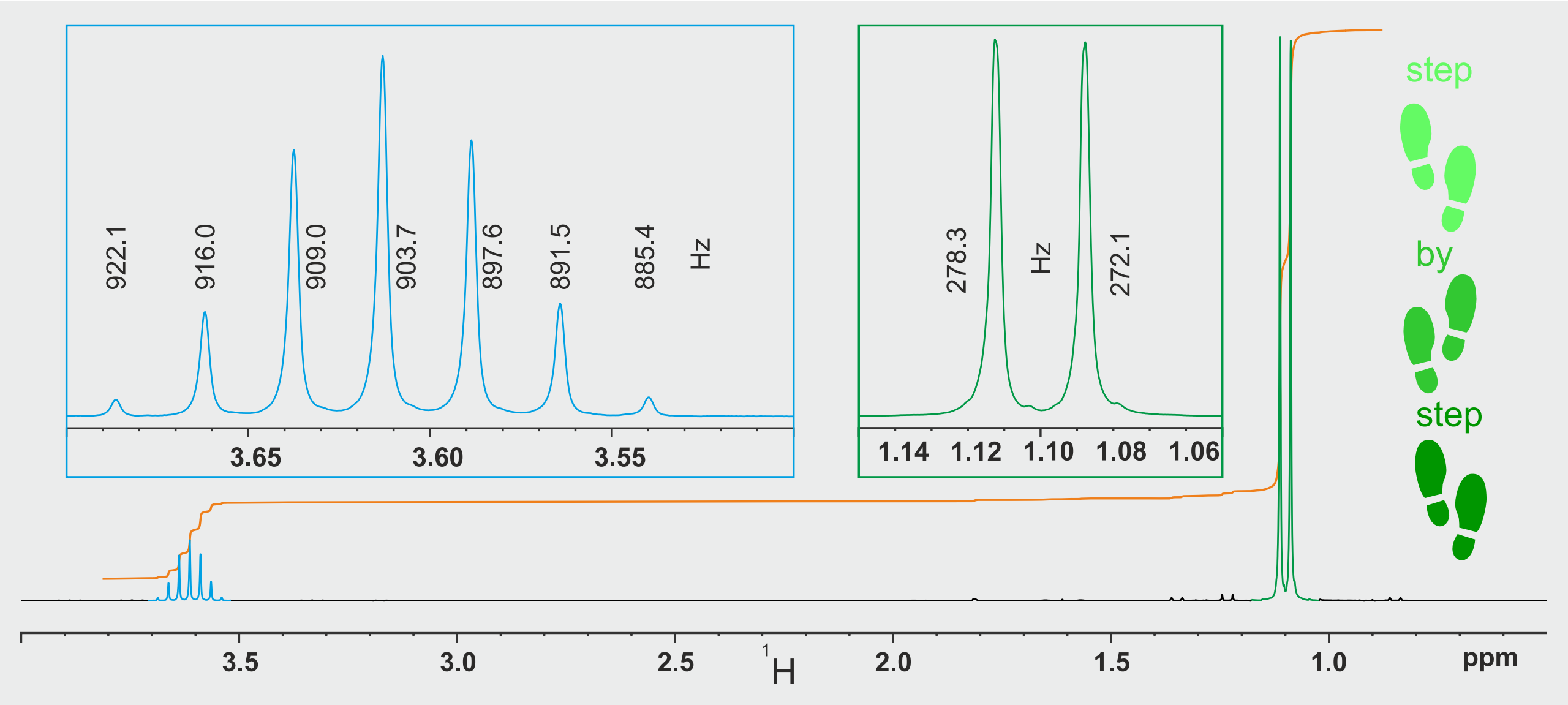
Exercise plus Solution – Quick PDF overview

