Excellent work!

JIGSAW 2B

October 14 2024

• Question 1

For a ^1H nucleus, the Larmor frequency in a 9.4 T magnetic field is:

$$\nu_{\text{ref}} = \gamma B_0 = (42.577\,\text{MHz/T}) \times 9.4\,\text{T} = 400.23\,\text{MHz}$$

The frequency difference of 2.0 kHz corresponds to a chemical shift difference of:

$$\Delta\delta = \frac{2000\,\text{Hz}}{400.23 \times 10^6\,\text{Hz}} \times 10^6 = 5\,\text{ppm}$$

Since C_2H_6 has a chemical shift of 1.2 ppm, C_2H_4 will have a chemical shift of:

$$\delta_{C_2H_4} = 1.2\,\text{ppm} + 5\,\text{ppm} = \mathbf{6.2\ ppm}$$

• Question 2

A) We use the Fourier transform to transform the time domain signal into a frequency domain signal. The Fourier transform decomposes a signal into its components in frequency domain.
B) Mathematically, the frequency domain is the integral of the time domain signal multiplied by sine-type functions over the frequency domain. A non-zero integral at a certain frequency means that the sine-type function fits well part of the signal. In effect, it can deconstruct a signal containing mixed frequencies into its components of frequency.

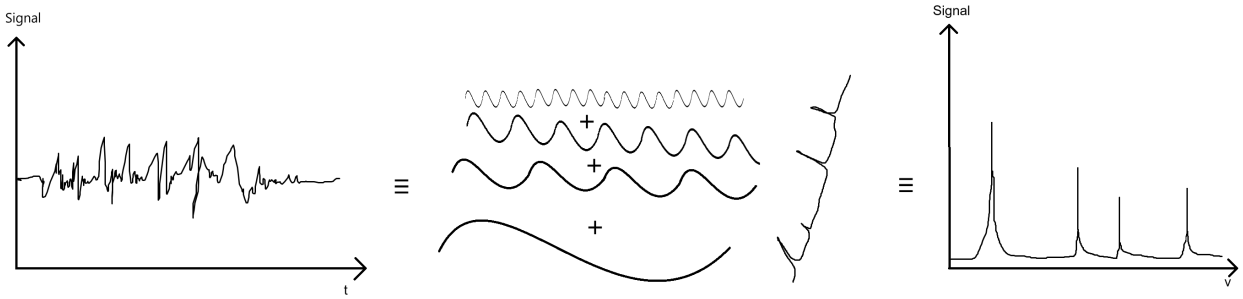


Figure 1: General schematic

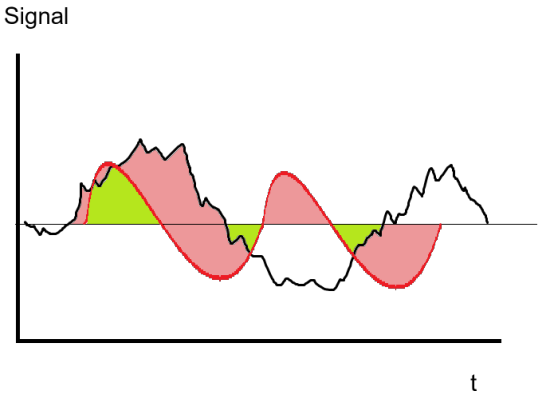


Figure 2: Bad frequency integration

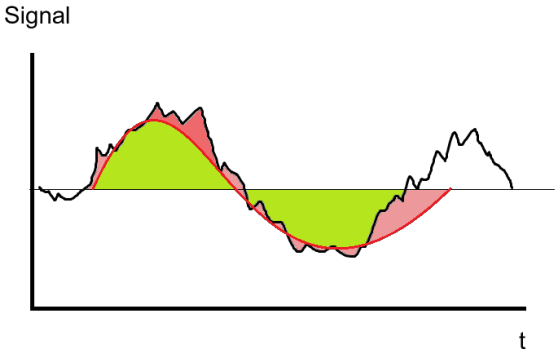


Figure 3: Good frequency integration

• Question 3

In a NMR spectra, each peak corresponds to a distinct type of atom. If a C NMR spectra shows three spikes, it means that there are three non equivalent types of carbon atoms in the sample. The same goes for H NMR spectra. Knowing this, one can guess the structure of a molecule based on the number of lines on each spectra. The procedure can also be done backwards, as one can guess the number of lines on each spectra based on the molecule's structure. These methods were employed to find the solutions to the exercise in the picture below.

