CH-314 Structural Analysis

Jigsaw 1C

Data: 3 spins: A, B and C

chemical shift:

- $\delta(A) = 120\ Hz$
- $\delta(B) = 1000\ Hz$
- $\delta(C) = 2000\ Hz$

- $J_{AB} = 12\ Hz$
- $J_{AC} = 4\ Hz$
- $J_{BC} = 6\ Hz$

Question 1:

A is coupled with spins B and C, each coupling is dividing the signal of A according to the multiplicity rule $(2nI+1)$

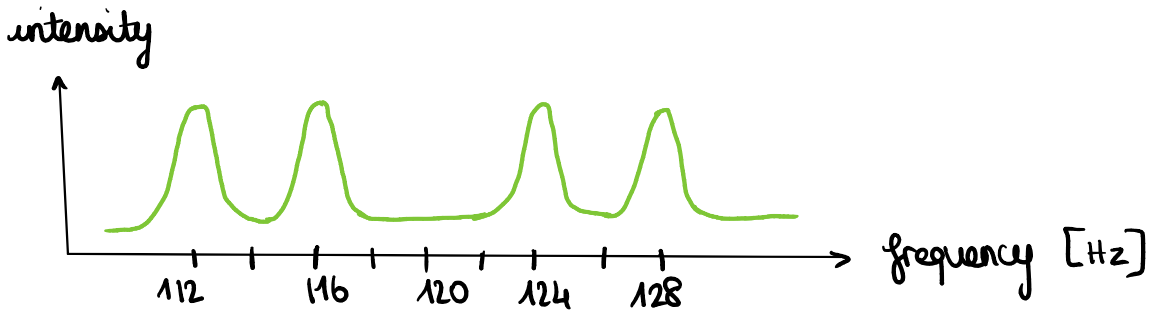
↳ coupling with B → doublet (2 lines, 12 Hz apart)

↳ coupling with C → each line of the doublet splits again into 2 lines (4 Hz apart)

There are 4 possible combinations for different B and C states, all with same probability, so same intensity.

	state of B	state of C	peak frequency:
①	α (up)	α	$120 + 6 + 2 = 128\ Hz$
②	α	β (down)	$120 + 6 - 2 = 124\ Hz$
③	β	α	$120 - 6 + 2 = 116\ Hz$
④	β	β	$120 - 6 - 2 = 112\ Hz$

↙ the center of the pattern is 120 Hz (chemical shift of A)

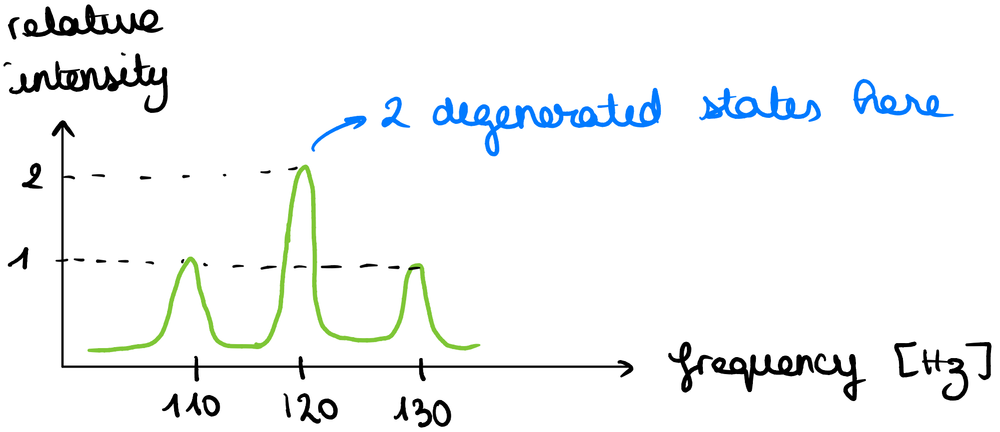


Question 2 now $J_{AB} = J_{AC} = 10\,Hz$ so $\frac{J_{AB}}{2} = \frac{J_{AC}}{2} = 5\,Hz$

state B	state C	peak frequency
α	α	$120 + 5 + 5 = 130$
β	β	$120 - 5 - 5 = 110$
α	β	$120 + 5 - 5 = 120$
β	α	$120 - 5 + 5 = 120$

the splitting overlaps.

