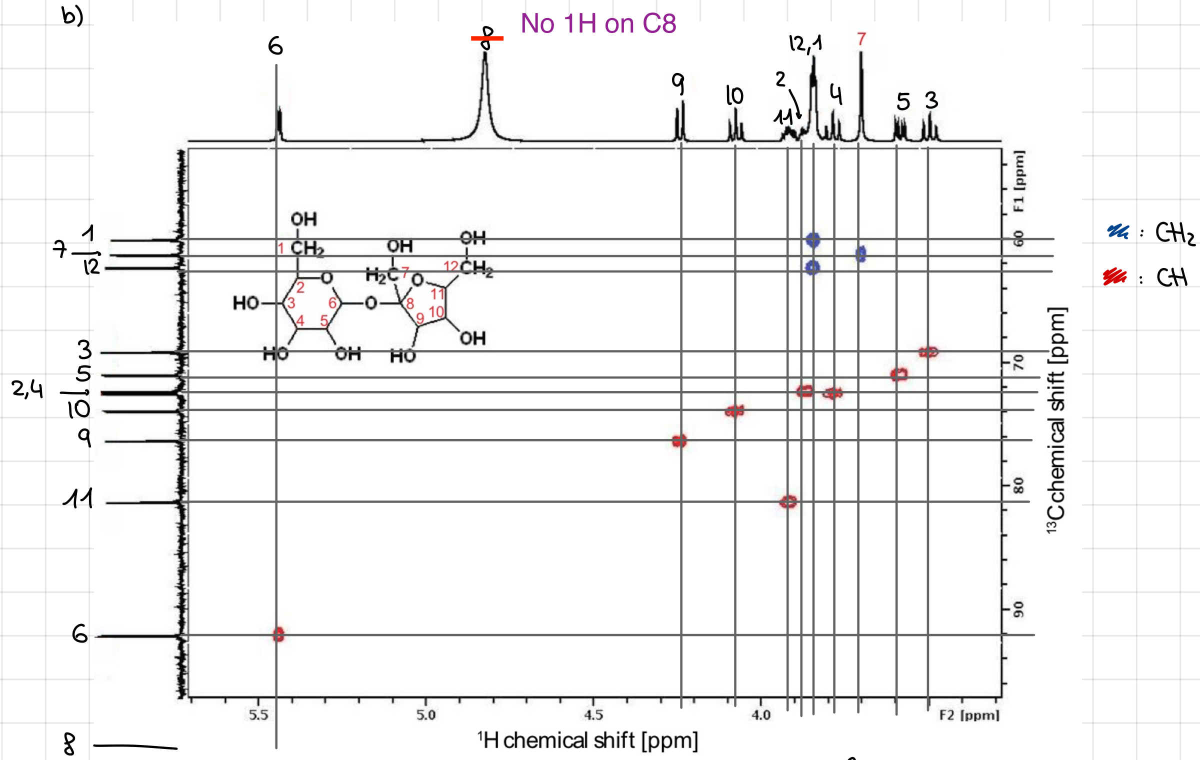
Jigsaw 4B - 2024

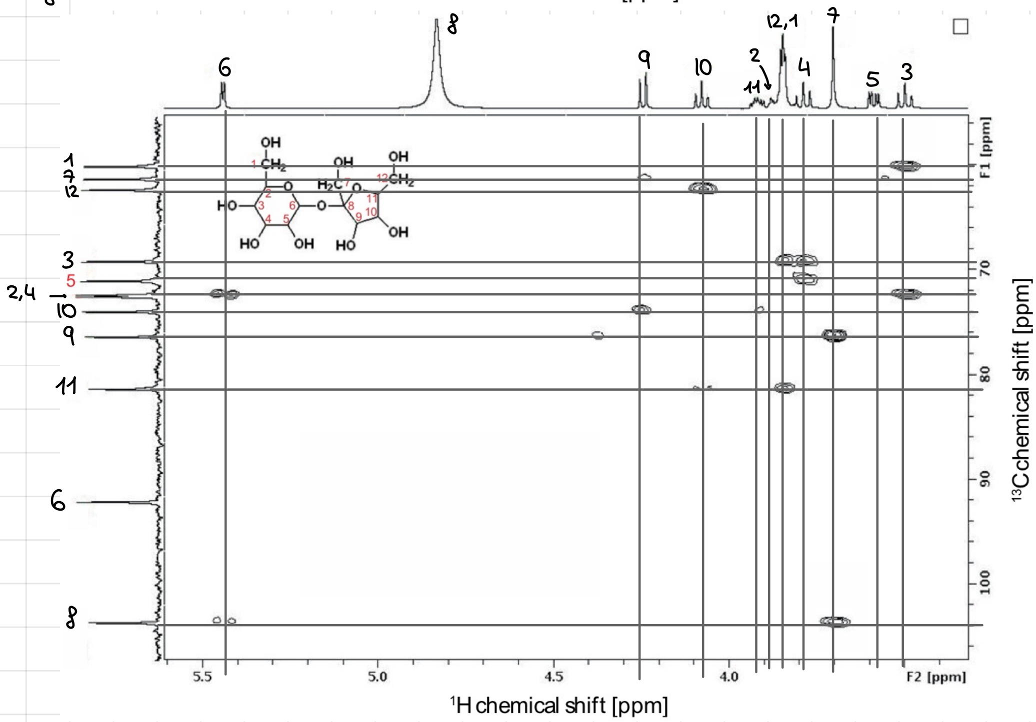
Excellent!!