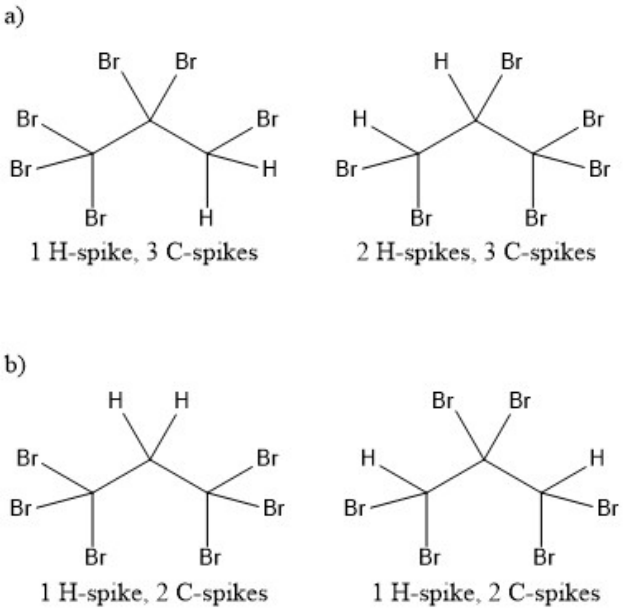


Figure 4: Question 3's solution

Jegrav 2B

Awesome job!

Problem 1

$\nu_0 \rightarrow$ Larmor frequency

$\nu \rightarrow$ NMR frequency

$\boxed{\nu = -\nu_0}$ for a given signal

$\left.\begin{array}{l} \nu_{0,C_2H_6} - \nu_{0,C_2H_4} = 2.0\ kHz \\ \nu_{0,C_2H_6} - \nu_{0,C_2H_4} = 2.0\ kHz \end{array}\right\} \Rightarrow \nu_{C_2H_4} - \nu_{C_2H_6} = 2.0\ kHz$

$\nu_{ref} \rightarrow$ NMR frequency for the reference

$$\nu_{ref} = \frac{|\gamma| B_0 (1-\bar{\sigma}_{ref})}{2\pi} \overset{1 \gg \bar{\sigma}_{ref}}{\simeq} \frac{|\gamma| B_0}{2\pi} =$$

$\gamma_H = 2.675 \cdot 10^8\ rad\ s^{-1} T^{-1}$

$$= \frac{2.675 \cdot 10^8\ rad\ s^{-1} T^{-1} \cdot 9.4\ T}{2\pi\ rad} \simeq 400\ MHz$$

$\left.\begin{array}{l} \nu_{C_2H_4} - \nu_{C_2H_6} = 2.0\ kHz = 2000\ Hz = 5.400\ Hz \\ \nu_{ref} = 400\ MHz \Rightarrow 1\ ppm = 400\ Hz \end{array}\right\} \Rightarrow$