⇒ the doublet of doublet collapses into a triplet because the combined splitting pattern is symmetric.



You could also have drown the tree diagram of the splitting. But good job.

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October 2025

1 Question 1

In order to answer the question of the multiplet structure, it is easier to first construct the coupling diagram, which can be seen in Figure 1.

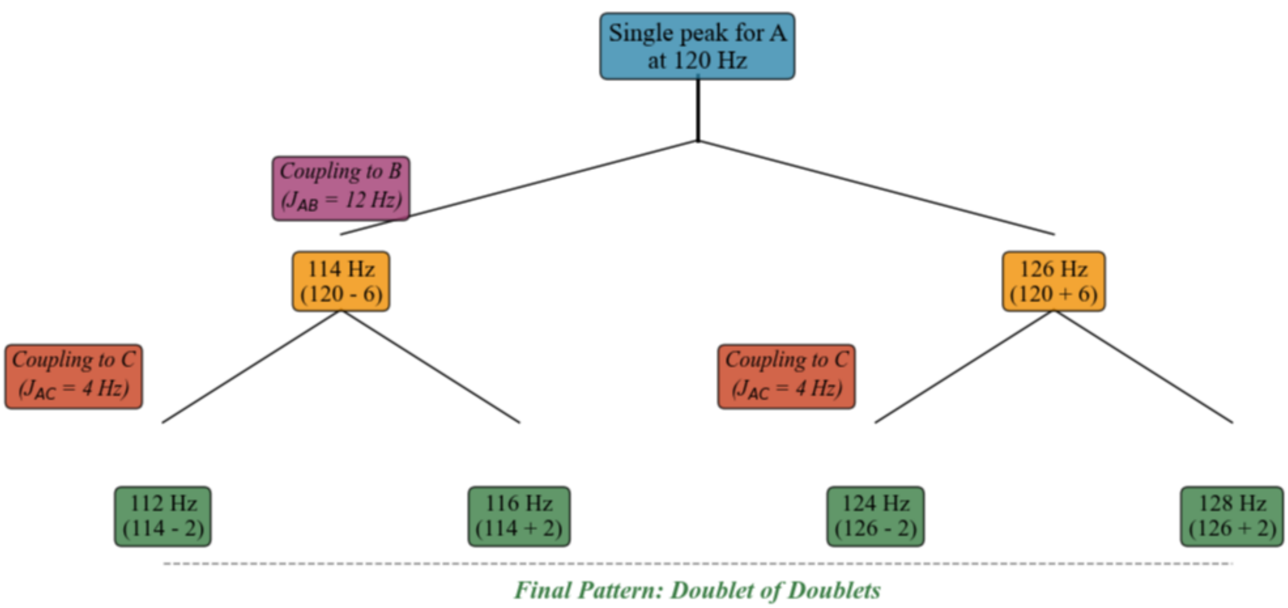

Figure 1: Coupling diagram of A when J_{AC}=4Hz and J_{AB}=12Hz

The relative intensities should be 1:1:1:1 in a doublet of doublets for this case

Then, from the different frequencies found for each peak, it is possible to plot a plausible structure for the multiplet, which can be seen in Figure 2.

