

Good! Be careful to use precise language, “the frequency of NMR” is a bit vague. It would be more clear to say “the strength of the magnetic field.”



NMR Jigsaw 1E

October 2024

1 Exercise 1

1.1

We use the following formula: $\delta(\text{ppm}) = 10^6 \times \frac{\nu - \nu_{\text{ref}}}{\nu_{\text{ref}}}$.

Plugging in the question's values we obtain the following:

$$\delta_1 = 10^6 \times \frac{400.135023 - 400.130000}{400.130000} = 12.5534201 \text{ ppm}$$

$$\delta_2 = 10^6 \times \frac{400.137921 - 400.130000}{400.130000} = 19.7960662 \text{ ppm}$$

1.2

Based on the chemical shifts for both peaks found in 1.1, we can find the new frequency based on the formula:

$$\begin{aligned} \nu_{\text{new}} &= \nu_{\text{ref}} + (\delta \times 10^{-6} \times \nu_{\text{ref}}) \\ \nu_1 &= 900.130000 + (12.553 \times 10^{-6} \times 900.130000) = 900.130000 + 0.01129971 = \\ &900.1413 \text{ MHz} \\ \nu_2 &= 900.130000 + (19.796 \times 10^{-6} \times 900.130000) = 900.130000 + 0.017819 = \\ &900.1478 \text{ MHz} \end{aligned}$$

The chemical shifts (in ppm) relative to both of these new peaks remain the same as in 1.1

1.3

We report peak locations in ppm so that their values are not dependant on the specific instrument and its properties (such as its magnetic field strength), but instead only to their distance to the relative frequency on the spectrometer, so

that the reported values are interpretable to anyone without having to know the exact specifics of the instrument they were measured with.

1.4

$$\nu_{sep} = |\delta_2 - \delta_1| \times \nu_{ref}$$

$$\nu_{sep,400} = |19.7960662 - 12.5534201| \times 400.130000 = 2897.99998 \text{ Hz}$$

$$\nu_{sep,900} = |19.7960662 - 12.5534201| \times 900.130000 = 6519.32303 \text{ Hz}$$

In rad/s:

$$\nu_{sep,400} = 2\pi \times 2897.99998 \text{ Hz} = 18219.37854 \text{ rad/s}$$

$$\nu_{sep,900} = 2\pi \times 6519.32303 \text{ Hz} = 40975.02689 \text{ rad/s}$$

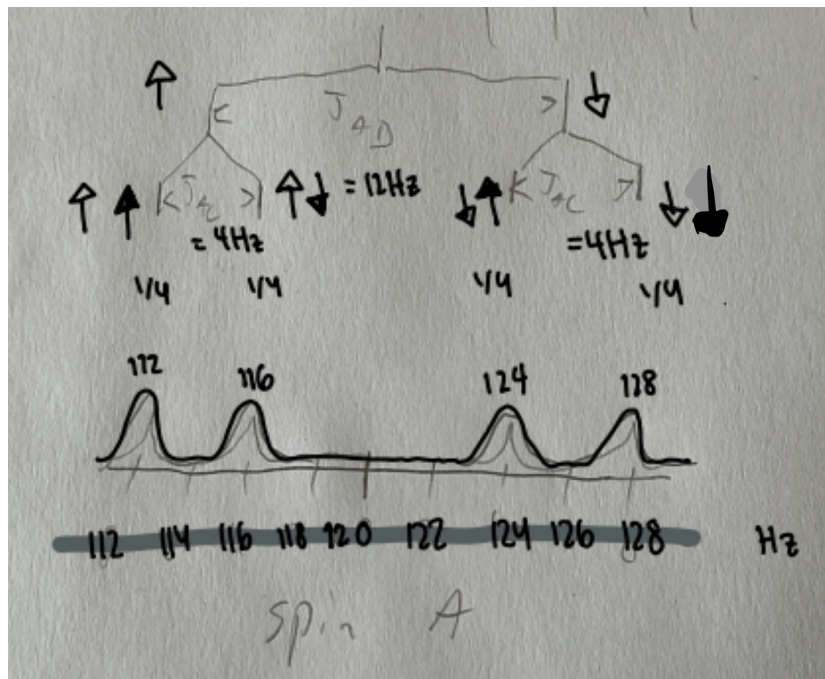
Good! Keep in mind that ν (v) is for frequency in time units (Hz), while ω (w) is used for angular frequency (in radians)

1.5

Yes, it is worth it to use higher magnetic fields: as shown by the previous question, higher magnetic fields allow for higher frequency separations in the spectrum, which may then allow us to distinguish them more easily and avoid overlaps. Higher magnetic-field spectrometers also tend to have a more significant resolution.

2 Exercise 2

2.1 Parts a and b

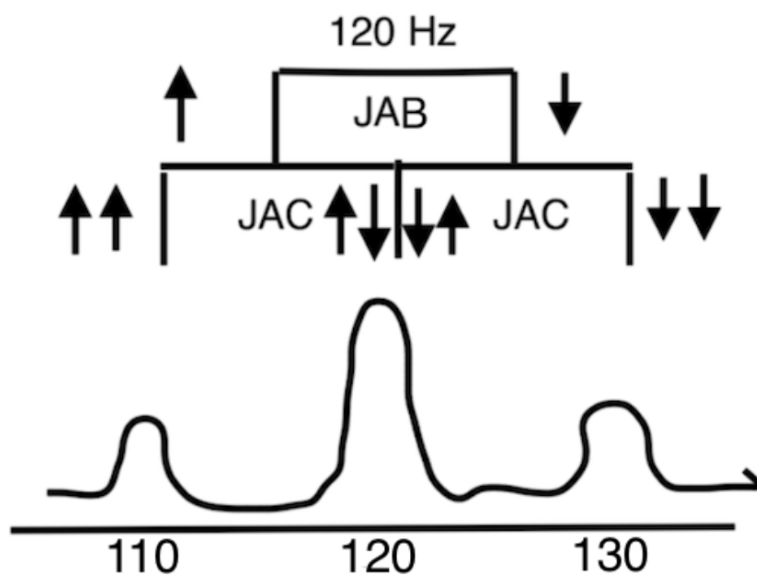


2.2 Part c

Between the 4 peaks, there is either a distance of 4 MHz or 8 MHz between the peaks, leading to the following

$$\begin{aligned}\Delta\delta_{400}(\text{ppm}) &= \frac{4}{400.130000} = 0.00999 \text{ ppm} \\ \Delta\delta_{400}(\text{ppm}) &= \frac{8}{400.130000} = 0.019998 \text{ ppm} \\ \Delta\delta_{900}(\text{ppm}) &= \frac{4}{900.130000} = 0.00444 \text{ ppm} \\ \Delta\delta_{900}(\text{ppm}) &= \frac{8}{900.130000} = 0.00888 \text{ ppm}\end{aligned}$$

2.3 Part d



From the above image, we see that when $J_{AB} = J_{AC}$, two of the four possible peaks end up at the exact same frequency so they end up merging. Instead of a doublet of doublets like previously, we now note a triplet-like pattern.