In-Class Exercise: Using NMR to Analyze a Typical Chemical Reaction

1. Let's say you were interested in conducting the reaction below.



Before running the reaction, you take an NMR spectrum of the starting material dissolved in $CDCl_3$ (shown below). Is the spectrum consistent with the structure of the starting material? To answer this question, follow these steps:

- a. How many resonances would you expect for this molecule? Put in other words, how many inequivalent types of protons are there in the molecule?
- b. Label each set of equivalent protons in the molecule structure with a lower-case letter (*a*, *b*...). Then, match each letter to one of the resonances in the spectrum, using a chemical shift table to help. Do things match up?



- So you run the reaction. Some initial analytical work shows that the reaction produced a mixture of two different materials, and you separate the components of the mixture by column chromatography. You take small amounts of the two isolated materials, which we'll call molecules A and B, and take NMR spectra of each in CDCl₃ (shown below and next page).
 - a. The spectra show that neither molecule is the starting material, which is a good thing—at least the reaction conditions did something. Is either molecule A or B the expected product? To answer this question, it might help to go through the same process that you went through in problem 1.
 - b. Given what you know about the reaction, can you identify the structure of the other product from the NMR spectrum? How might the reaction have generated this product?



