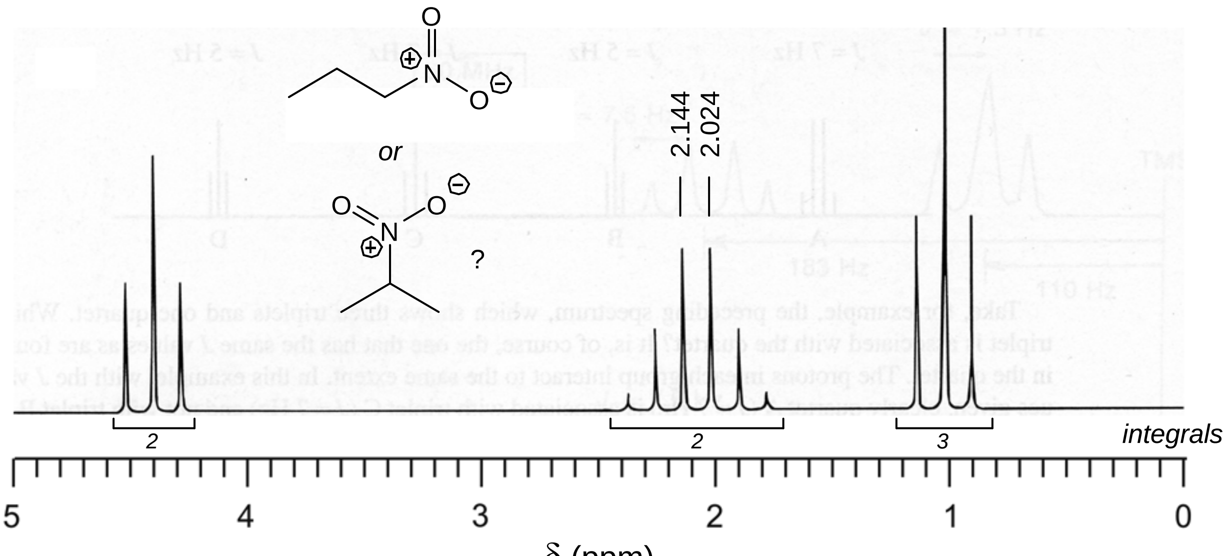
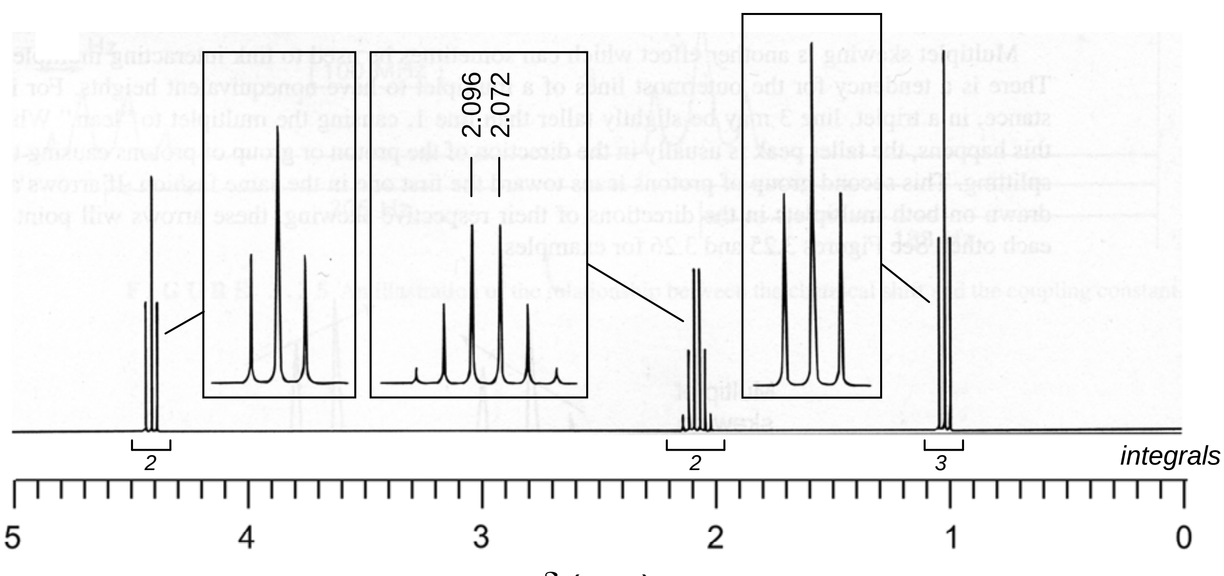
In-Class Exercise:
Splitting Patterns in NMR

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



^{1}H NMR, 60 MHz, $CDCl_3$



^{1}H NMR, 300 MHz, $CDCl_3$

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,

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

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