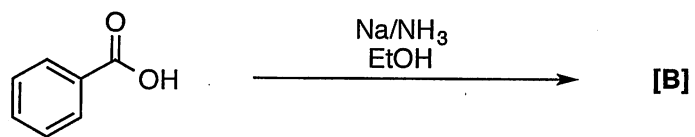
CS-00-344

Compound 5 (Can you figure this one out without ^1H NMR?)

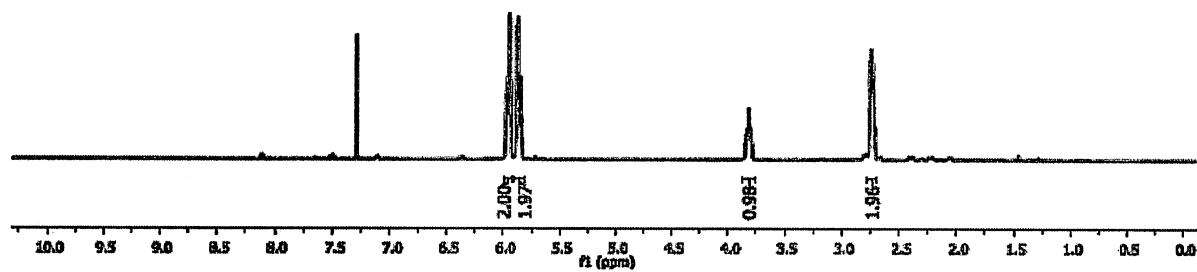
Molecular Formula: $\text{C}_5\text{H}_{10}\text{O}_2$

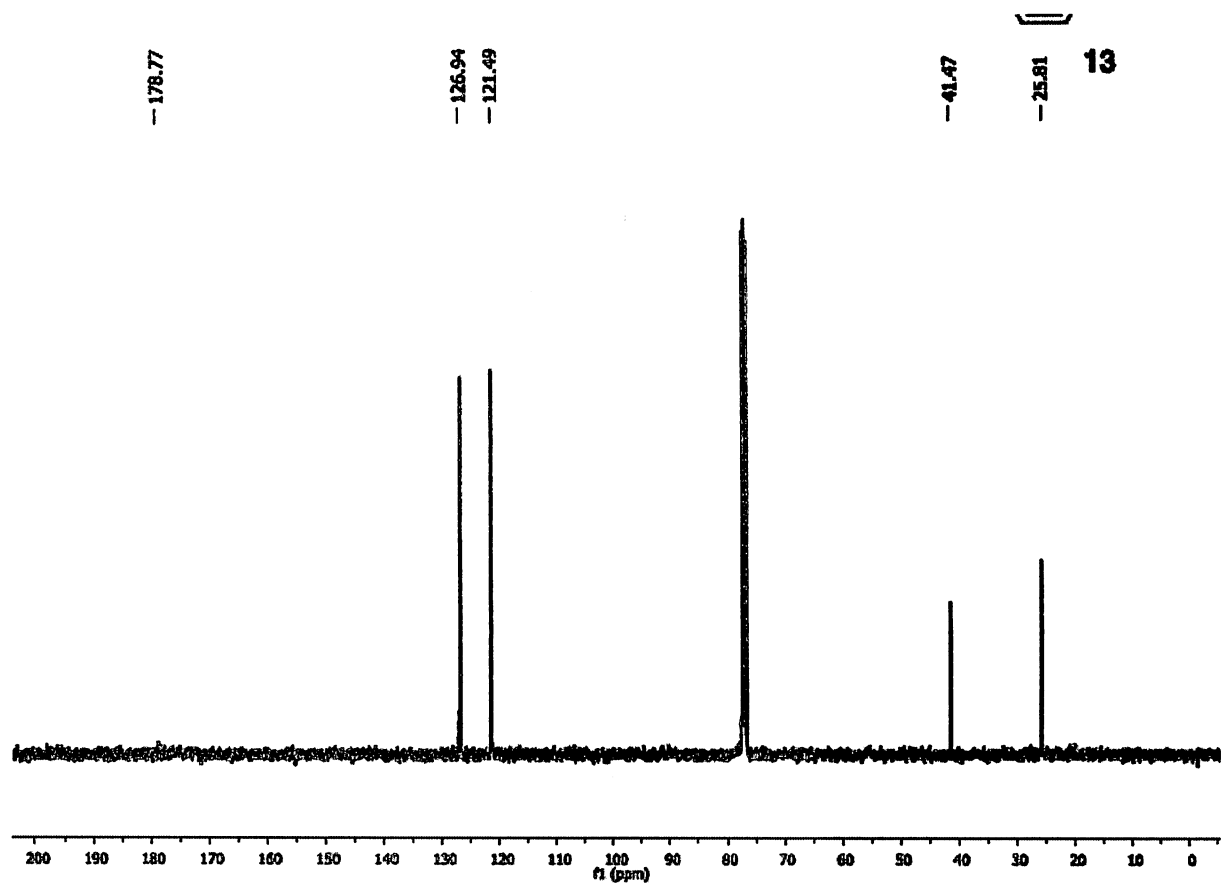


3.



The ^{13}C and ^1H spectra of **B** are shown below. What is the structure of **B**?





What is the mechanism of the transformation from the starting material to product B?