Question 1 :

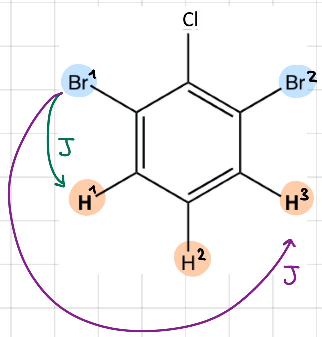
a) The first spectrum corresponds to HSQC because each carbon associate to one hydrog
The second spectrum corresponds to HMBC because one can observe multiple protons per carbon.

b)





Question 2 :



- the two bolded H of the molecule and the 2 Br are chemically equivalent but not magnetically equivalent.

- chemically equivalent because of the symmetry of the molecule.
- not magnetically equivalent because the coupling constant $J(Br^1-H^1) \neq J(Br^1-H^3)$.

Jigsaw 4 B

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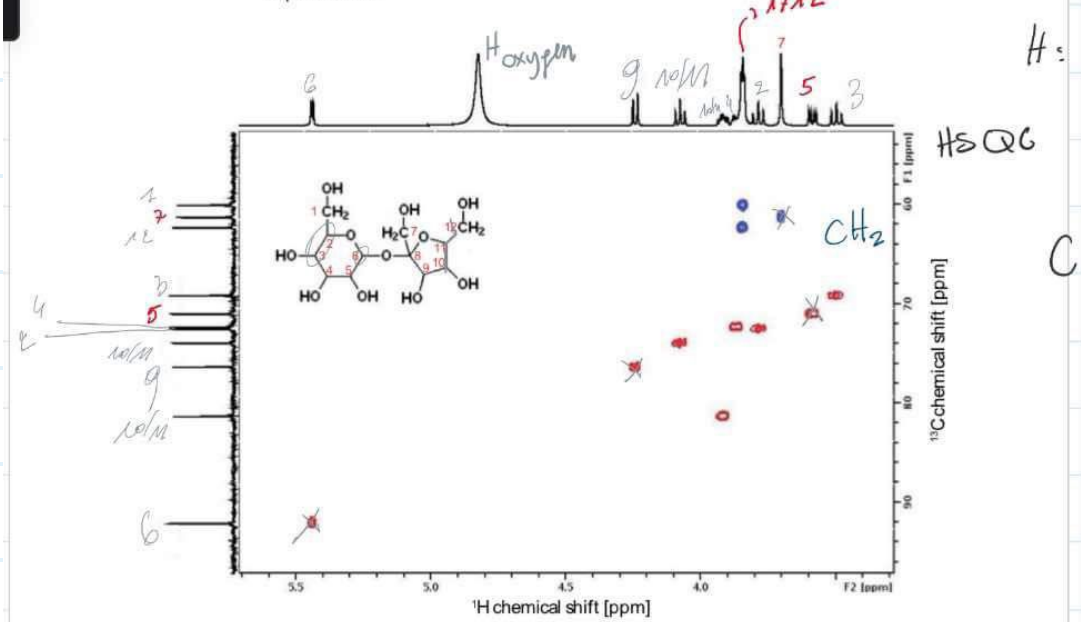
1. a. HSQC : first spectrum

