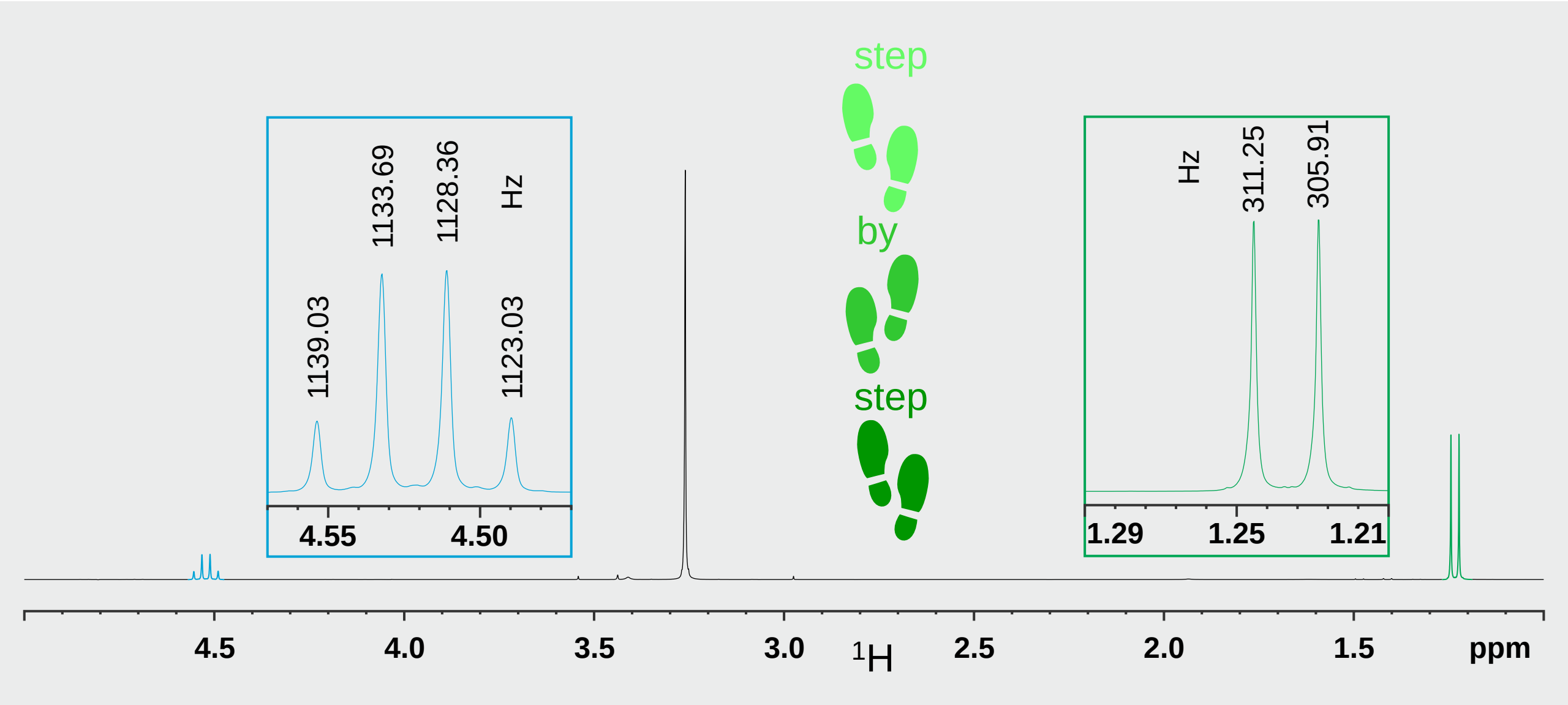
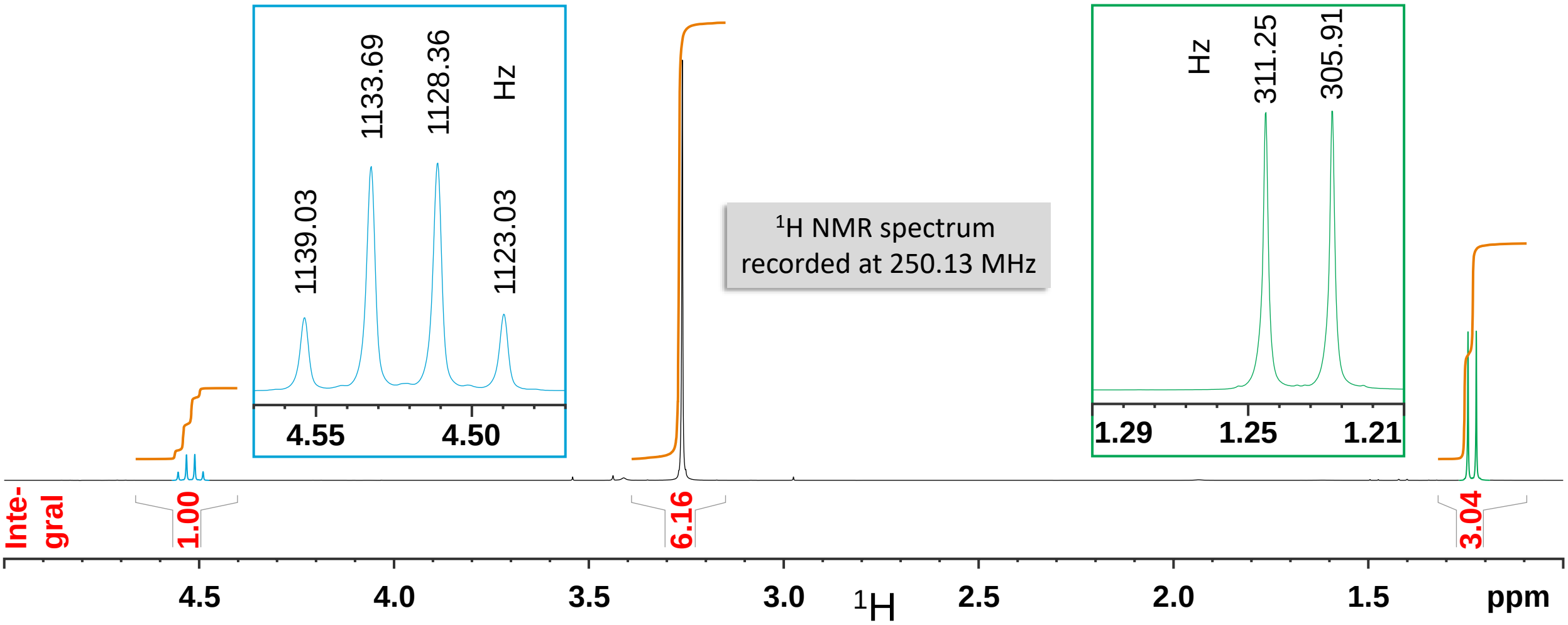
Exercise plus Solution – Quick overview