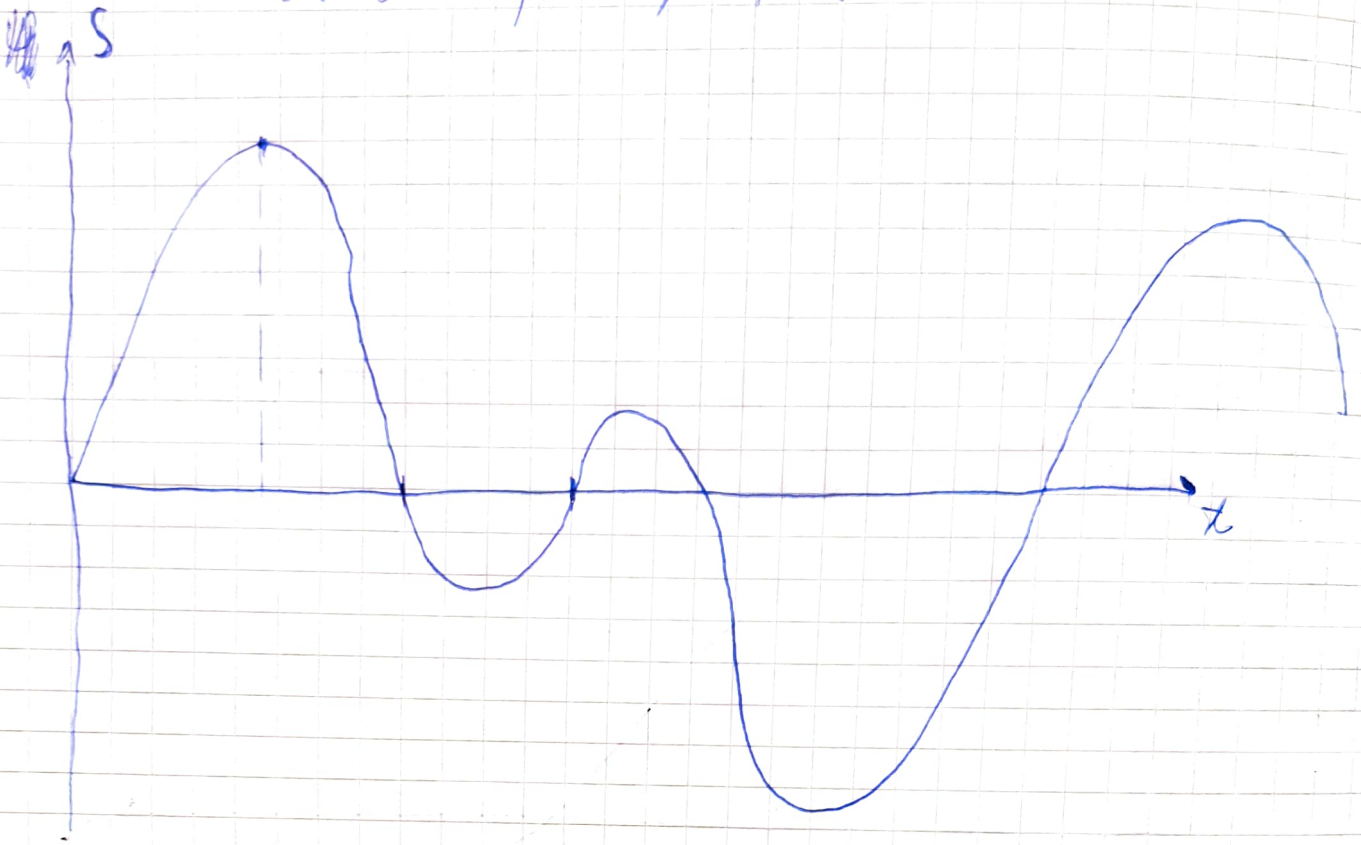
$\left.\begin{array}{l} \Rightarrow \bar{\sigma}_{C_2H_4} - \bar{\sigma}_{C_2H_6} = 5\ ppm \\ \bar{\sigma}_{C_2H_6} = 1.2\ ppm \end{array}\right\} \Rightarrow \boxed{\bar{\sigma}_{C_2H_4} = 6.2\ ppm}$

Problem 2

a. The mathematical procedure used is a Fourier transform, which transforms the time-domain signal into a frequency domain.

b. A time domain signal is a periodic function. As the functions sin and cos (oscillating with different values of frequency) form a complete set, the time domain signal function can be written as a linear expansion of sin and cos functions. Therefore, when performing a Fourier transform, one needs to determine which ~~frequency of a~~ frequencies of oscillation contribute to the time domain signal, so that large coefficients of the linear expansion.

We can consider the following signal:



