CH-314 Structural Analysis
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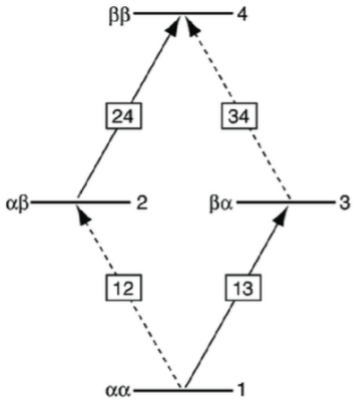
Jigsaw 1A

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*



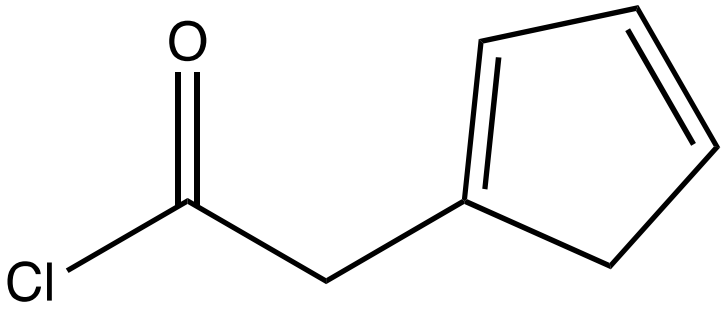
transition	spin states	frequency/Hz
$1 \rightarrow 2$	$\alpha\alpha \rightarrow \alpha\beta$	$-\nu_{0,2} - \frac{1}{2}J_{12} =$
$3 \rightarrow 4$	$\beta\alpha \rightarrow \beta\beta$	$-\nu_{0,2} + \frac{1}{2}J_{12} =$
$1 \rightarrow 3$	$\alpha\alpha \rightarrow \beta\alpha$	$-\nu_{0,1} - \frac{1}{2}J_{12}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

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

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

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

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



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

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