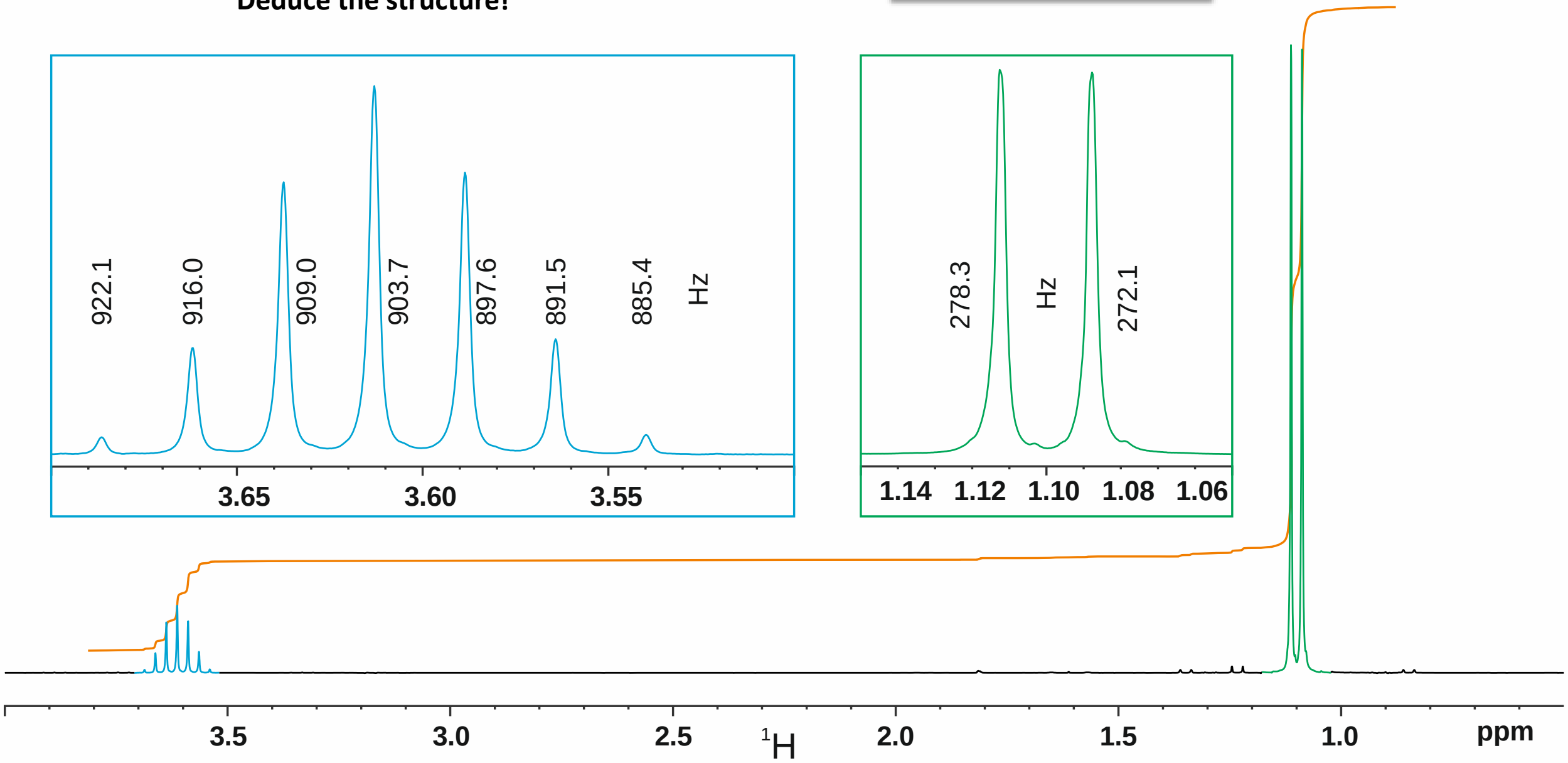
It is recommended to use this PDF version only for a quick overview of the NMR challenge. All animations of the PowerPoint version are missing, under certain circumstances quality deficiencies may also occur.
The higher quality PowerPoint files are freely available for download at any time.



$C_6H_{14}O$ measured in $CDCl_3$

Deduce the structure!