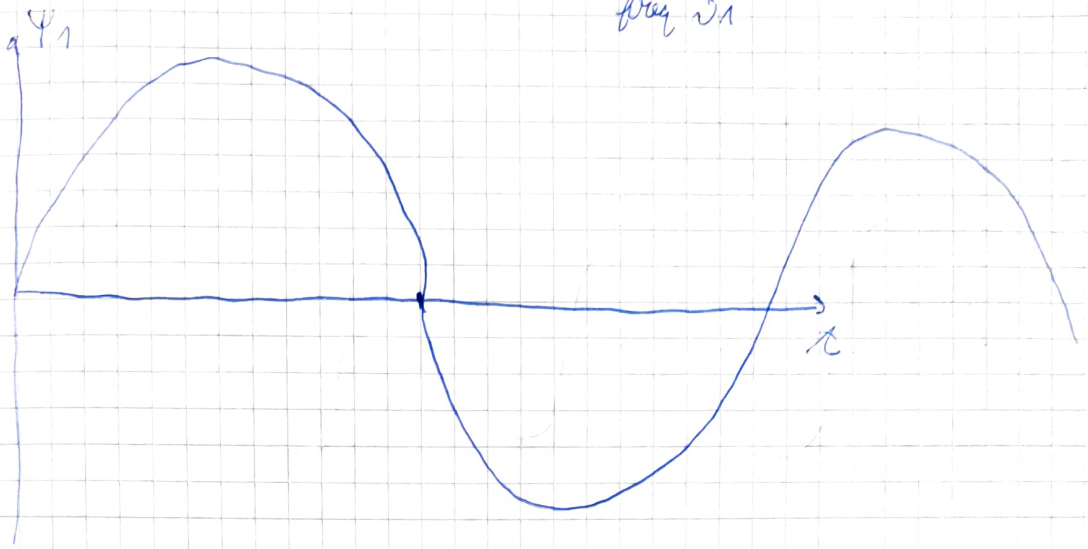
The Fourier transform formula is

$$\mathcal{F}(\omega) = \int S(t) e^{-i\omega t} dt \; ; \int S(t) e^{-i \cdot 2\pi \nu t} = \mathcal{F}(\nu)$$

for $\omega = 2\pi\nu$

with $\omega = 2\pi\nu$. This represents taking the product between the signal and ~~an e a function oscillating~~ a pure sin or cos function oscillating with frequency ν and then computing the area of the product of the two functions. If the pure function contributes to the signal, then the product (the overlap) should have an overall all large positive area. If not, the area of the product should be close to 0.

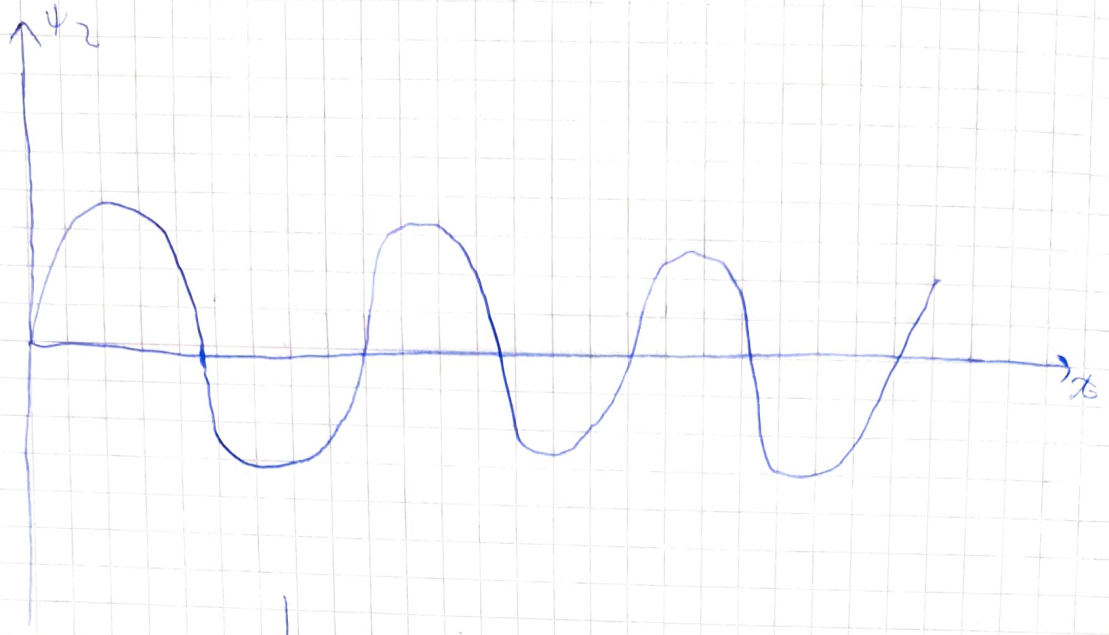
One can try the following pure function of freq ν_1



