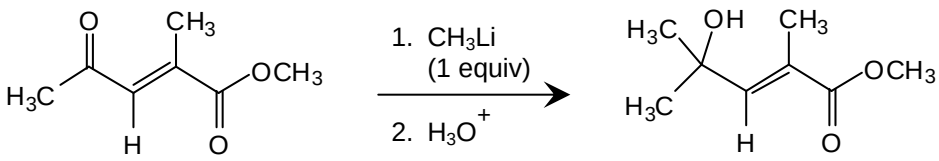
Chemistry 2331H Monday, November 25

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

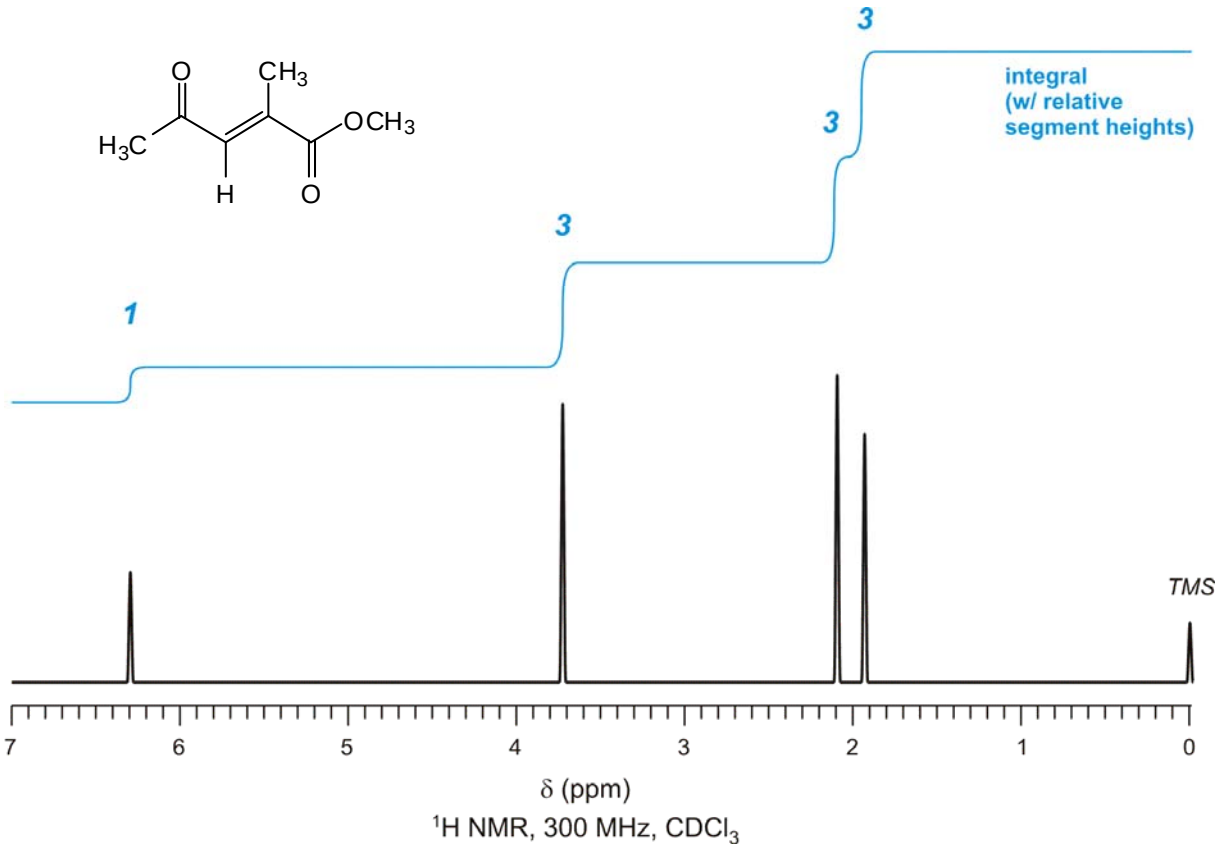
1. Sydney, a chemist, is interested in conducting the reaction below.