^{1}H NMR spectrum recorded at 250.13 MHz

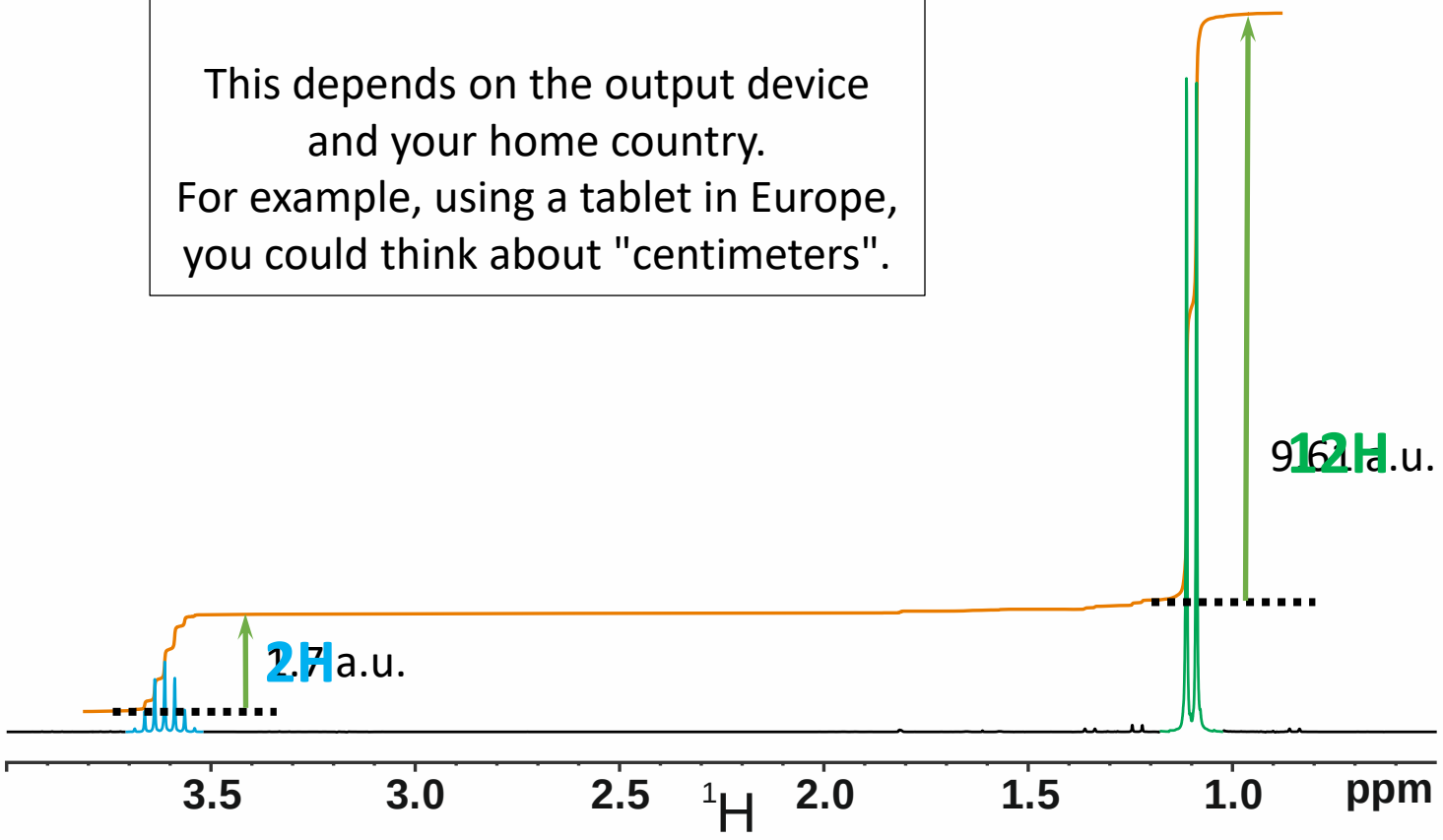


Solution

a.u. ???

arbitrary units

This depends on the output device and your home country.
For example, using a tablet in Europe, you could think about "centimeters".