It is recommended to use this 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.



$C_4H_{10}O_2$ measured in $CDCl_3$

Deduce the structure!



$C_4H_{10}O_2$ recorded in $CDCl_3$

Step-by-step-solution

There is no **double bond equivalent**.

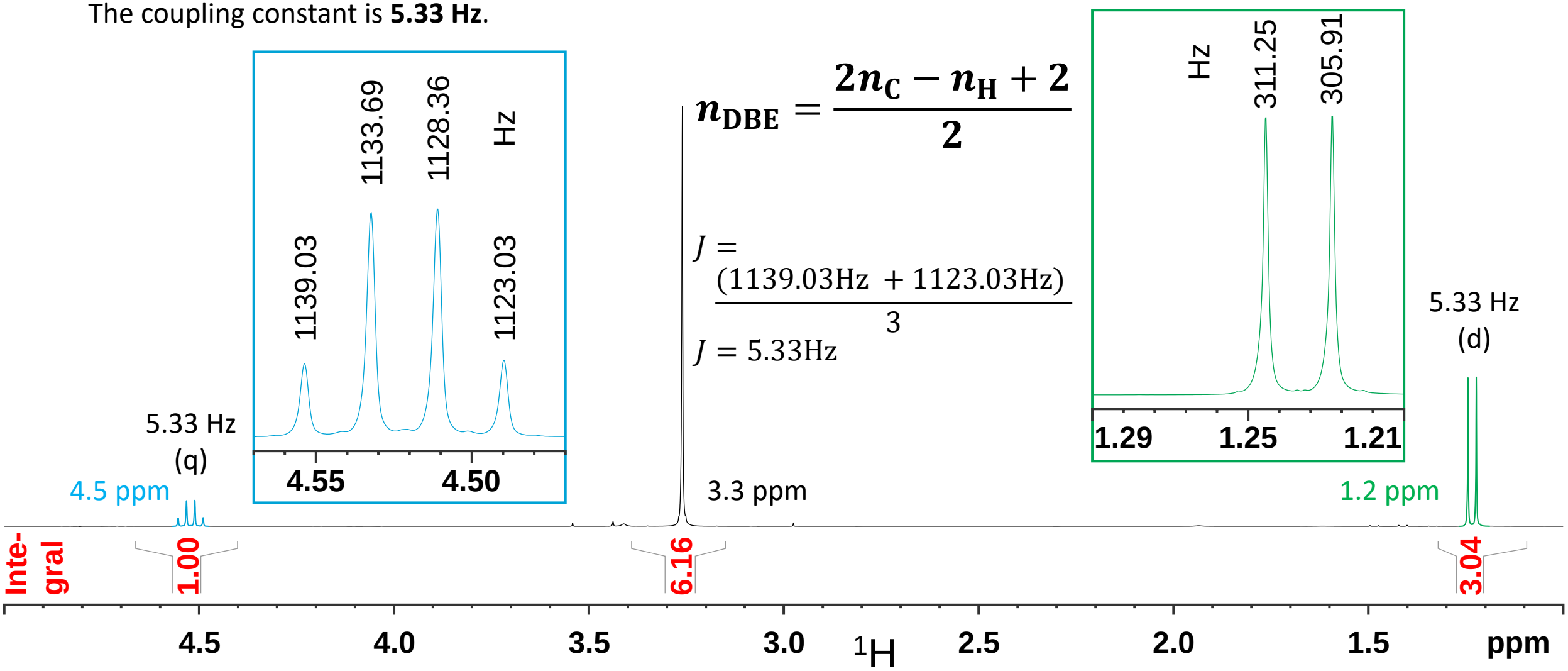
The chemical shifts are not particularly important in this example.
There are only two multiplets, i.e. they can only be "pure" multiplets – in this case a **doublet** and a **quartet**.
An estimation is sufficient.

The coupling constant is **5.33 Hz**.