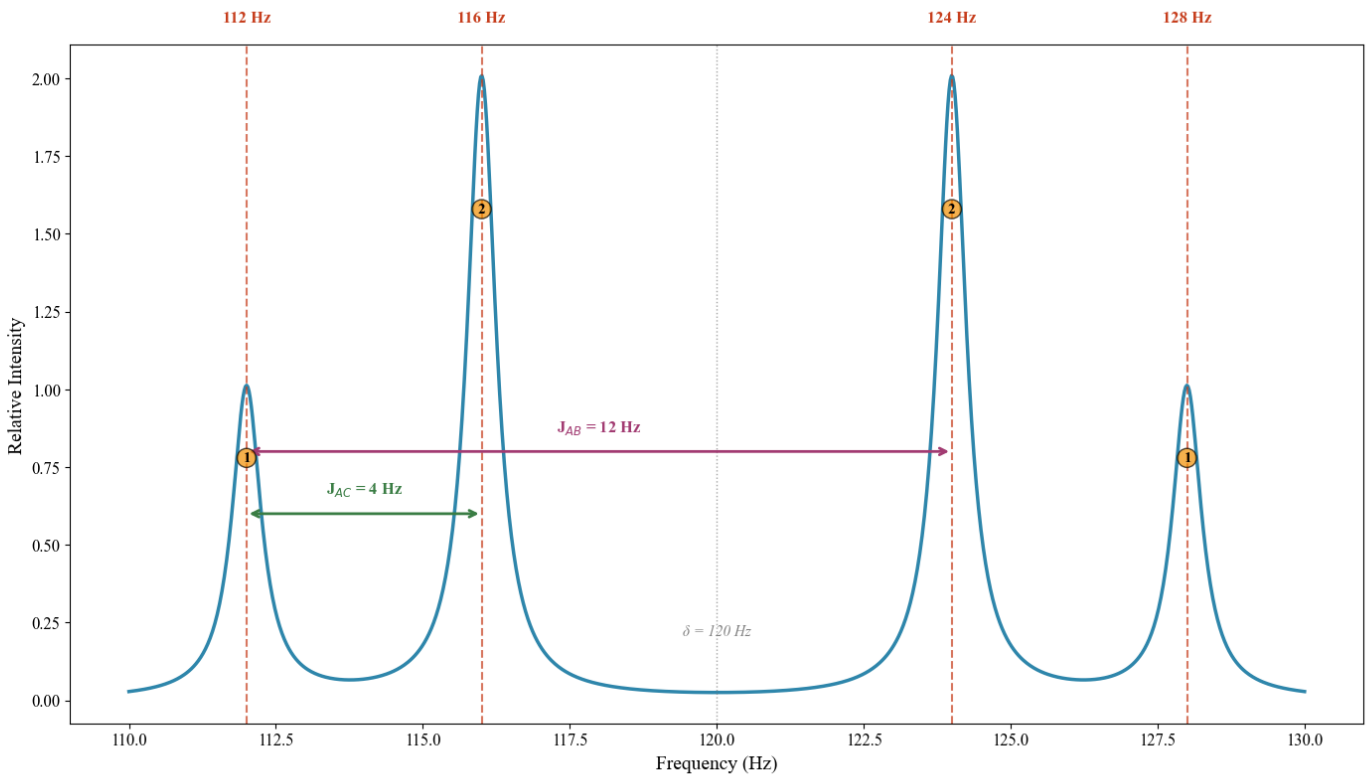

Figure 2: NMR Multiplet Pattern for A .The coupling with B (J_{AB}), i.e. C (J_{AC}) is represented on the figure. The frequency of each peak is also indicated above the figure, in the unit of Hz.

2 Question 2

Similary to the previous, to answer the question of the multiplet structure, it is easier to first construct the coupling diagram, which can be seen in Figure 3.