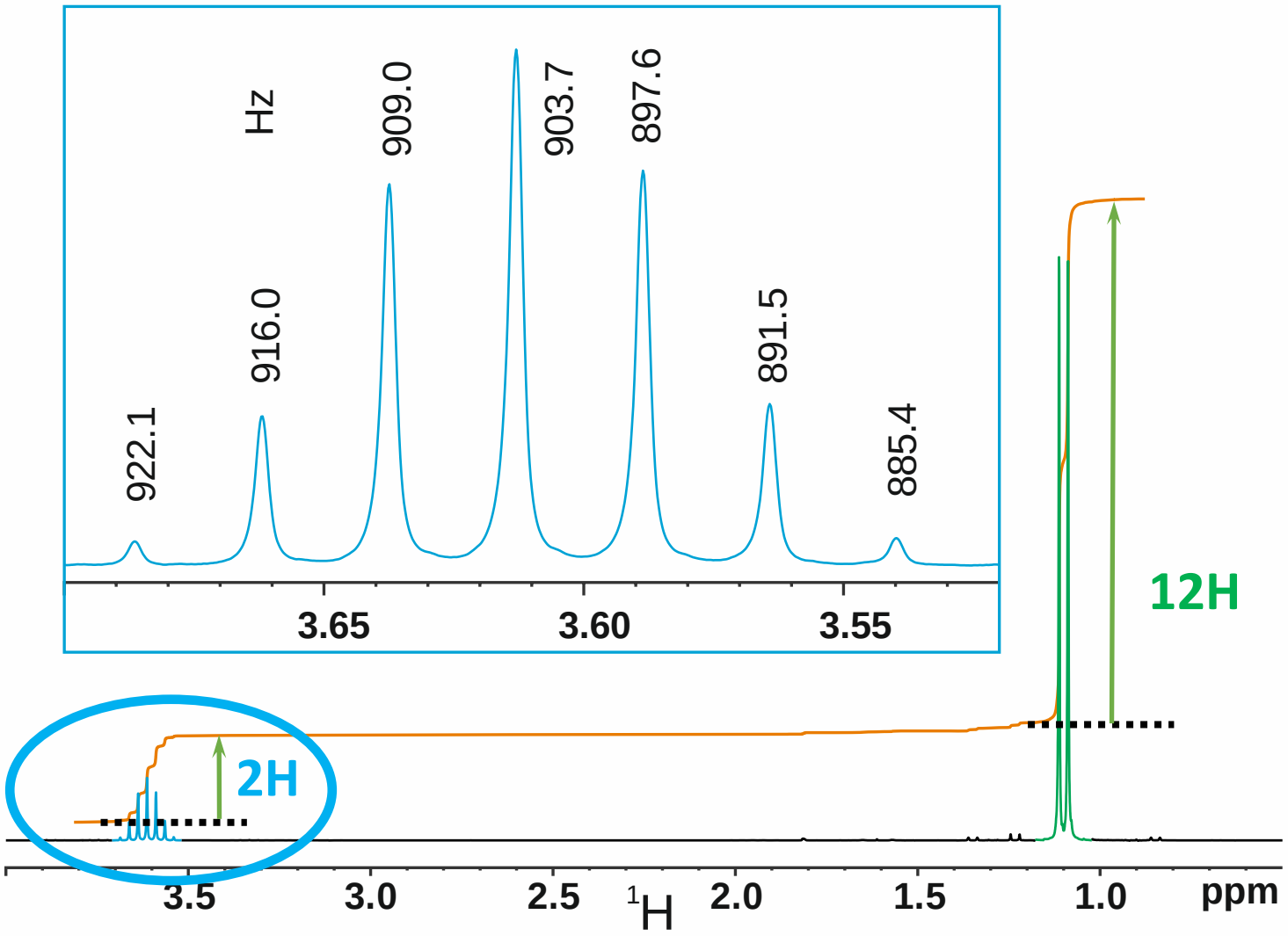
$C_6H_{14}O$

- no degree of unsaturation (double bond equivalents)
- fourteen protons and two signal groups only – there has to be some kind of symmetry
- Integration:

low field multiplet	-	1.7 a.u.
high field multiplet	-	9.61 a.u.
all 14 protons	-	11.31 a.u.
1 proton	≙	0.81 a.u.
low field multiplet	≙	**2.1** H
high field multiplet	≙	**11.9** H

Let us start with the septet.

Solution



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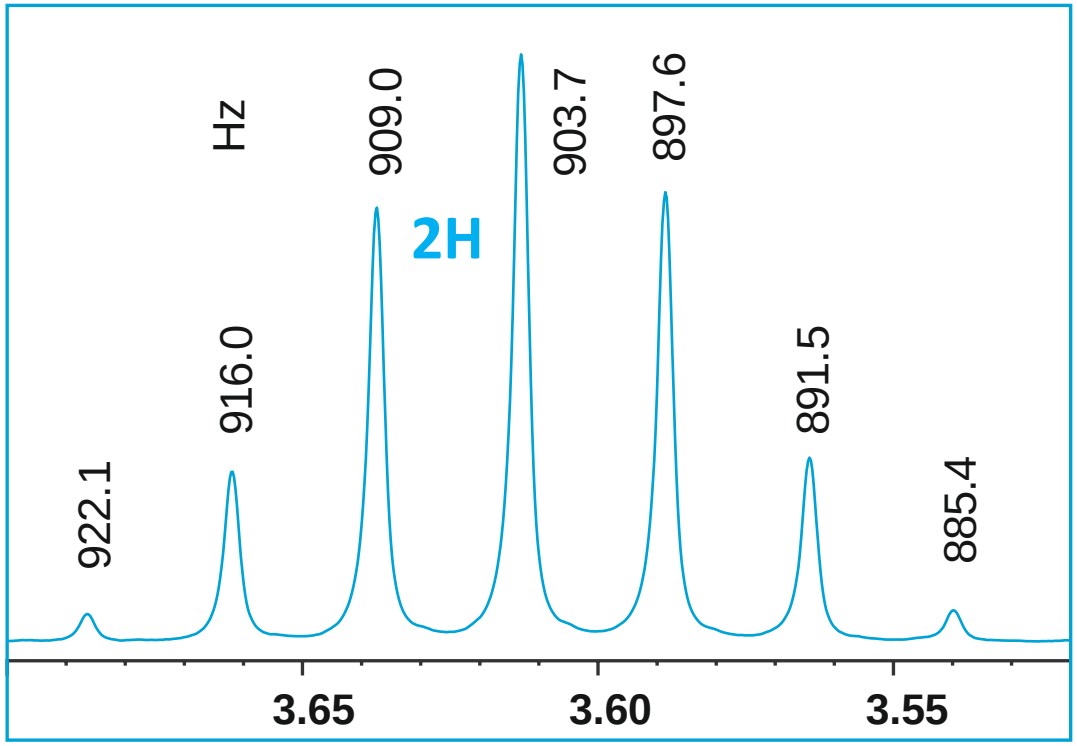
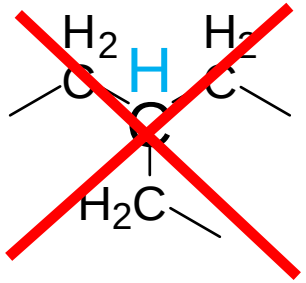
According to the *n-1 rule*, we need 6 equivalent neighbour protons to observe a septet.

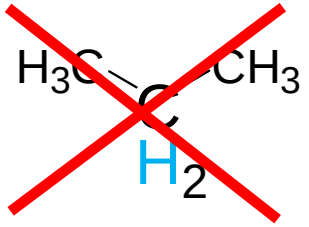
$C_6H_{14}O$



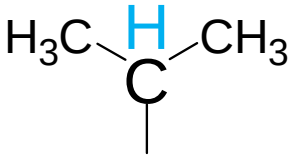
Because of the integral of **2** the fragment is needed twice, resulting in 8 C-atoms.