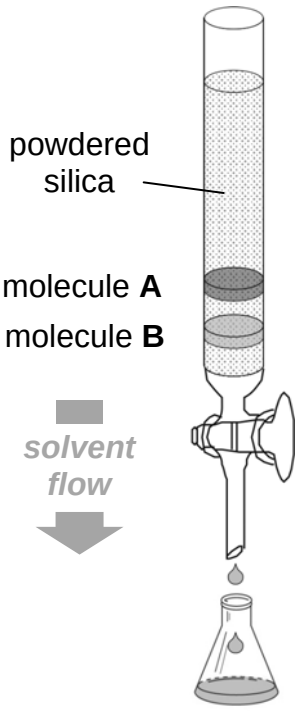
Before running the reaction, Sydney takes an NMR spectrum of the starting material dissolved in deuterated solvent (shown below). Is the spectrum consistent with the structure of the starting material? To answer this question, follow these steps:

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?



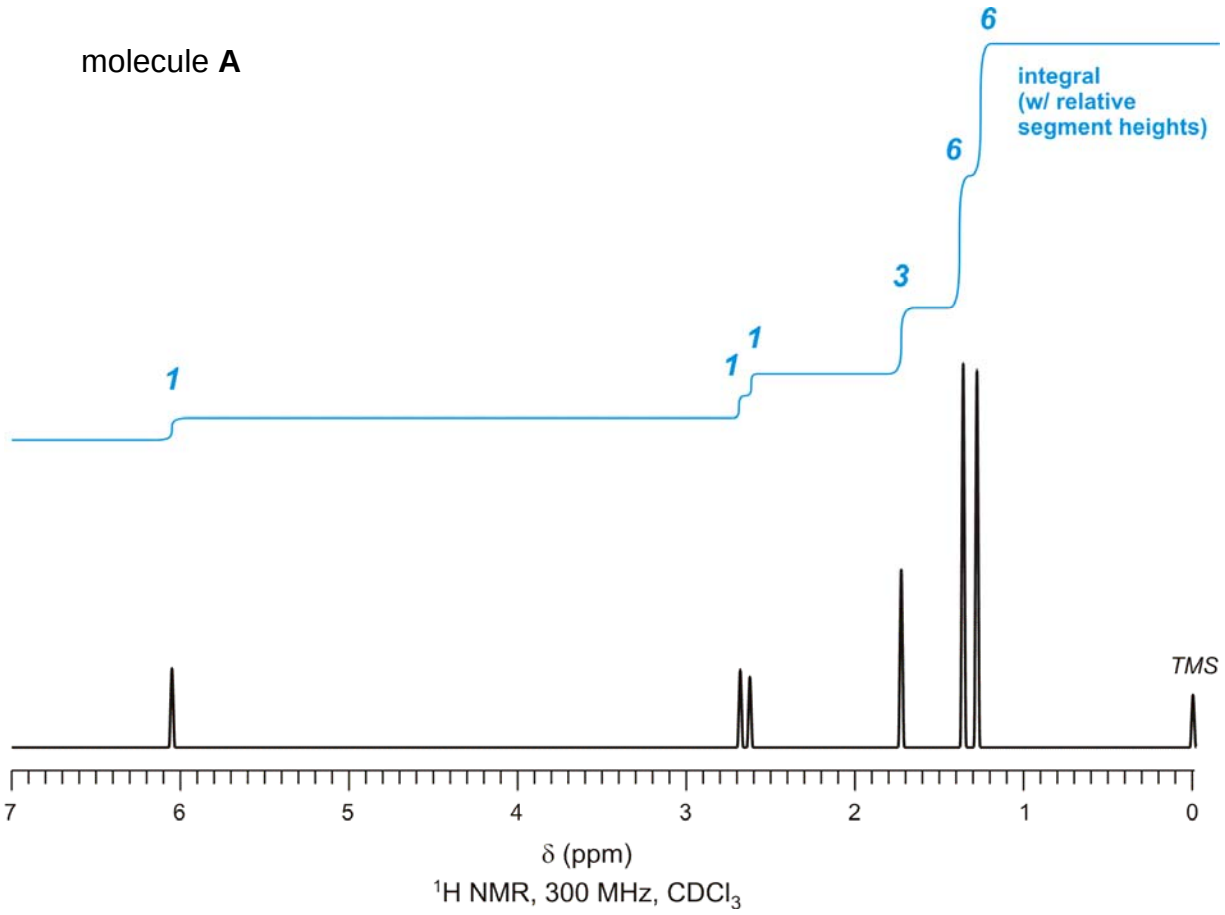
2. So Sydney runs the reaction. Some initial analytical work shows that the reaction produced a mixture of two different materials, and so Sydney separates the components of the mixture by column chromatography (diagrammed at right). She takes small amounts of the two isolated materials, which we'll call molecules **A** and **B**, and takes NMR spectra of each in $CDCl_3$ (shown below and next page).



