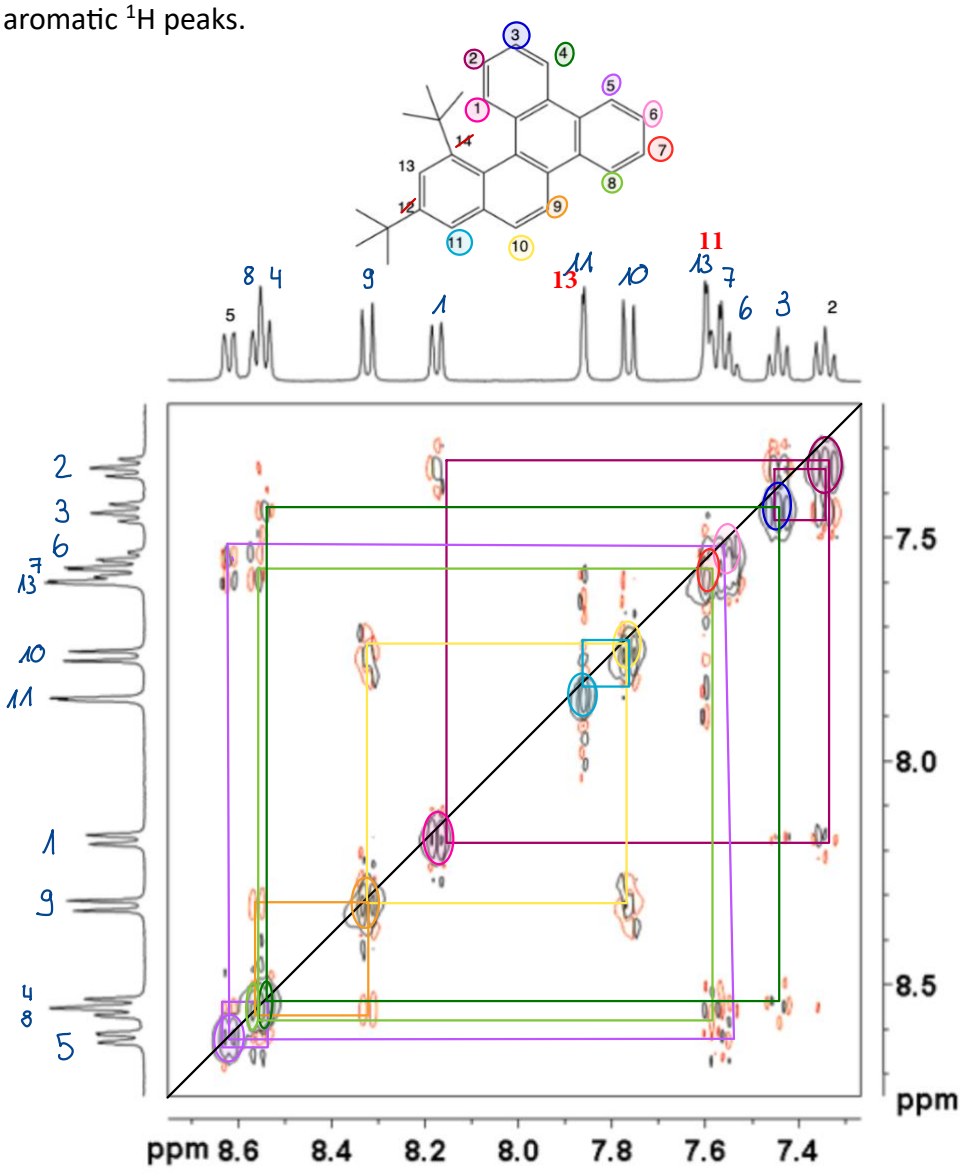
CH-314 Structural Analysis
ruben.rodriguezmadrid@epfl.ch
ray.cowen@epfl.ch

Jigsaw 4A

1. [Keeler Section 9.7.4] The 2D NOESY (Nuclear Overhauser Effect SpectroscopY) experiment gives information on through-space interactions, which can be used to identify protons which are close in space. Below, you have the aromatic region of the ^{1}H 2D NOESY spectrum of 12,14-di^{t}butylbenzo[g]chrysene. Assign the different aromatic ^{1}H peaks.