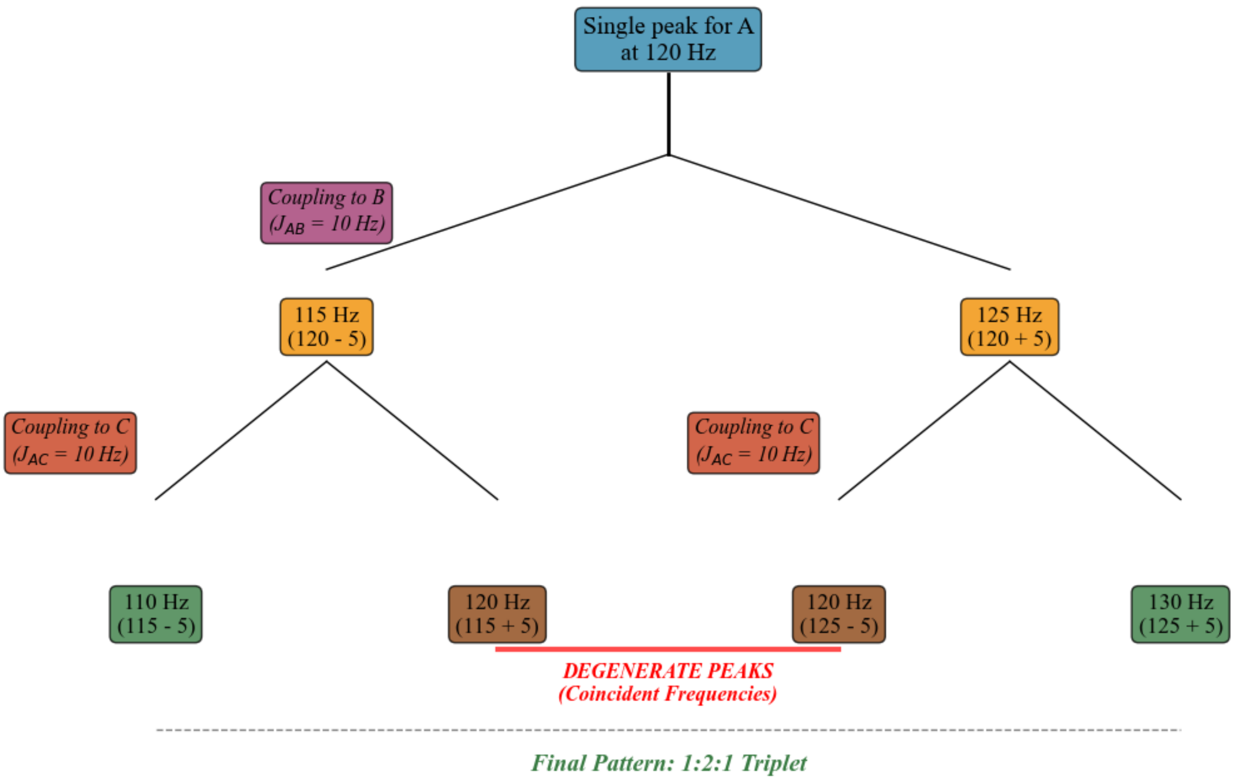

Figure 3: Coupling diagram of A when J_{AC}=J_{AB}=10Hz

Then, from the different frequencies found for each peak, it is possible to plot a plausible structure for the multiplet, which can be seen in Figure 4. When the coupling constants J_{AC} and J_{AB} are equal, a simplification occurs in the NMR spectrum due to peak degeneracy. Instead of the expected four-line doublet of doublets pattern, only three peaks are observed, forming a characteristic 1:2:1 triplet. This degeneracy arises because two of the four theoretically possible transitions occur at identical frequencies, as it can be seen by the calculation in Figure 4.

Here the relative intensities are correct.

