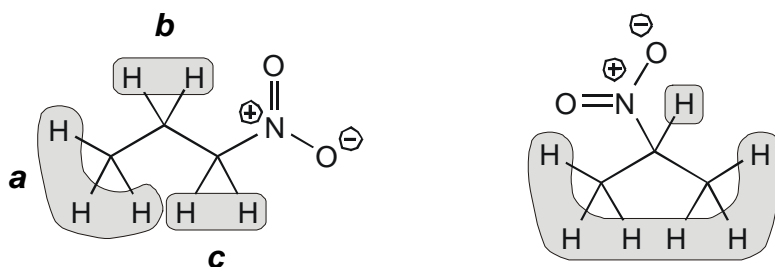


In-Class Exercise Solutions: Splitting Patterns in NMR

- a. Each spectrum has three multiplets. Each multiplet is a single resonance, representing a single set of equivalent protons. So that means our molecule must have three inequivalent sets of protons.

The chemical shift of each multiplet is the center of the multiplet. So that means our three resonances have chemical shifts $\delta = 4.41$, 2.08, and 1.02 ppm. As we discussed in class, chemical shift doesn't vary with spectrometer field strength, so it doesn't matter which spectrum you use to calculate these values.

- b. Only 1-nitropropane has three inequivalent sets of protons; 2-nitropropane only has two sets.



So only 1-nitropropane is consistent.

- c. protons a:

Only one of the three multiplets, the one at $\delta = 1.02$ ppm, has integrated intensity 3. Only group **a** has that many protons. It makes sense that this group should be the farthest upfield (at the lowest frequency); these protons are farthest from the positively charged, electron-withdrawing nitrogen that deshields the nearer H's. The multiplet is a triplet, corresponding to splitting with the two neighbors **b**.

protons b:

These protons have five neighbors—all of the protons at **a** and **c**. So, assuming simple splitting where all J values are the same (which doesn't always happen, but let's see if it does here), the resonance corresponding to protons **b** should be a sextet. The multiplet at $\delta = 2.08$ ppm fits that bill.

protons c:

These are the closest to the electron-withdrawing nitro group, so it makes sense that these protons should appear the farthest downfield (at highest frequency), at $\delta =$

4.41 ppm. They couple only to the two protons at **b**, and so we'd expect this resonance to be a triplet, which it is.

- d. In the case of simple splitting, the coupling constant J can be calculated as the distance between any pair of peaks. Using the pair of labeled peaks in the upper spectrum,

$$\begin{aligned}\Delta\delta &= (2.144 \text{ ppm}) - (2.024 \text{ ppm}) \\ &= 0.120 \text{ ppm}\end{aligned}$$

To convert this to J in Hz, we have to multiply by the spectrometer frequency:

$$\begin{aligned}J \text{ (Hz)} &= \Delta\delta \text{ (ppm)} \times \nu_0 \text{ (MHz)} \\ &= (0.120 \text{ ppm}) \times (60 \text{ MHz}) \\ &= 7.2 \text{ Hz.}\end{aligned}$$

So, to sum up,