1.75/2



2. [Keeler Section 12.2 and Hore Section 3.3] For each of the following compounds determine whether the protons are magnetically or chemically equivalent. Explain why.

   a. Benzene

   b. [From Past Exam] The 2,5 protons in furan

1. Starting from 2, it is observed that it exchanges with two other protons as expected. It is expected for the atom 3 to have a triplet and for atom 1 to have a singlet, therefore the atoms 1 and 3 can be identified.
Starting from 5, it is known that it will exchange with 6 and weakly with 4. The peak for 6 should be a triplet and for 4 a doublet. It is however observed that a triplet appears for 4. This may be explained further by since it may be an overlap of doublets.

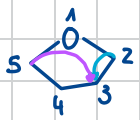
11 and 13 swapped

Starting from the singlet, only two choices open themselves: 11 or 13. It is known that there is a correlation between this proton and another, 11 is therefore chosen and 13 is isolated. 10 is therefore identified as the doublet next to it as it exchanges with it. 10 interacts strongly with 9, so the doublet on the left is identified as being 9. 9 is known to interact weakly with 8, as observed on the spectrum. The observed triplet was therefore the superposition of the doublet of 4 and 8. 8 is expected to interact strongly with 7, as it can be seen at the bottom right. Finally, 13 is identified to be in the mix of 6 and 7.

2. The condition to be chemically equivalent is that there must be a symmetry. And to be magnetically equivalent the nuclei must firstly be chemically equivalent, and secondly, it must have the same coupling with the other nuclei and/or all the nuclei are the same. 2/2

a) All the protons are chemically equivalent and magnetically equivalent.

b) Protons 2 and 5 are chemically equivalent but not magnetically equivalent because the proton 2 and 5 have not the same coupling with proton 3.



