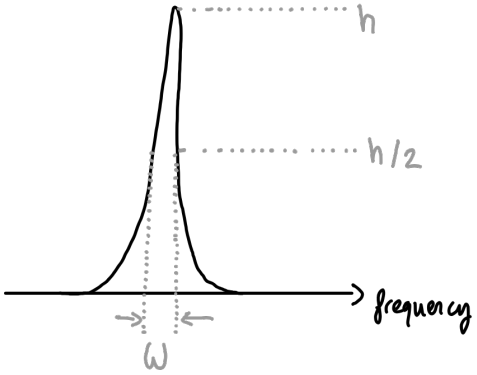
Great work!

Jigsaw 1D

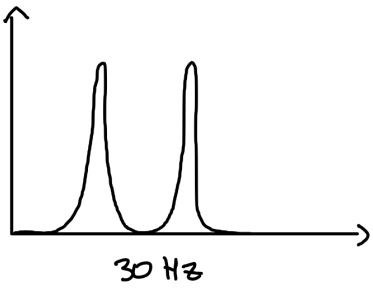
Question 1

The linewidth of an absorption mode lineshape is measured by taking the width of the peak at half the peak height.

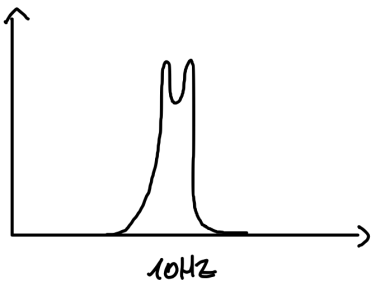


Question 2

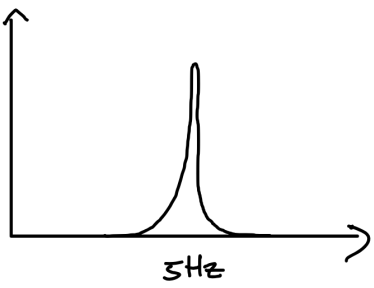
a)



b)



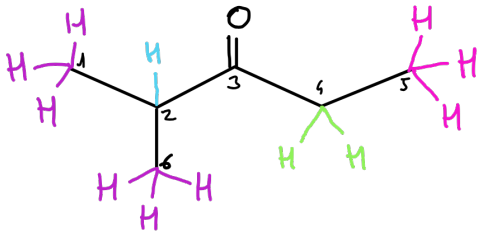
c)



d) In case c) the separation is half of the linewidth, so the two peaks are no longer distinct and a single line is seen. This would be the case for any lower frequencies.

Question 3

a)



The multiplicity can be determined by counting the neighbour H and is due to the spin coupling between the H.
The purple hydrogens appear as a doublet since they only have one neighbour H (the blue one). As there is 6 equivalent purple hydrogens, the doublet will integrate for 6.
The blue hydrogen appears as an heptuplet because of the 6 neighbour hydrogens (the purple ones). This will integrate for 1.
The green hydrogens will appear as a quadruplet because of the 3 neighbour hydrogens (the pink ones) and integrate for 2.
The pink hydrogens will appear as a triplet because of the 2 neighbour hydrogens (the green ones) and integrate for 3.

carbon number	# of H	multiplicity	intensity	
1	3	doublet	6	} same peak
6	3	doublet	6	
2	1	heptuplet	1	
3	0	—	0	
4	2	quadruplet	2	
5	3	triplet	3	

The question also asks for a predicted spectrum (i.e., draw where the peaks would show up and what they look like)

b) i) Without coupling all carbon appears as singulet and since 1 & 6 are equivalent we should have 5 signals (4 that integrate for 1 and 1 that integrate for 2).

ii) By considering the proton coupling, the singulet change to multiplet depending on the hydrogen linked to the carbon. We should have 14 signals.

carbon number	# of H	multiplicity	intensity	
1	3	quadruplet	2	} same peak
6	3	quadruplet	2	
2	1	doublet	1	
3	0	singulet	1	
4	2	triplet	1	
5	3	quadruplet	1	

Good! Be aware that a lot of times, to measure 13C faster, we use some techniques (cross polarization/ etc.) that make the spectrum not quantitative, so the peak intensities don't provide the same information

c) Generaly ^{13}C spectra are measured with decoupling for two main reasons:

① The spectra is more readable because there is only singulet for each chemically different carbon
② The coupling with hydrogen break down the singulet in multiplet thus lowering the intensity of the peak thus lowering the $\frac{\text{signal}}{\text{noise}}$ ratio.

