2/2 Great job!

CH-314 Structural Analysis
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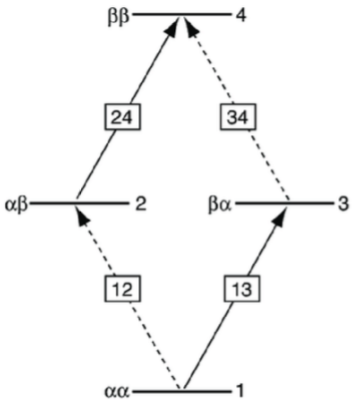
Jigsaw 3A

Hore Section 3.1. Effect on NMR spectra

1. 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.



transition	spin states	frequency/Hz
$1 \rightarrow 2$	$\alpha\alpha \rightarrow \alpha\beta$	$-\nu_{0,2} - \frac{1}{2}J_{12} = -(-180) - \frac{16}{2} = 172$ Hz
$3 \rightarrow 4$	$\beta\alpha \rightarrow \beta\beta$	$-\nu_{0,2} + \frac{1}{2}J_{12} = -(-180) + \frac{16}{2} = 188$ Hz
$1 \rightarrow 3$	$\alpha\alpha \rightarrow \beta\alpha$	$-\nu_{0,1} - \frac{1}{2}J_{12} = -(-130) - \frac{16}{2} = 122$ Hz
$2 \rightarrow 4$	$\alpha\beta \rightarrow \beta\beta$	$-\nu_{0,1} + \frac{1}{2}J_{12} = -(-130) + \frac{16}{2} = 138$ Hz

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

$1 \rightarrow 2$ $\quad -(-180) - \frac{16}{2} = 172$ Hz

$3 \rightarrow 4$ $\quad -(-180) + \frac{16}{2} = 188$ Hz

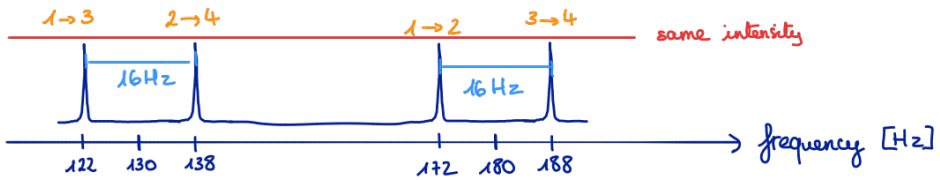
$1 \rightarrow 3$ $\quad -(-130) - \frac{16}{2} = 122$ Hz

$2 \rightarrow 4$ $\quad -(-130) + \frac{16}{2} = 138$ Hz

   b. What is the selection rule in NMR? Are the transitions in part (a) allowed?

Transitions are allowed if $\Delta m = \pm 1$, that is just one spin changes its magnetic quantum number. ($\Delta m_x = \pm 1$ or $\Delta m_x = \pm 1$)
Since each transition above shows one single change of magnetic moment (α to β or β to α), all transitions are allowed.

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



2/2 Nice work!

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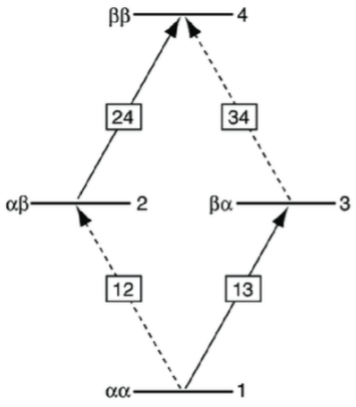
Hore Section 3.1. Effect on NMR spectra

1. 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.



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

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

$\nu_{0,1} = -130\,Hz$, $\nu_{0,2} = -180\,Hz$, $J_{1,2} = 16\,Hz$

$1 \rightarrow 2: -\nu_{0,2} - \frac{1}{2}J_{1,2} = -188\,Hz$
$3 \rightarrow 4: -\nu_{0,2} + \frac{1}{2}J_{1,2} = -172\,Hz$
$1 \rightarrow 3: -\nu_{0,1} - \frac{1}{2}J_{1,2} = -138\,Hz$
$2 \rightarrow 4: -\nu_{0,1} + \frac{1}{2}J_{1,2} = -122\,Hz$

Careful with the negative signs!
These should all be positive values

b. What is the selection rule in NMR? Are the transitions in part (a) allowed?

selection rule for magnetic dipole transitions: $\Delta m = \pm 1$
In a transition, only 1 nuclear spin can flip at a time.
Using this and based off the 4 states we have, we find:

Transition	state change
$1 \rightarrow 2$	$\alpha\alpha \rightarrow \alpha\beta$
$3 \rightarrow 4$	$\beta\alpha \rightarrow \beta\beta$
$1 \rightarrow 3$	$\alpha\alpha \rightarrow \beta\alpha$
$2 \rightarrow 4$	$\alpha\beta \rightarrow \beta\beta$

So, yes, all the transitions in (a) are allowed

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