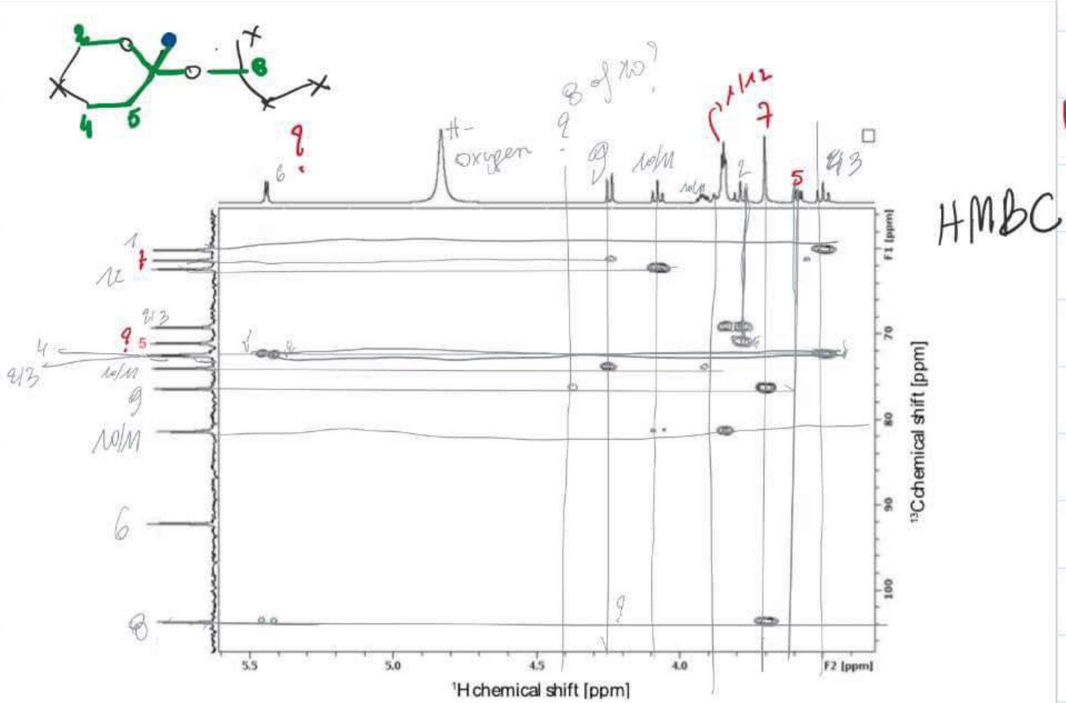
HMBC : second spectrum

b. b. Assign the ^1H and ^{13}C. Notice that the axis limits vary between the experiments.

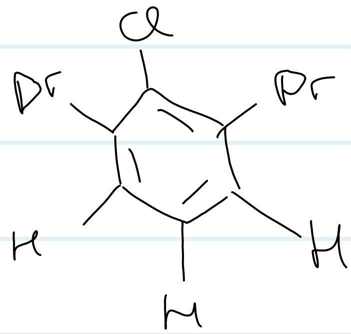


H:

C:



2.



Bromides : chemically but not magnetically

Hydrogens : chemically but not magnetically

JIGSAW 4B

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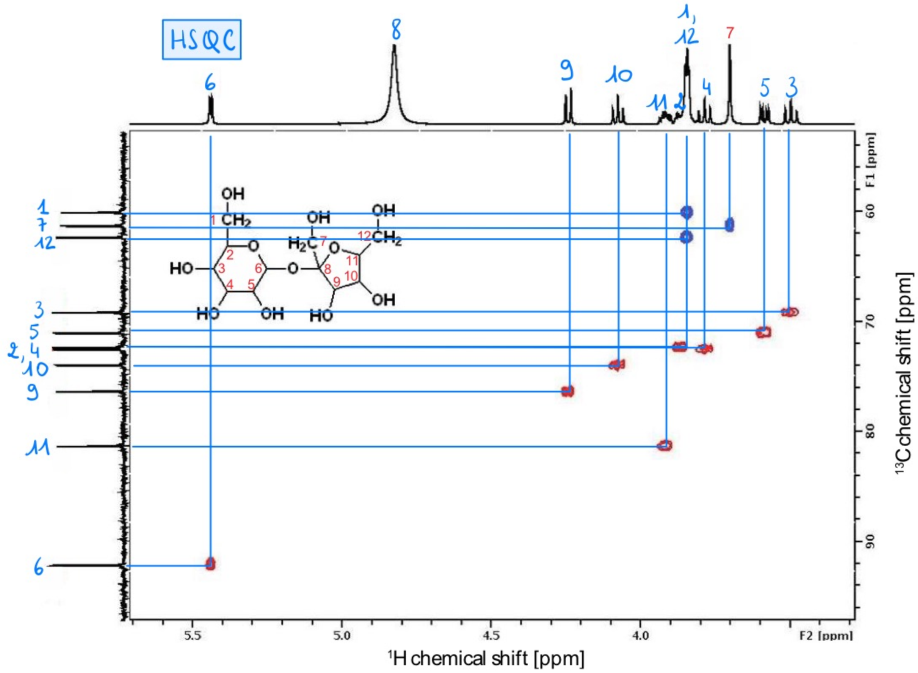
Question 1

