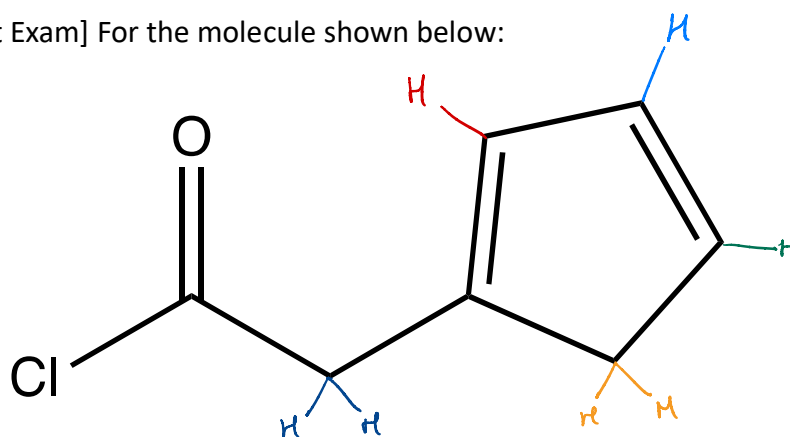


2. [From Past Exam] For the molecule shown below:

2/2



- a. [Week 1 Slide 14] How many unique chemical shifts are present in the ^1H spectrum? Ignore splitting due to scalar couplings.

5 unique chemical shifts

- b. [Keeler Section 2.3] For each ^1H site, label the expected peak intensity and multiplet pattern.

m singular, intensity: 1

m doublet, intensity: 1:1

m triplet of doublet 1:1:2:2:1:1 or doublets of triplets 1:2:1:1:2:1

m doublet of doublet 1:1:1:1

m doublet, intensity 1:1

It will appear as a doubled of doublets, this is true. However, depending on the coupling constant it might also appear as a "triplet"-like with intensities 1:2:1

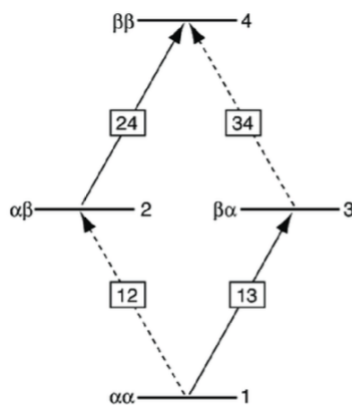
The same thing happens in the green protons. Depending on the coupling constants there are many possibilities and the ones you have mentions are some of them. Those are also referred as multiplets.

Jigsaw 1A

Introduction to Nuclear Magnetic Resonance

1. [Keeler Sections 2.3 and 3.6] Consider a system of two coupled spins with the energy levels shown below. Let the Larmor frequency of the first spin be -130 Hz and that of the second spin be -180 Hz, and let the coupling between the two spins be 16 Hz. See also: Jigsaw 1E.2

2/2



transition	spin states	frequency/Hz
$1 \rightarrow 2$	$\alpha\alpha \rightarrow \alpha\beta$	$-\nu_{0,2} - \frac{1}{2}J_{12} = 122 \text{ Hz}$
$3 \rightarrow 4$	$\beta\alpha \rightarrow \beta\beta$	$-\nu_{0,2} + \frac{1}{2}J_{12} = 198 \text{ Hz}$
$1 \rightarrow 3$	$\alpha\alpha \rightarrow \beta\alpha$	$-\nu_{0,1} - \frac{1}{2}J_{12} = 122 \text{ Hz}$
$2 \rightarrow 4$	$\alpha\beta \rightarrow \beta\beta$	$-\nu_{0,1} + \frac{1}{2}J_{12} = 138 \text{ Hz}$

- a. Compute the frequencies (in Hz) of the four transitions according to the table.

$$\left. \begin{array}{l} \nu_{0,2} = -180 \text{ Hz} \\ J_{12} = 16 \text{ Hz} \\ \nu_{0,1} = -130 \text{ Hz} \end{array} \right\} \text{ substituting the values in the formula:}$$

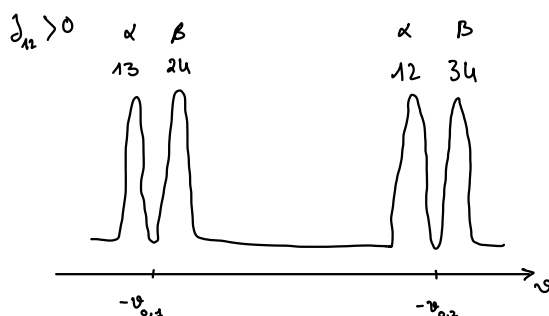
- b. * [Keeler Section 3.6] What is the selection rule in NMR? Are the transitions in part (a) allowed?