Where should the remaining C_3H_6O be bound?



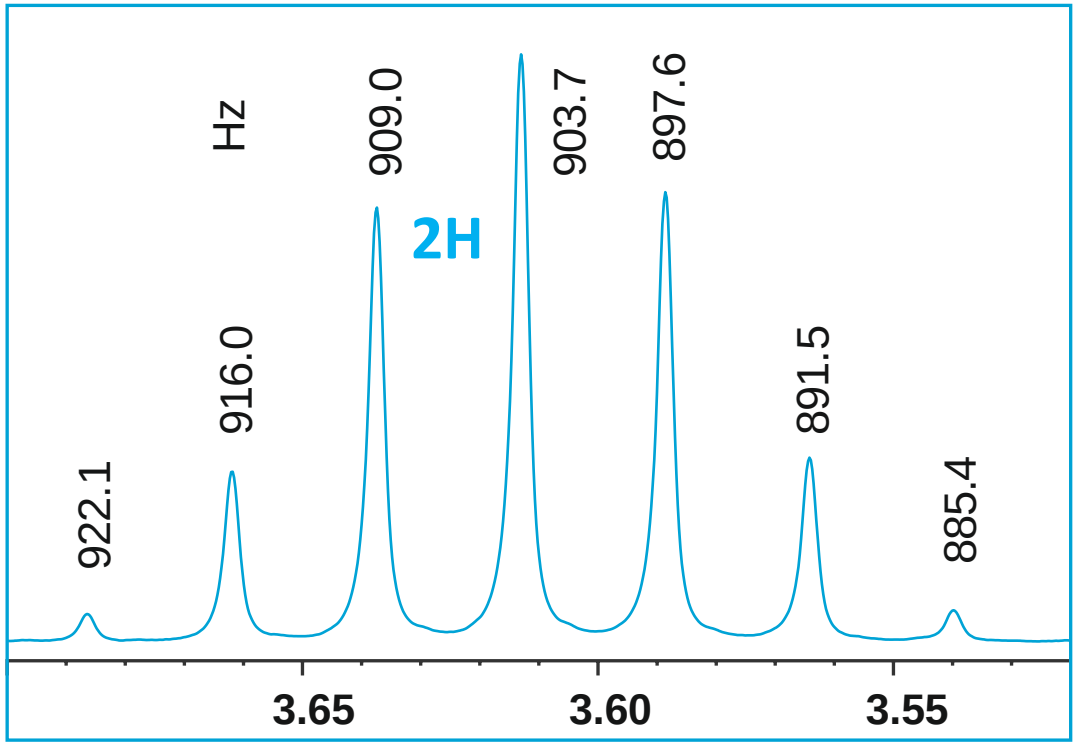
third possibility



According to the *n-1 rule*, we need 6 equivalent neighbour protons to observe a septet.

And why do we see an integral of 2?

$C_6H_{14}O$



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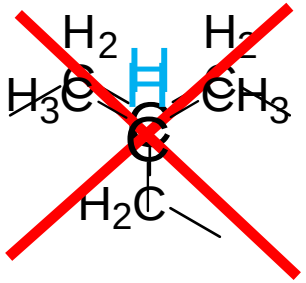

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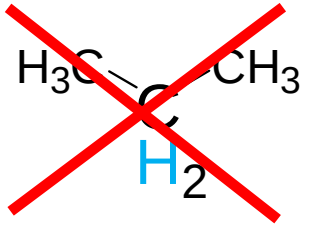

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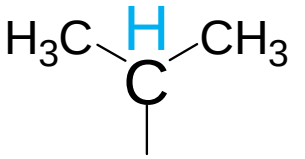