So to resume the decoupled spectrum is more readable and ~~less~~ more sensitive.

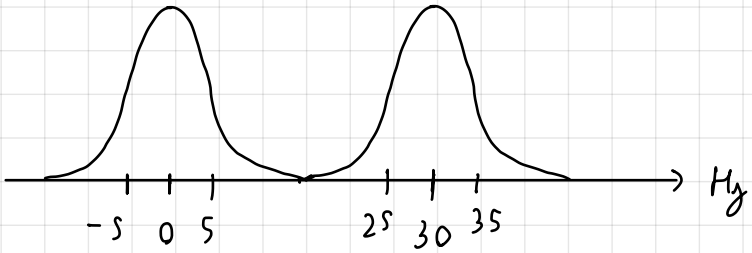
Serie 10:

Nice job!

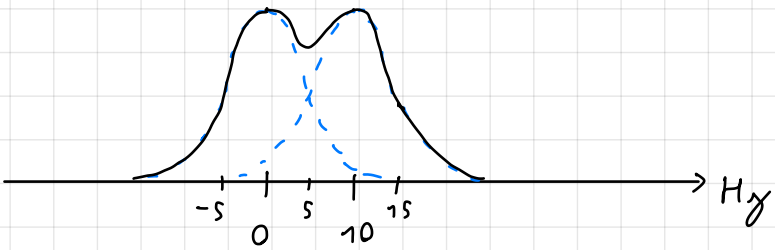
1. The linewidth is the width of the peak at the half of the height of the peak.

2. w = 10 Hz

a. Δ=30 Hz

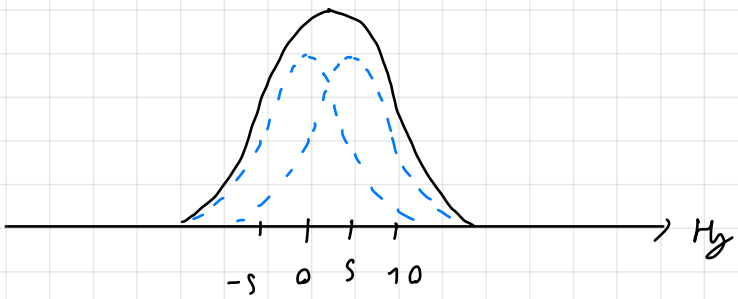


b. Δ=20 Hz



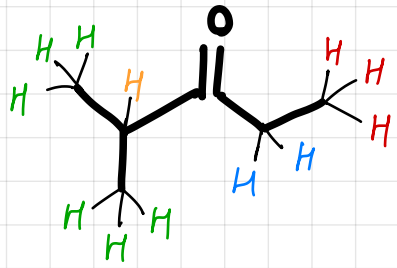
single peaks
seen signal

c. Δ = 5 Hz



d. In the c. case, the doublet is analyzed as a singlet because there is not enough resolution.

3. a.



Good! Usually for NMR we report relative intensities by scaling to integers -- these percentages correspond to intensities of 6, 1, 2, and 3, respectively

H is see as a doublet (coupling with one H) of relative intensity of 100 % ;

H " heptuplet (" six H) " ~17 % ;

H " quadruplet (" three H) " ~33 % ;

H " triplet (" two H) " 50 % .

The question also asks for a predicted spectrum (i.e., draw where the peaks would show up and what they look like)

b. i) with coupling

14 signal (doublet count as two)

ii) without coupling

5 signals

c. The ^{13}C spectra with decoupling show to read quicker the graph because the ration signal/noise increases.