One spin changed $\Rightarrow \Delta m = \pm 1$

In all cases, only one spin changes (either α or β)

$\hookrightarrow$ All transitions are allowed

- c. Make a sketch of the spectrum. Label the frequencies.

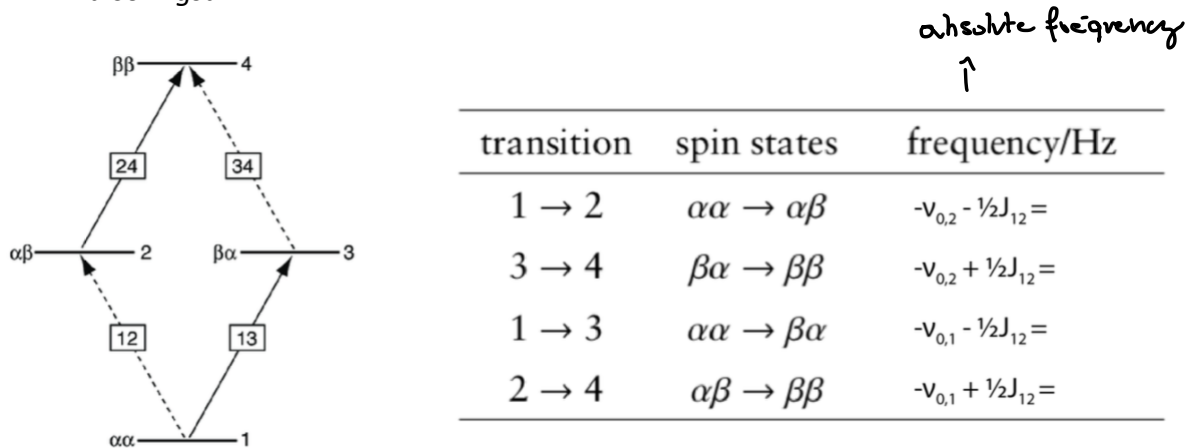


Jigsaw 1A

Introduction to Nuclear Magnetic Resonance

2/2

1. [Keeler Sections 2.3 and 3.6] Consider a system of two coupled spins with the energy levels shown below. Let the Larmor frequency of the first spin be -130 Hz and that of the second spin be -180 Hz, and let the coupling between the two spins be 16 Hz. See also: Jigsaw 1E.2



- a. Compute the frequencies (in Hz) of the four transitions according to the table.

$$\begin{aligned}
 J_{12} &= 16 \text{ Hz} \\
 \nu_{0,2} &= -180 \text{ Hz} \\
 \nu_{0,1} &= -130 \text{ Hz} \\
 -\nu_{0,2} - \frac{1}{2}J_{12} &= 180 - 8 = 172 \text{ Hz} \\
 -\nu_{0,2} + \frac{1}{2}J_{12} &= 180 + 8 = 188 \text{ Hz} \\
 -\nu_{0,1} - \frac{1}{2}J_{12} &= 130 - 8 = 122 \text{ Hz} \\
 -\nu_{0,1} + \frac{1}{2}J_{12} &= 130 + 8 = 138 \text{ Hz}
 \end{aligned}$$

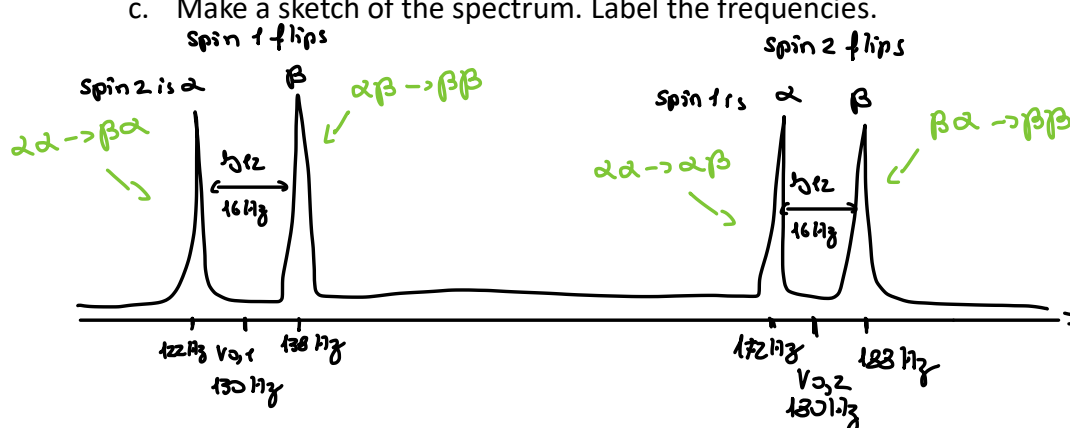
- b. * [Keeler Section 3.6] What is the selection rule in NMR? Are the transitions in part (a) allowed?