$C_6H_{14}O$

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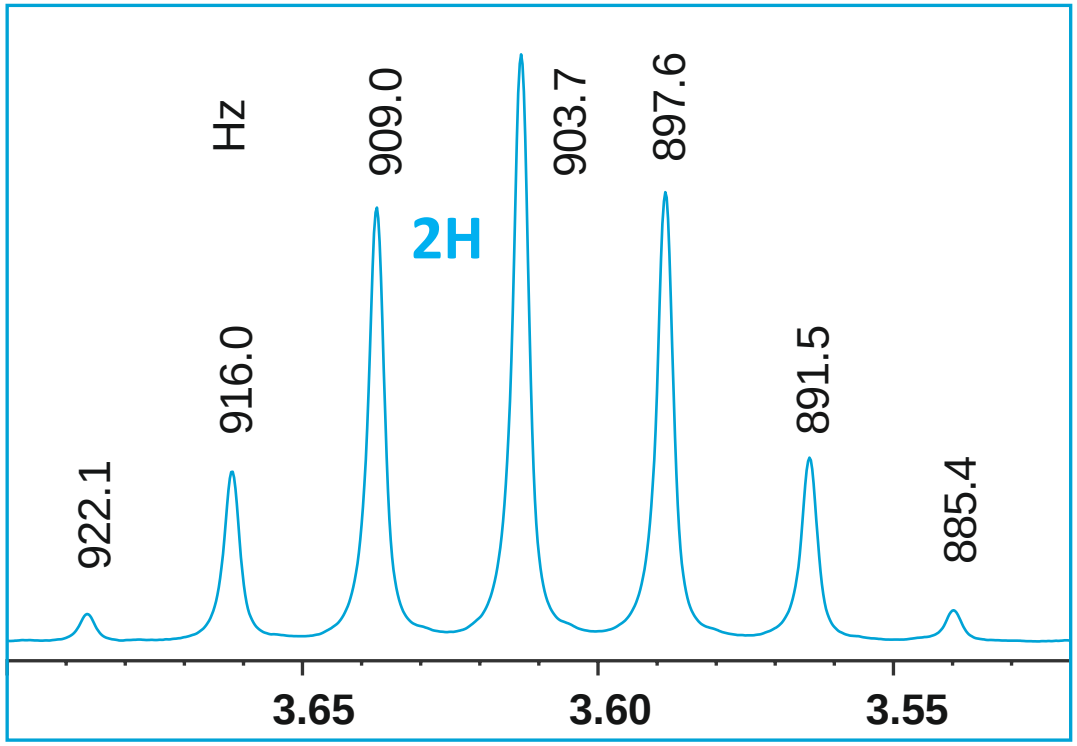
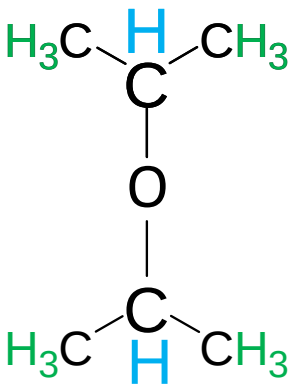


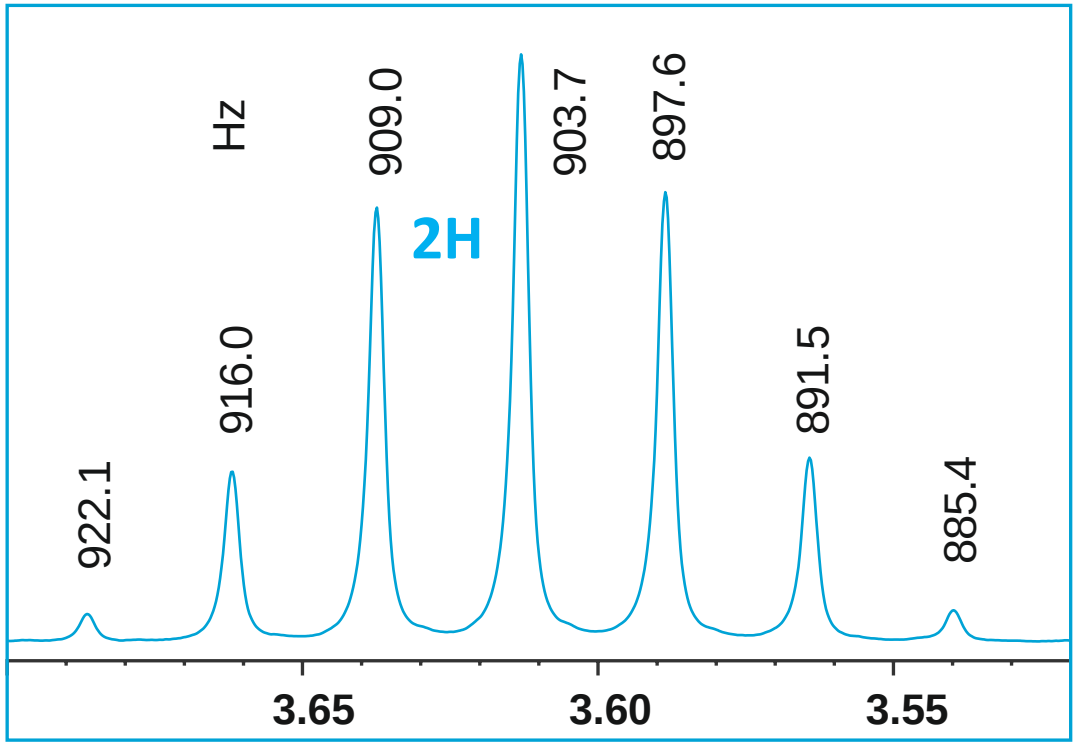
And now only one oxygen atom is missing from the molecular formula. The two isopropyl fragments can be connected using the oxygen atom.