$$n_{DBE} = \frac{2n_C - n_H + 2}{2}$$

$$J = \frac{(1139.03\text{Hz} + 1123.03\text{Hz})}{3}$$

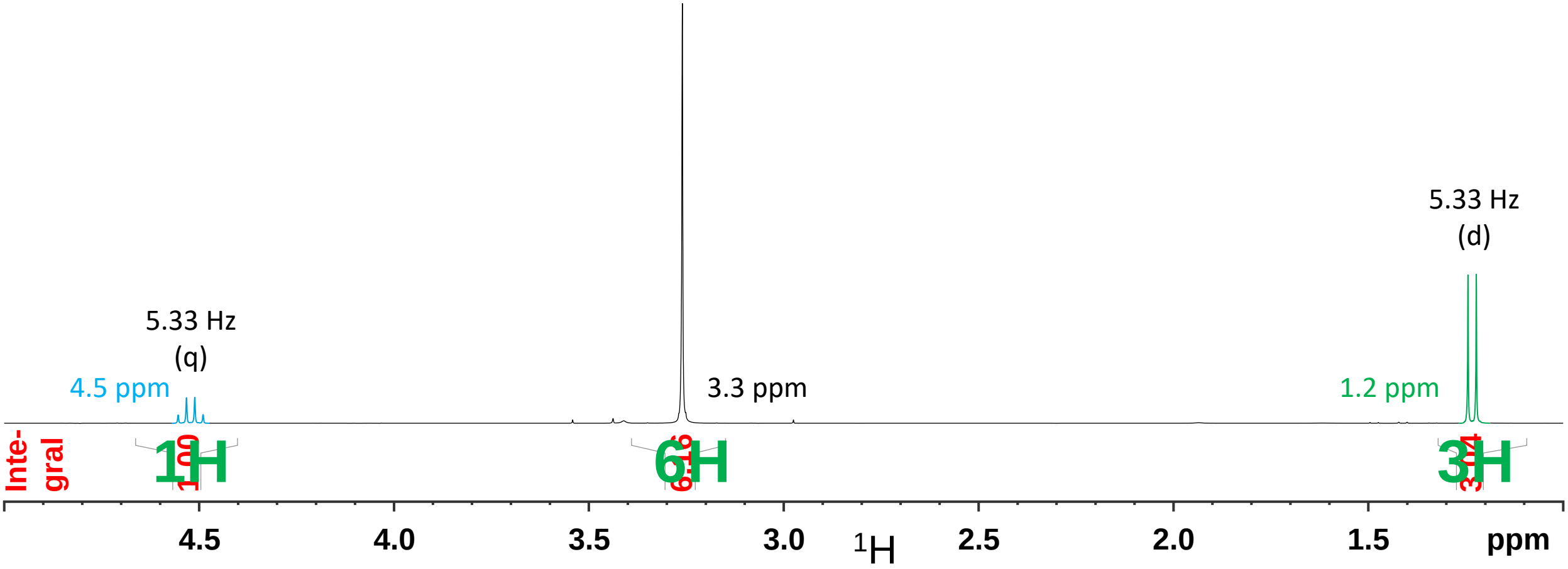
$$J = 5.33\text{Hz}$$



There is no **double bond equivalent**.

Integration is simple, the proportionality factor between the measured integral (in arbitrary units) and the proton number is just 1.