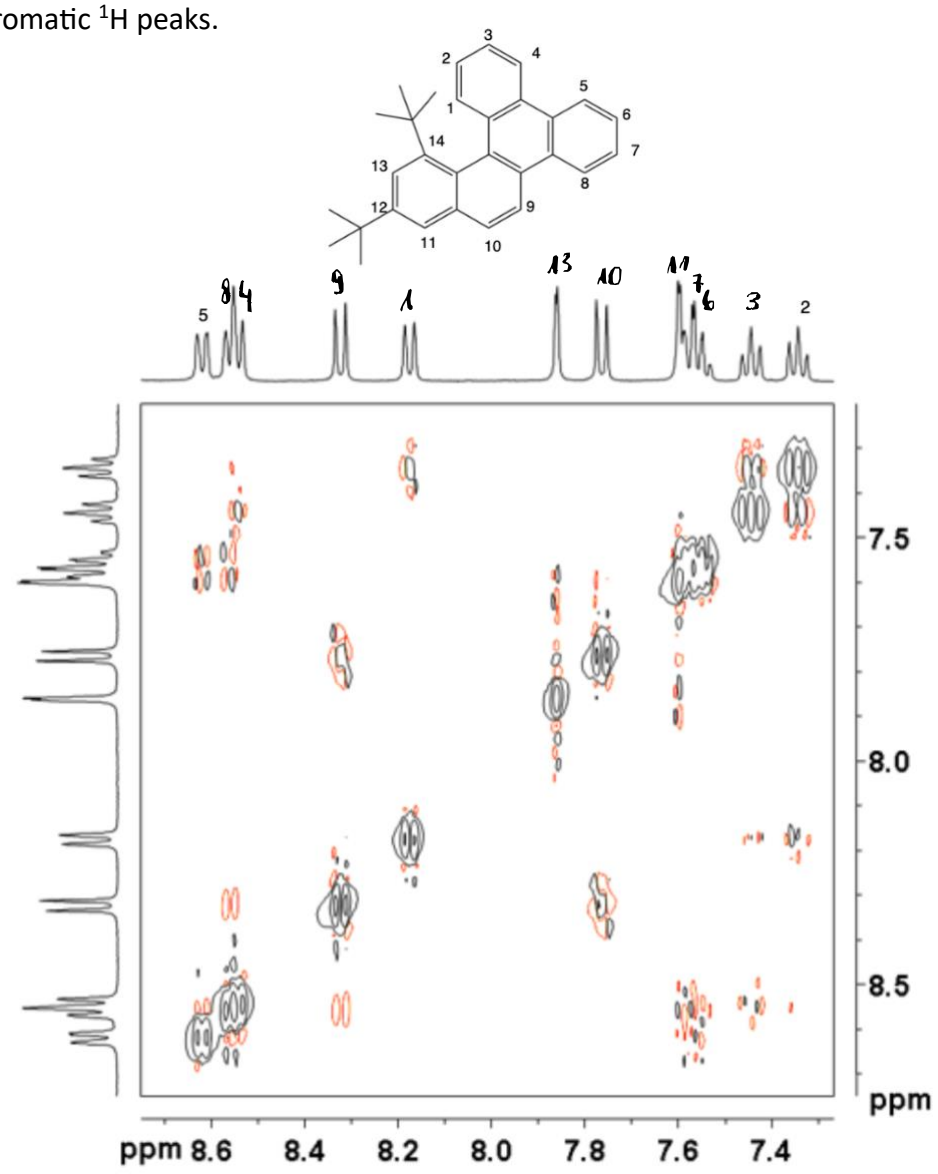
Victoire Kezeu T.
Matéo Tatzber

CH-314 Structural Analysis
ruben.rodriguezmadrid@epfl.ch
ray.cowen@epfl.ch

Jigsaw 4A

1. [Keeler Section 9.7.4] The 2D NOESY (Nuclear Overhauser Effect SpectroscopY) experiment gives information on through-space interactions, which can be used to identify protons which are close in space. Below, you have the aromatic region of the ^{1}H 2D NOESY spectrum of 12,14-di^{t}butylbenzo[g]chrysene. Assign the different aromatic ^{1}H peaks.

2/2

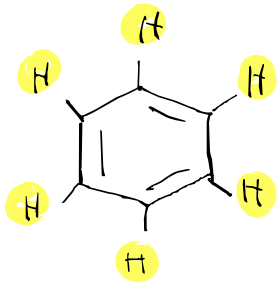


2. [Keeler Section 12.2 and Hore Section 3.3] For each of the following compounds determine whether the protons are magnetically or chemically equivalent. Explain why.

   a. Benzene

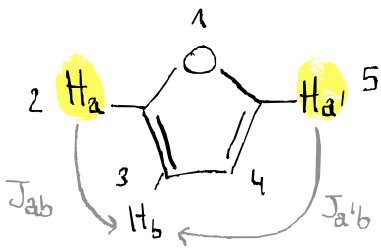
   b. [From Past Exam] The 2,5 protons in furan

(1)



Due to the aromatic nature of benzene, all H are magnetically equivalent and they are chemically equivalent because if protons are magnetically equivalent, they will also be chemically equivalent. The reverse is not true though.

(2)



$J_{ab} \neq J_{a'b}$

2,5 H are chemically equivalent because the carbons are equivalent by symmetry and H will have the same chemical shift.

NB :

- chemically equivalent : identical chemical shift / configuration
- magnetically equivalent : identical linkage / coupling to any atom

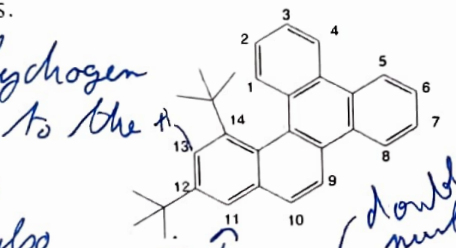
CH-314 Structural Analysis
ruben.rodriguezmadrid@epfl.ch
ray.cowen@epfl.ch