The selection rule is that $\Delta m = \pm 1$

The transition of part a are:

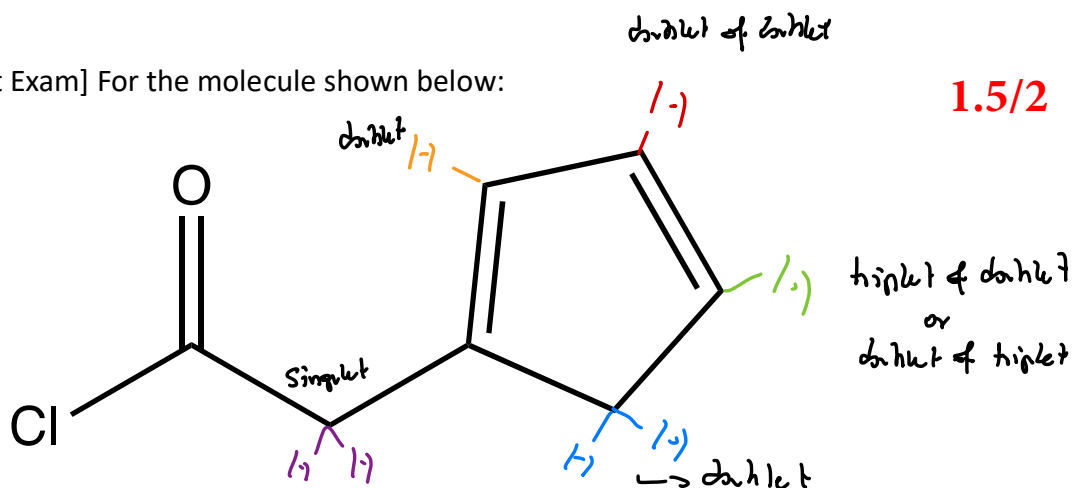
$\alpha\alpha \rightarrow \alpha\beta$: +1	$\left. \begin{array}{l} \alpha\alpha \rightarrow \alpha\beta : +1 \\ \beta\alpha \rightarrow \beta\beta : -1 \\ \alpha\alpha \rightarrow \beta\alpha : +1 \\ \alpha\beta \rightarrow \beta\beta : -1 \end{array} \right\} \text{done per the transition are allowed}$
$\beta\alpha \rightarrow \beta\beta$: -1	
$\alpha\alpha \rightarrow \beta\alpha$: +1	
$\alpha\beta \rightarrow \beta\beta$: -1	

- c. Make a sketch of the spectrum. Label the frequencies.



2. [From Past Exam] For the molecule shown below:

1.5/2



a. [Week 1 Slide 14] How many unique chemical shifts are present in the ^1H spectrum? Ignore splitting due to scalar couplings.

5 unique chemical shifts

b. [Keeler Section 2.3] For each ^1H site, label the expected peak intensity and multiplet pattern.

Singlet because no H around.

doublet because one H around it (the red one)

doublet of doublet because 2 different H around it (the orange and green one)

doublet because one H around it (the green one)

triplet of doublet or doublet of triplet because 3 H around it but 2 H of the same color (triplet) and 1 H of the other color (doublet)

For the intensity, the purple and blue H have twice the intensity of the orange, red and green H, because there are twice as many of them.

For the peak intensities we expect a Pascal triangle as a rule of thumb:

purple = (intensity) 1

yellow = 1:1

blue = 1:1

red = 1:1:1

green = 1:1:2:2:1:1 or 1:2:1:1:2:1 for example

The red one will appear as a doubled of doublets, this is true. However, depending on the coupling constant it might also appear as a "triplet"-like with intensities 1:2:1

The same thing happens in the green protons. Depending on the coupling constants there are many possibilities and the ones you have mentioned are some of them. Those are also referred as multiplets.