$C_4H_{10}O_2$ recorded in $CDCl_3$

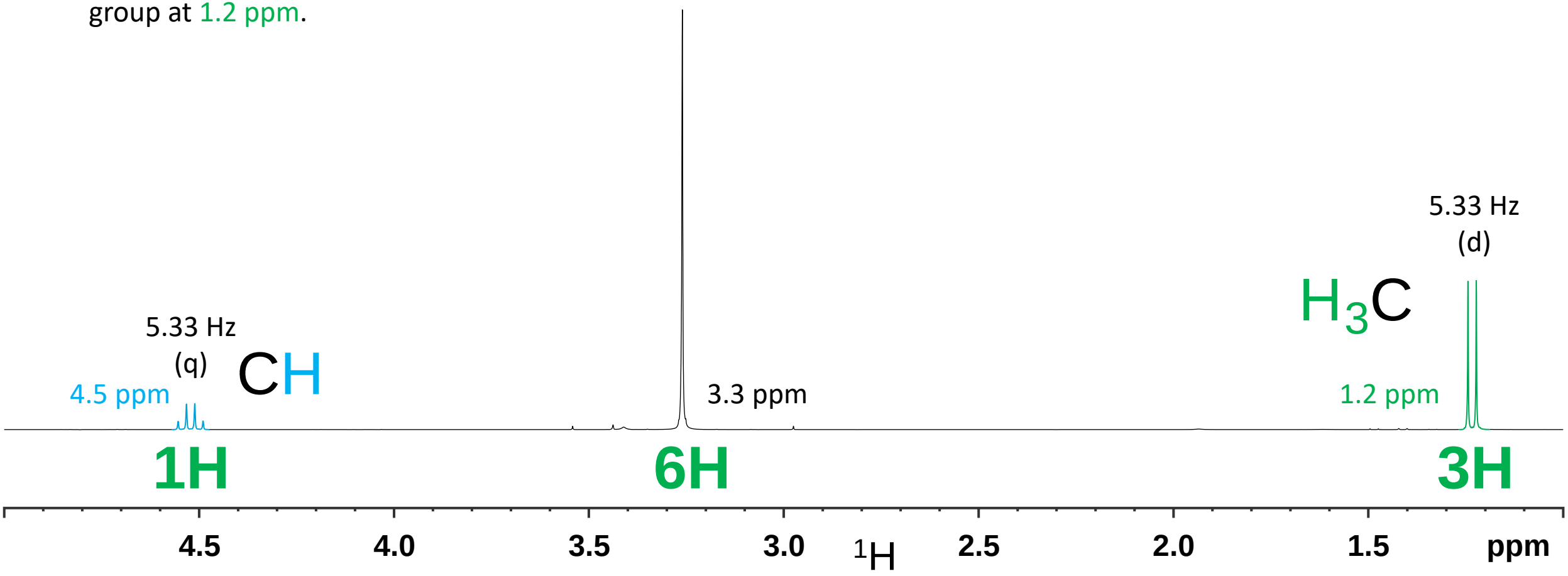


There is no **double bond equivalent**.

$C_4H_{10}O_2$ recorded in $CDCl_3$

Let us first assume that all three signal groups originate from CH_n fragments. The reason why OH is out of question follows in a few steps.

Then we would have a CH group at 4.5 ppm and a CH_3 group at 1.2 ppm.



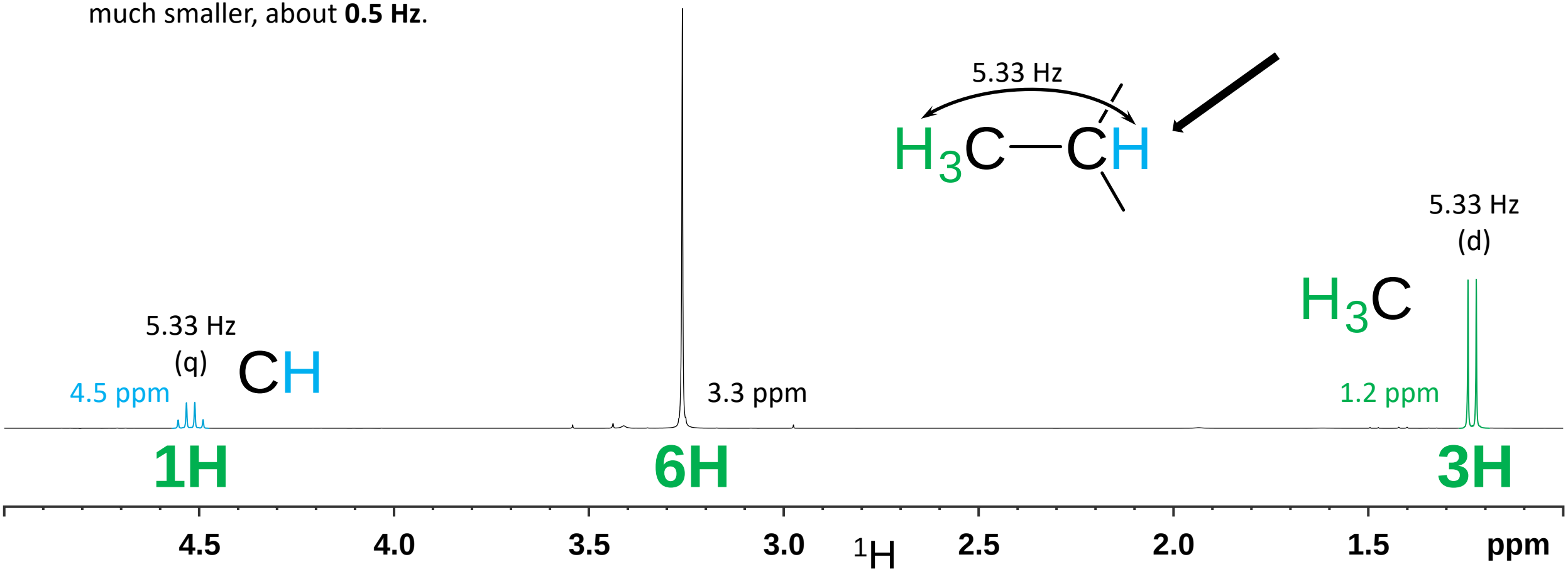
$C_4H_{10}O_2$

If the carbon atoms of the two fragments are joined together, the coupling patterns of both multiplets can be well explained.