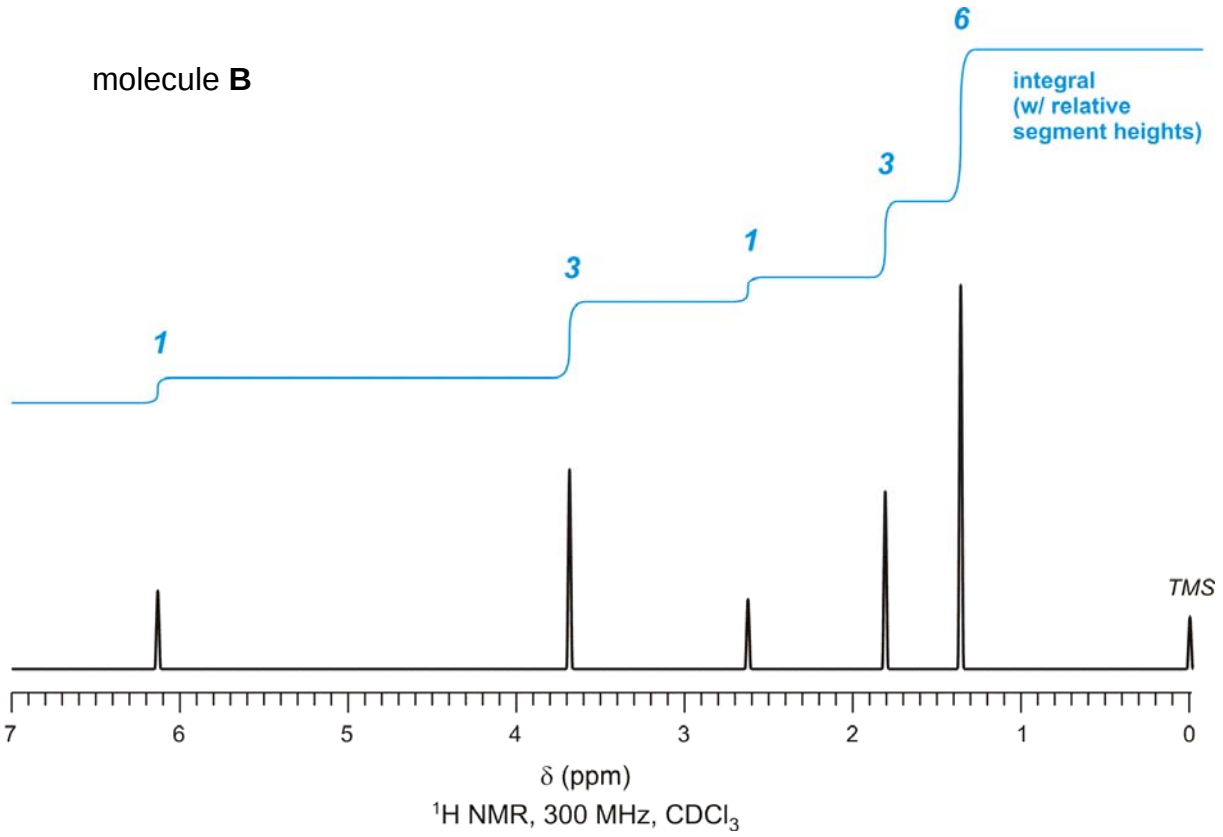
Column chromatography. A glass column is packed with a granular material, and then a solution of a mixture of molecules is flowed through the column. Because molecules A and B stick differently to the silica (here, A sticks more), the two molecules drip out of the end of the column at different times.

   a. The spectra show that neither molecules are 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.

molecule **A**



molecule **B**



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?