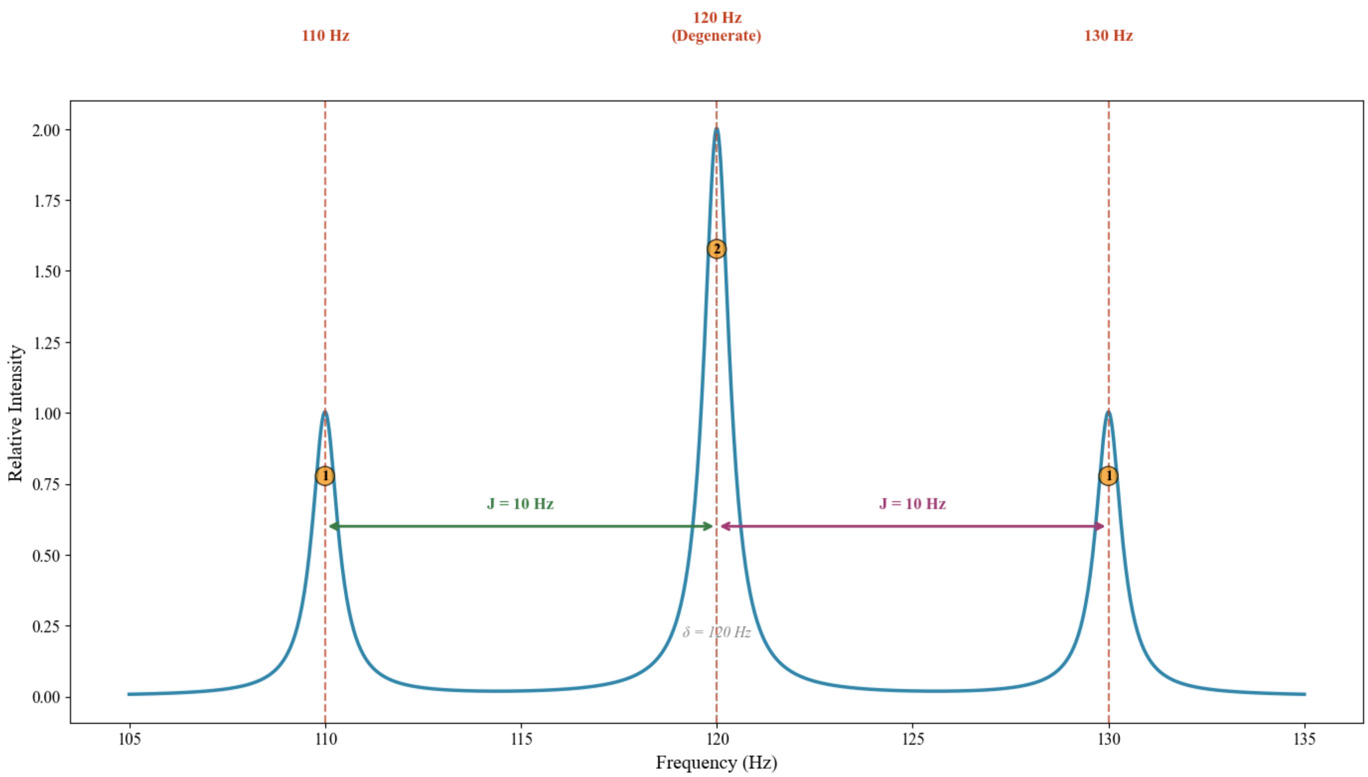

Figure 4: NMR Multiplet Pattern for A .The coupling with B (J_{AB}), i.e. C (J_{AC}) is represented on the figure, when they are both equal. The frequency of each peak is also indicated above the figure, in the unit of Hz.

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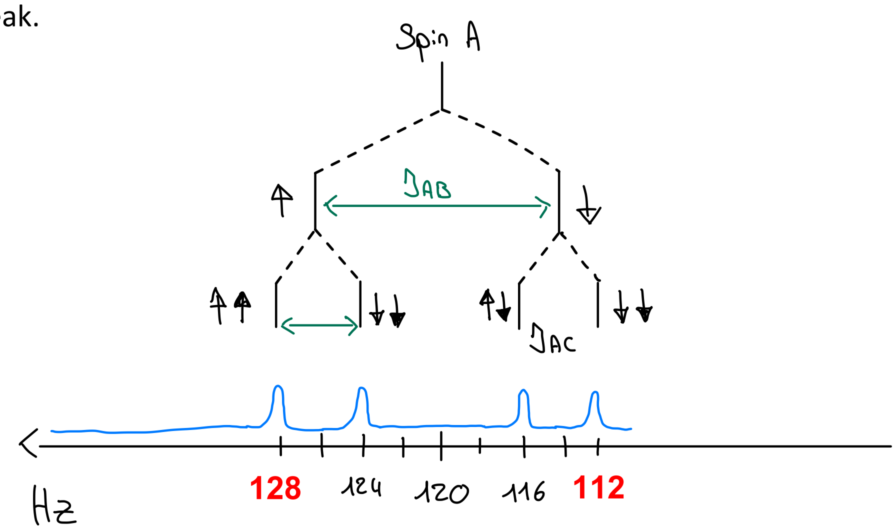
Keeler Section 2.3. Scalar coupling

[From Past Exam] Consider 3 spins, A, B, and C. The chemical shift of A is 120 Hz, and J_{AB} = 12 Hz, J_{AC} = 4 Hz, and J_{BC} = 6 Hz. The chemical shifts of B and C are 1000 and 2000 Hz, respectively.

1. Draw the multiplet pattern that would be seen for spin A. Label the frequencies of each peak.



2. Repeat step (1) for J_{AB} = 10 Hz and J_{AC} = 10 Hz. What special feature arises when J_{AB} = J_{AC}?

What special feature in the intensities?