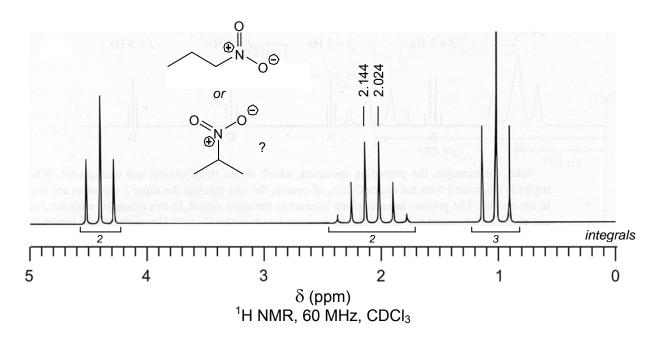
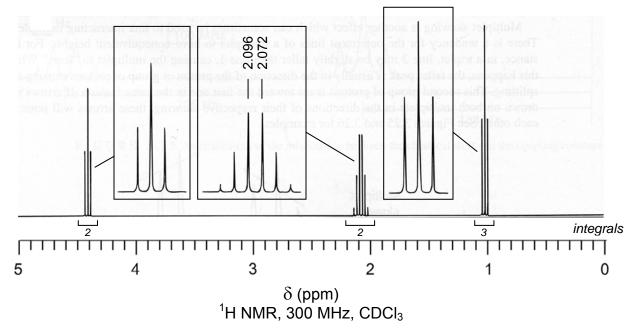
In-Class Exercise: Splitting Patterns in NMR

The two NMR spectra of nitropropane ($C_3H_7NO_2$) shown below were taken on different NMR spectrometers, with different field strengths.





In the lower spectrum, the boxes show expanded views of the indicated multiplets.

- a. How many inequivalent protons are represented in these spectra? In other words, how many resonances are there? (Keep in mind that a multiplet is still just a single resonance.)
- b. Which isomer of nitropropane (1-nitropropane or 2-nitropropane) do the spectra represent?
- c. Assign each multiplet to a distinct proton in the nitropropane structure. (You might think you need a chemical shift table to do this, but you really don't.) Explain each splitting pattern in the spectrum in terms of the number of neighbors each proton has.
- d. What is the J value for coupling between all of the protons in nitropropane? The values shown on the marked peaks are in ppm; you can calculate a frequency difference $\Delta\delta$ in ppm, but you'll have to convert that value to Hz to express it as a J value. Use the equation I showed in class,

$$chemical \ shift, \ ppm \ \delta = \frac{shift \ downfield \ from \ TMS \ (in \ Hz)}{spectrometer \ frequency \ (in \ MHz)}$$

There is no need to convert units in the equation; 1 ppm = 1 Hz/MHz.