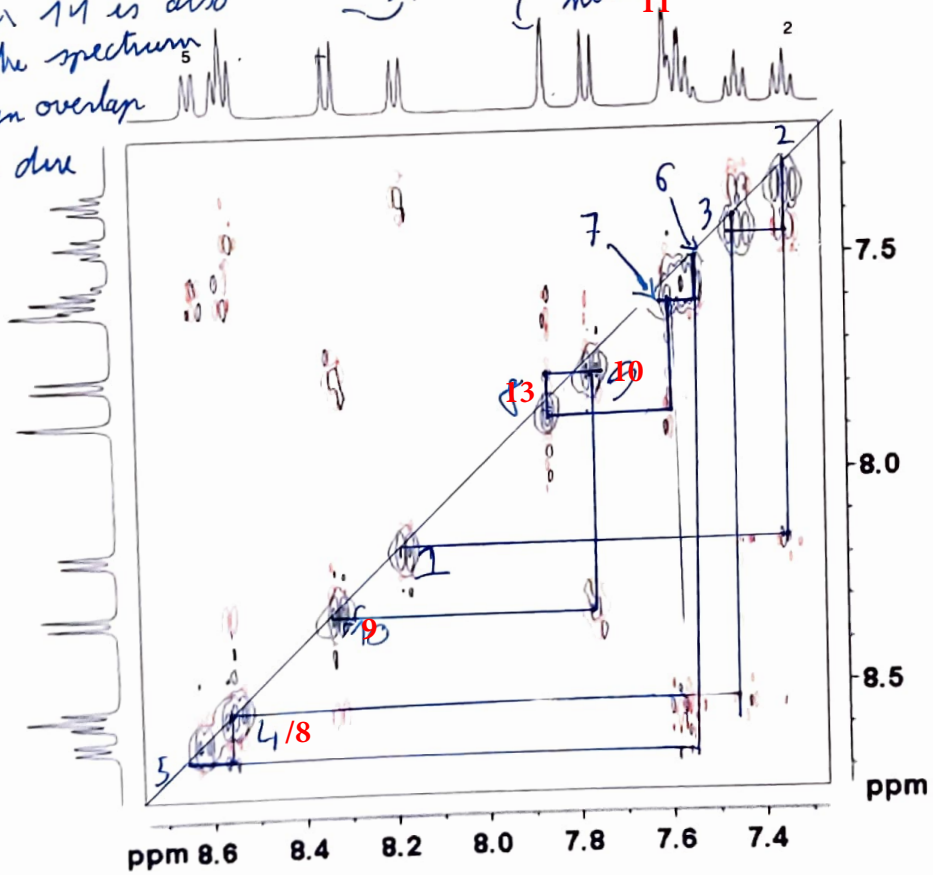
Jigsaw 4A

1. [Keeler Section 9.7.4] The 2D NOESY (Nuclear Overhauser Effect SpectroscopY) experiment gives information on through-space interactions, which can be used to identify protons which are close in space. Below, you have the aromatic region of the ^{1}H 2D NOESY spectrum of 12,14-di^{t}butylbenzo[g]chrysene. Assign the different aromatic ^{1}H peaks.

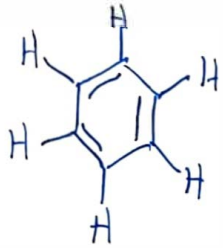
We do not see the hydrogen on carbon 13 due to the tert-butyl groups

Proton on carbon 14 is also not visible in the spectrum perhaps due to an overlap in the peaks or due to t-butyl.





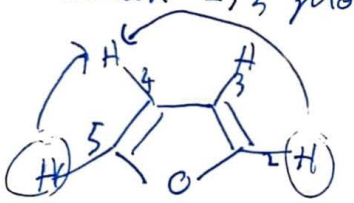
Benzene



All hydrogens are in equal chemical environments, so they are chemically equivalent

All hydrogen atoms experience the same magnetic environment so they are magnetically equivalent

Furan 2, 5 protons



The hydrogens 2,5 are bonded to the same atoms so they are chemically equivalent.

The hydrogens 2 and 5 are not magnetically equivalent since they have different J-coupling with proton 4 and 3.