In the case of CH, of course, two free valences are missing.

A coupling constant of **5.33 Hz** is somewhat small for vicinal coupling. **7 Hz** would be ideal. On the other hand, a wide-range coupling across four single bonds would be much smaller, about **0.5 Hz**.

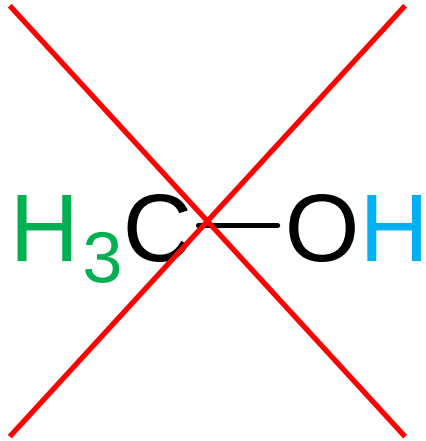
Let us now replace CH with OH on a trial basis.



This would give us methanol. Further connections are not possible, but the part of the molecule responsible for the singlet at approx. **3.3 ppm** still has to be connected somehow.

$C_4H_{10}O_2$

Lets return to CH_3–CH<.

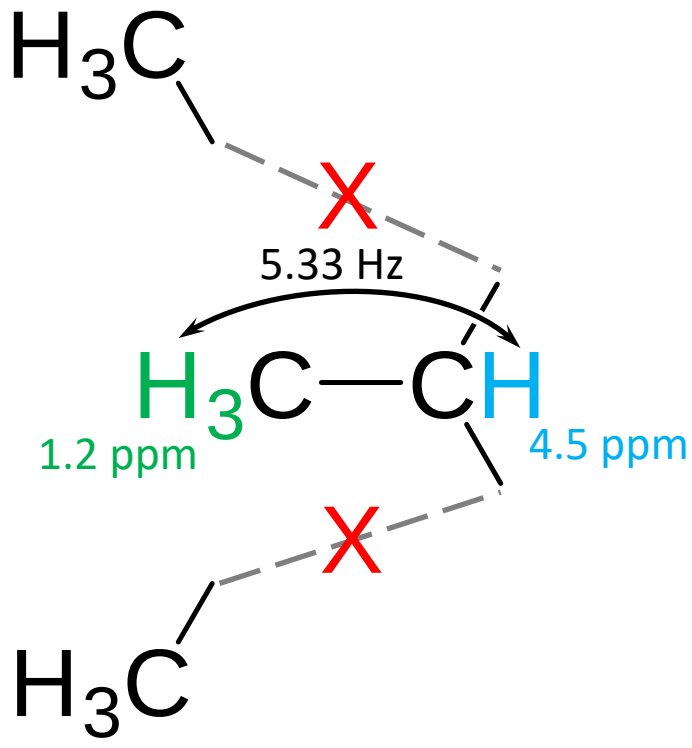


$C_4H_{10}O_2$

A singlet with 6 protons might be due to two equivalent CH_3 or three equivalent CH_2 groups.

Two out of a total of four C atoms are already assigned. Three more carbon atoms are impossible. The signal at 3.3 ppm comes from **two equivalent methyl groups**.

The methyl groups cannot be directly attached to the CH group. If they were directly attached, we would see a doublet at **3.8 ppm**.



A short inventory is sufficient for a complete structural elucidation.