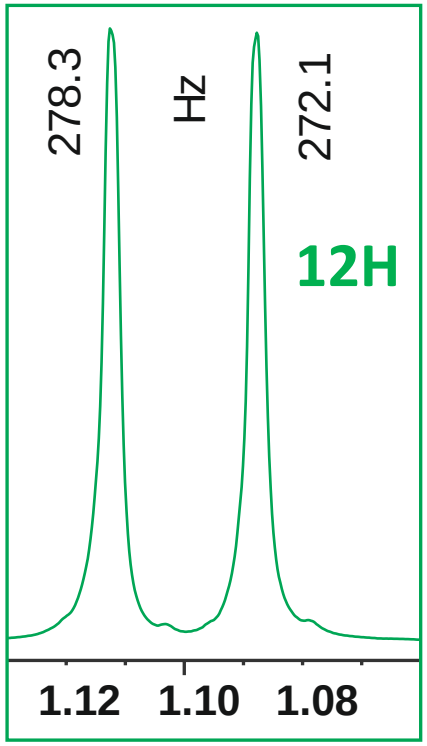


The integral of **2** is obtained via an identical second isopropyl fragment.

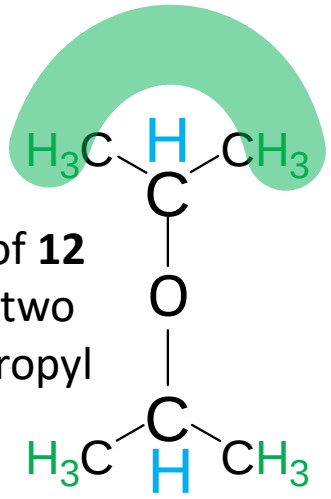
$C_6H_{14}O$

What about the methyl groups?





The integral of **12** results from two identical isopropyl groups.

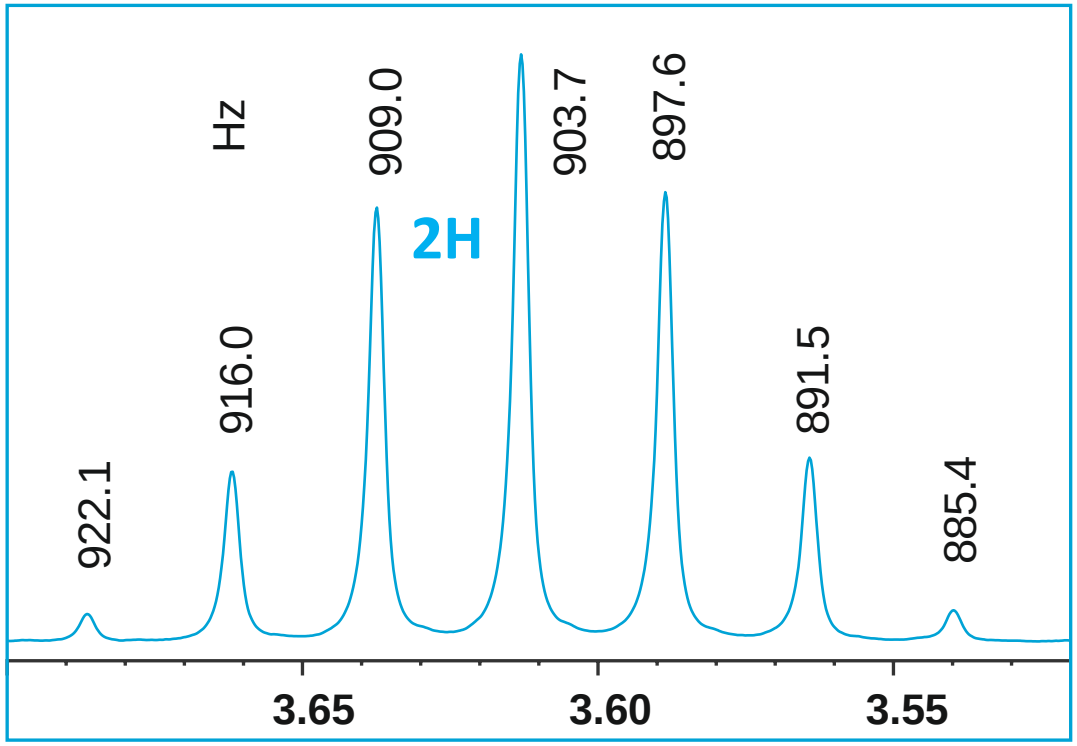


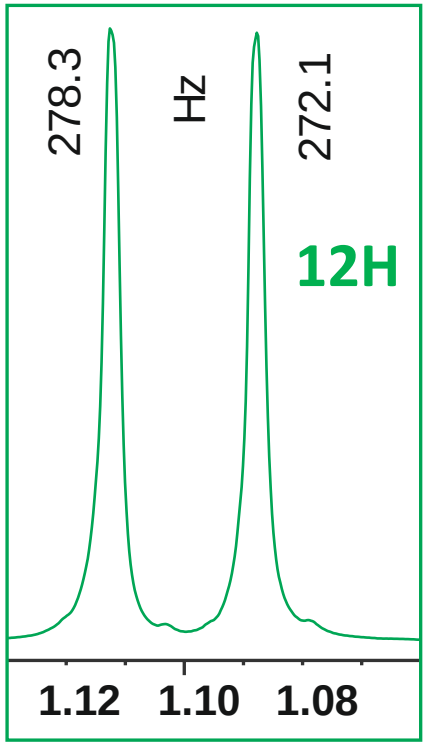
All six methyl protons within the isopropyl group are chemically equivalent and are three bonds separated from the same neighbour proton.