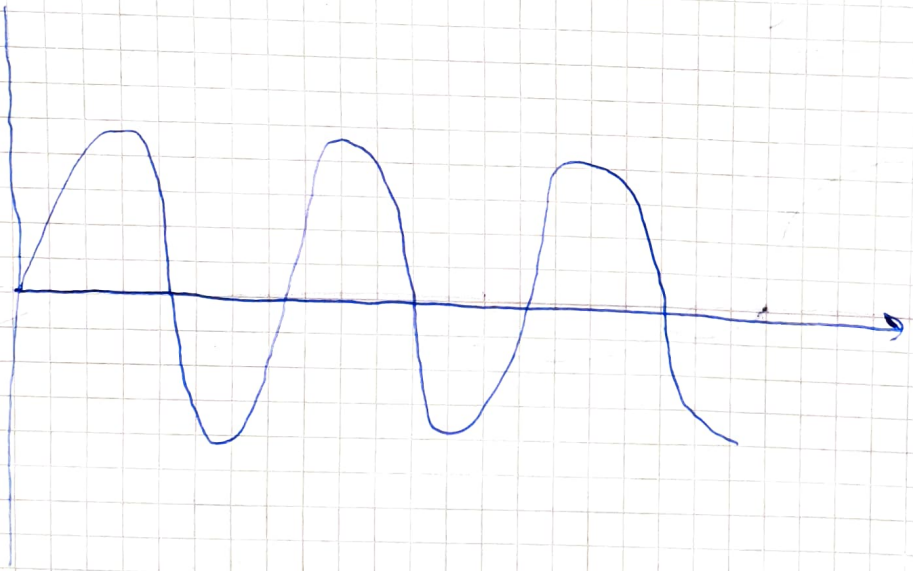
product with $S(t)$

⇒ it is observed that the positive areas are greater than negative ones ⇒ ν_1 contributes to the signal S

Now, one can take the pure function oscillating with ν_2

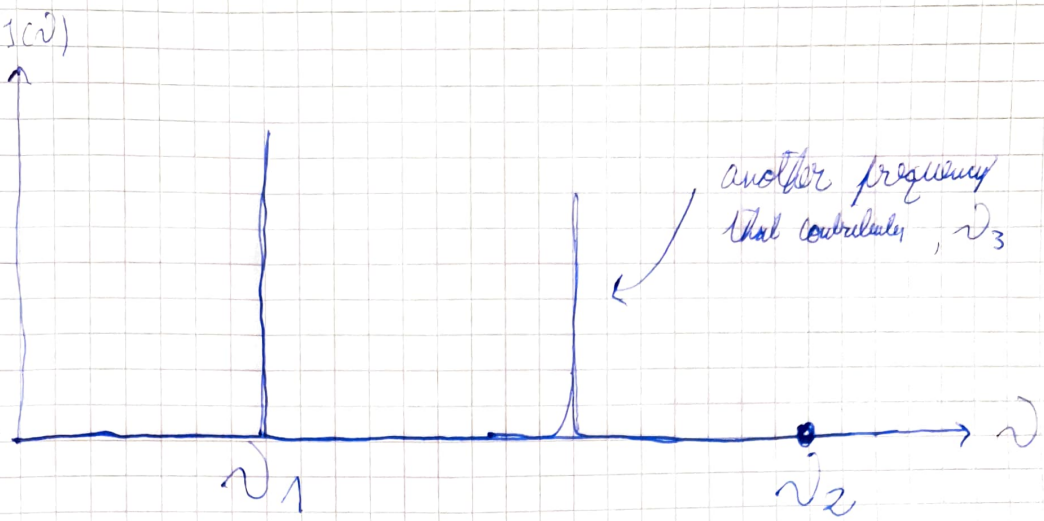


product with S



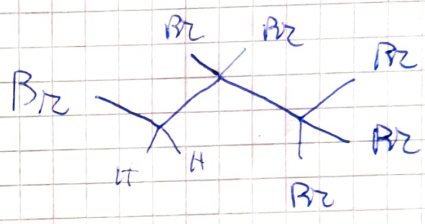
$\Rightarrow$ each positive area is compensated by a negative area
$\Rightarrow \nu_2$ doesn't contribute to S

By applying the Fourrier transform to a train of segments, one obtains the following frequency domain signal:

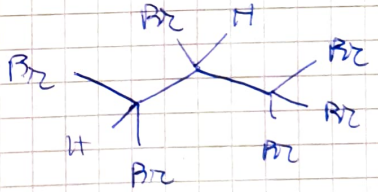


Problem 3

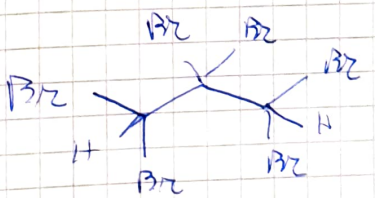
a. Isomer 1:



Isomer 2:



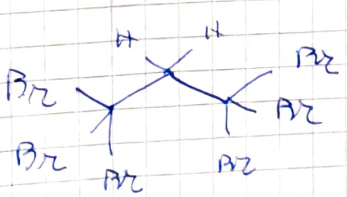
b. Isomer 3:



^{13}C: 2 peaks

^{1}H: 1 peaks

Isomer 4:



^{13}C: 2 peaks

^{1}H: 1 peak