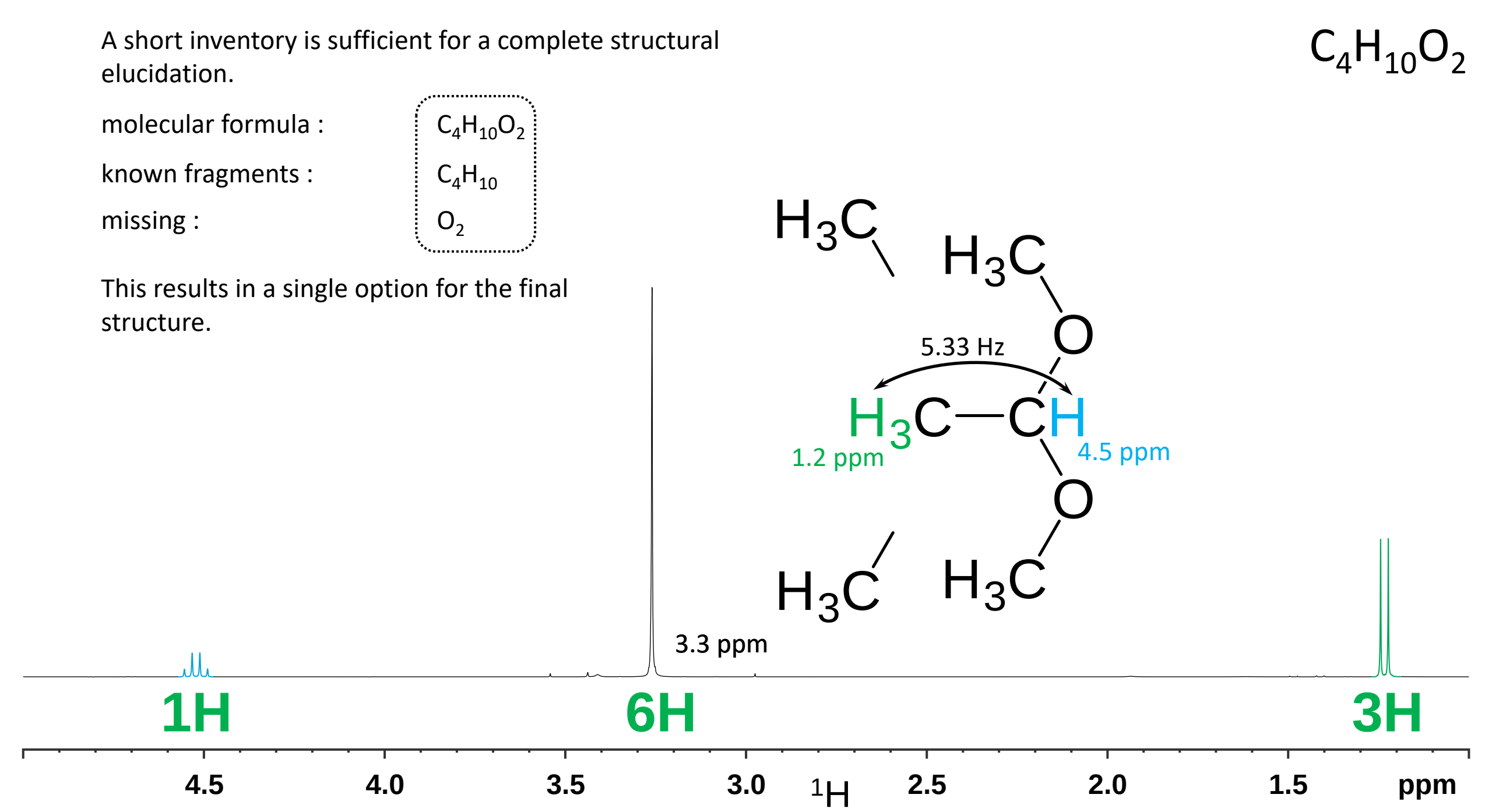
$C_4H_{10}O_2$

molecular formula : $C_4H_{10}O_2$

known fragments : C_4H_{10}

missing : O_2

This results in a single option for the final structure.