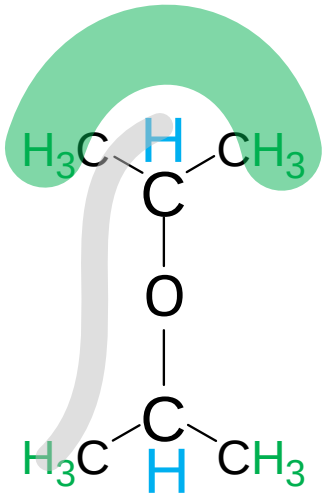
We expect a doublet.

One final remark.

$C_6H_{14}O$







In principle there is a second way for the scalar coupling across 5 bonds. Normally, only couplings over up to three bonds may be seen. Here we are not able to see this coupling.

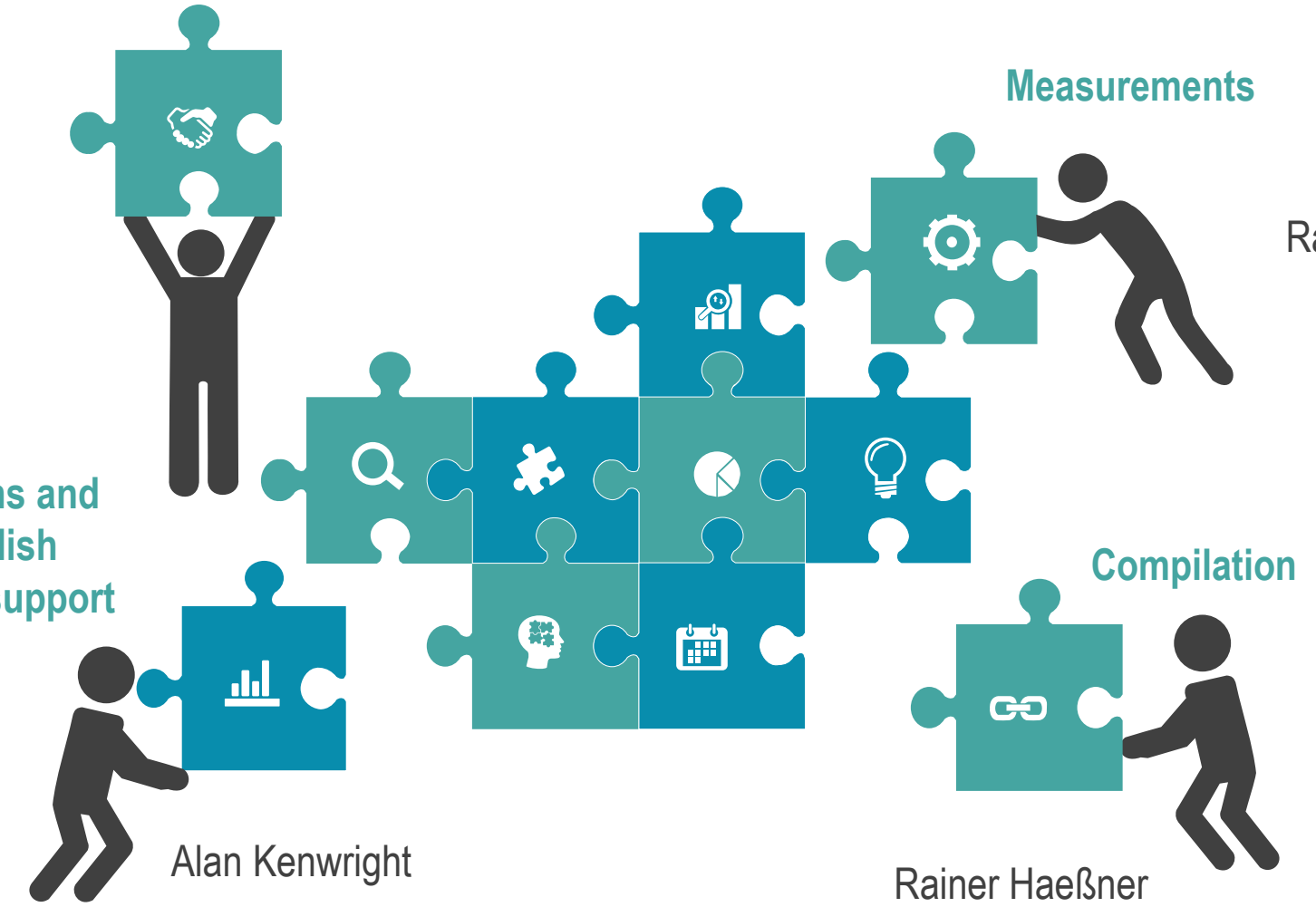
Contributions

Spectrometer time

TU Munich

Measurements

Rainer Haeßner



Discussions and native English language support

Alan Kenwright

Compilation

Rainer Haeßner

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