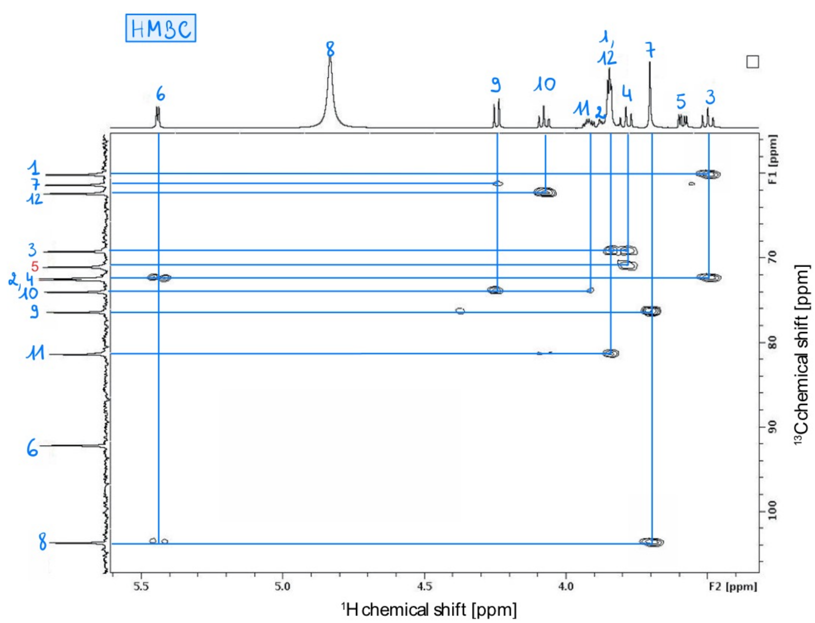
1. [Keeler Sections 8.7 and 10.6] 2D NMR experiments are not limited to one nucleus, but we can also perform heteronuclear 2D NMR experiments. One example is the Heteronuclear Single Quantum Coherence (HSQC) experiment, which detects 1H13C single bond correlations. Another is the Heteronuclear Multiple Bond Correlation (HMBC) experiment, which gives correlations between carbons and protons that are separated by two or three bonds. Direct one-bond correlations are suppressed. The intensity of cross peaks depends on the coupling constant. Thus, the absence of a cross peak doesn't confirm that carbon-proton pairs are many bonds apart.

a. Two spectra for sucrose are shown below. Which spectrum corresponds to HSQC and which corresponds to HMBC? How do you know?

HSQC peaks represent one-bond correlations between hydrogen and directly attached carbon atoms, whilst HMBC shows correlation between hydrogens and carbons that are two to three bonds apart. Thus, HSQC presents fewer correlations than HMBC: spectra 1 corresponds to HSQC and HMBC to the second one.

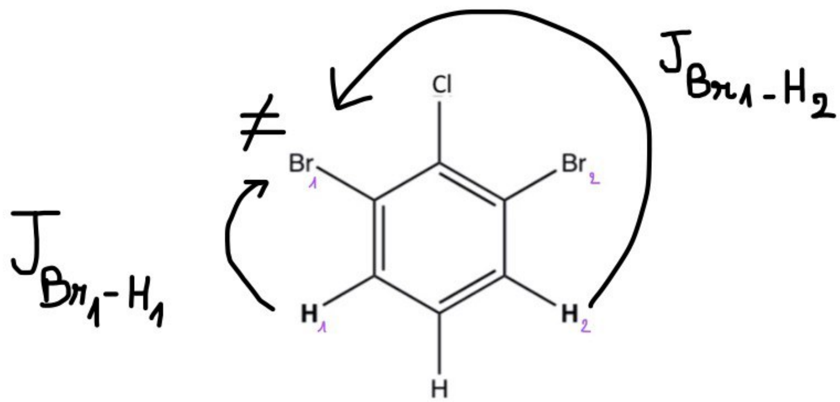
b. Assign the ^{1}H and ^{13}C. Notice that the axis limits vary between the experiments.





Question 2

[Keeler Section 12.2 and Hore Section 3.3] Are the two bolded protons in the following molecule chemically or magnetically equivalent? What about the two bromine atoms?



The two bolded proton are chemically equivalent due to the symmetry of the molecule (symmetry allows them to have the same local environment). However, the coupling between these protons and one bromine is different ($J_{Br1\text{-}H1} \neq J_{Br1\text{-}H2}$) so they aren't magnetically equivalent.

The two Bromine atoms are also chemically equivalent due to symmetry, but they aren't magnetically equivalent because of their different coupling with the two hydrogens.

Figure 1: Signal intensity as a function of tau