Contributions

Spectrometer time

TU Munich

Measurements

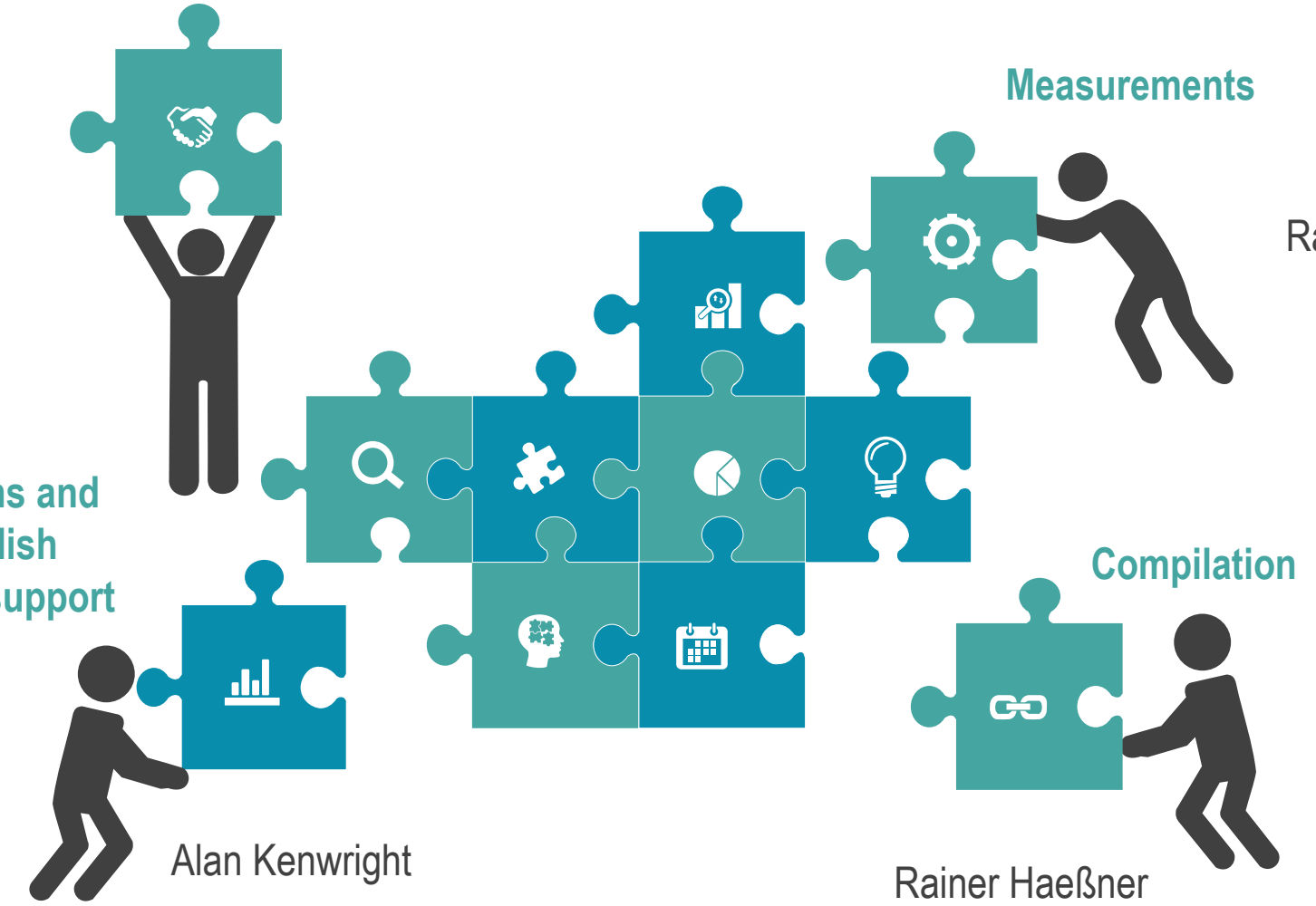
Rainer Haeßner

Discussions and native English language support

Alan Kenwright

Compilation

Rainer Haeßner



More exercises …