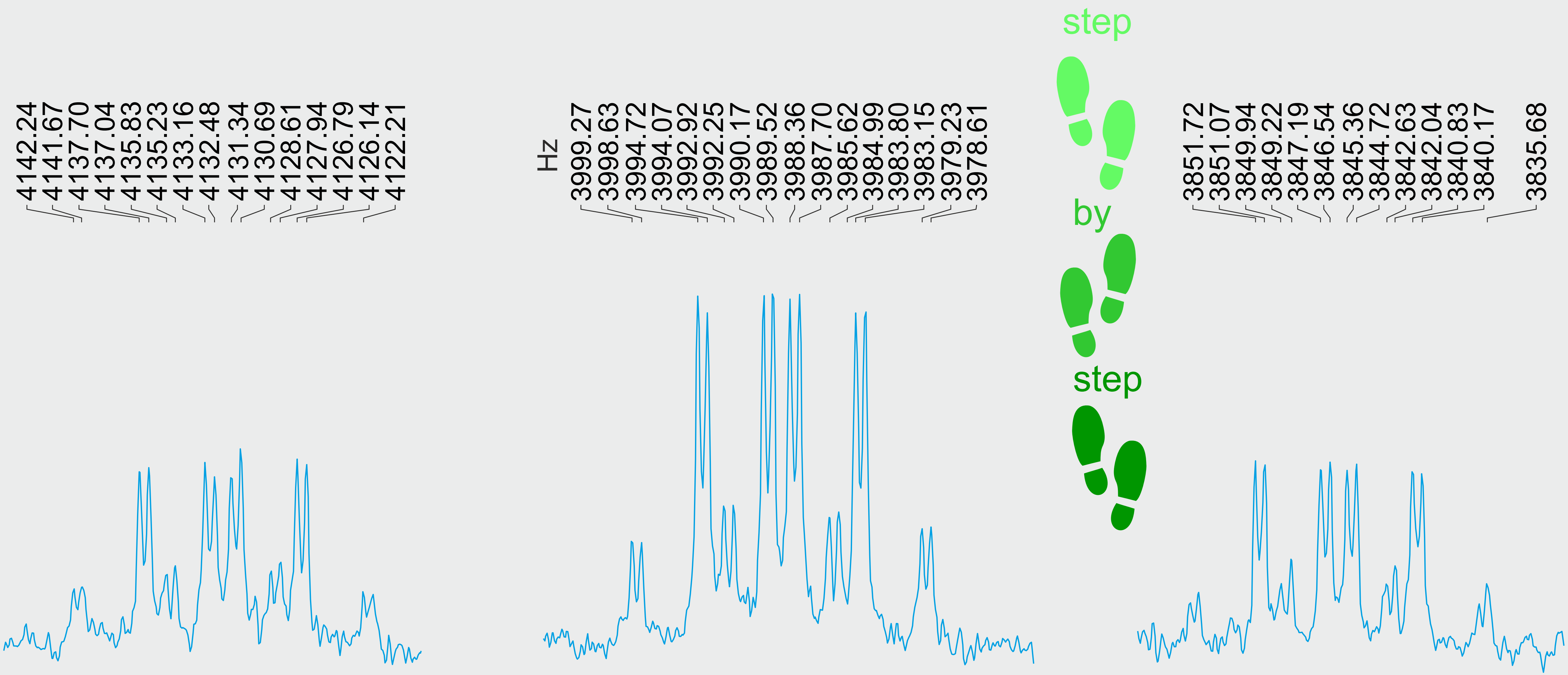
Exercise plus Solution – Quick overview

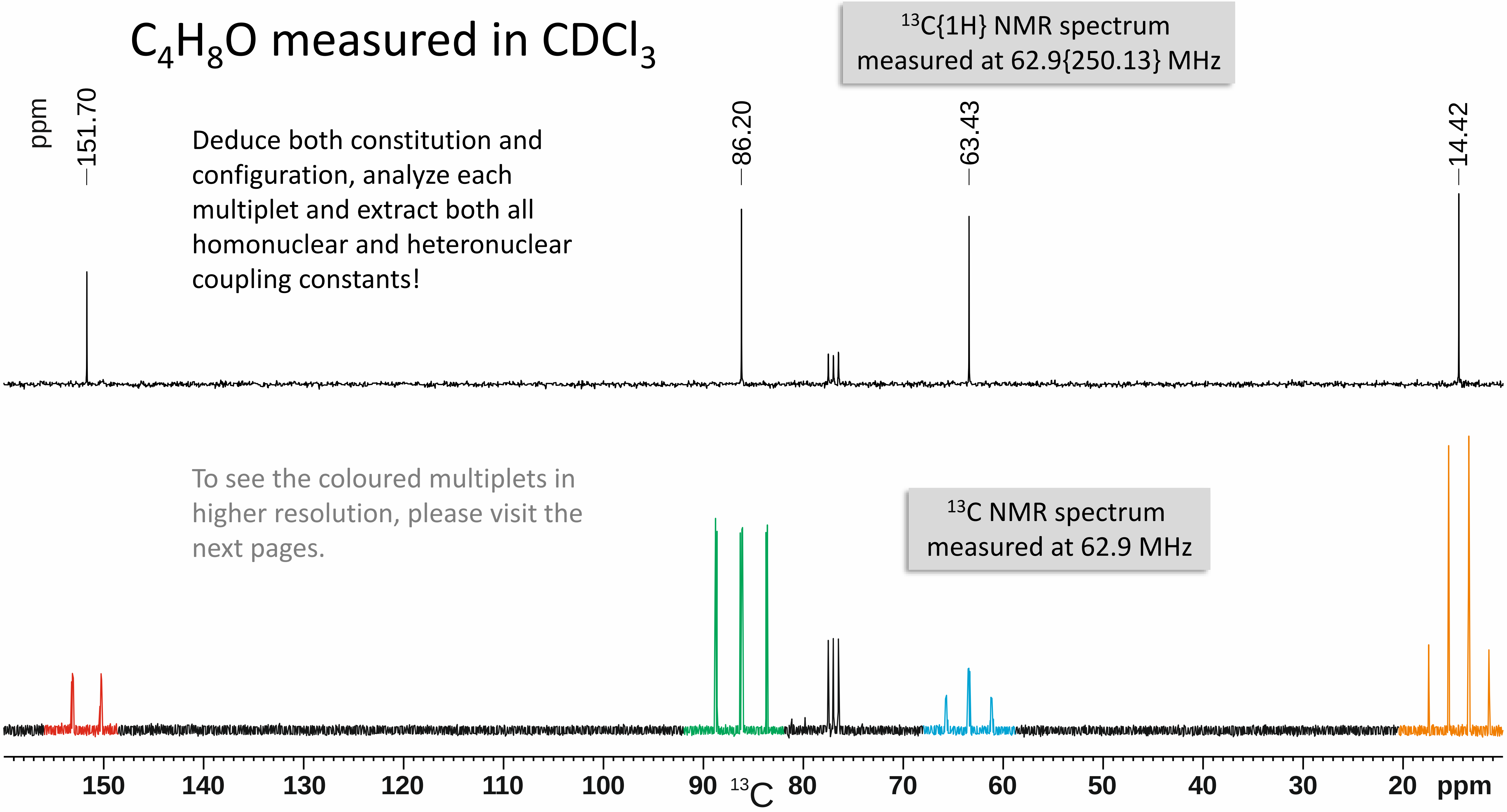
It is recommended to use this version only for a quick overview of the NMR challenge. All animations of the PowerPoint version are missing, under certain circumstances quality deficiencies may also occur.
The higher quality PowerPoint files are freely available for download at any time.



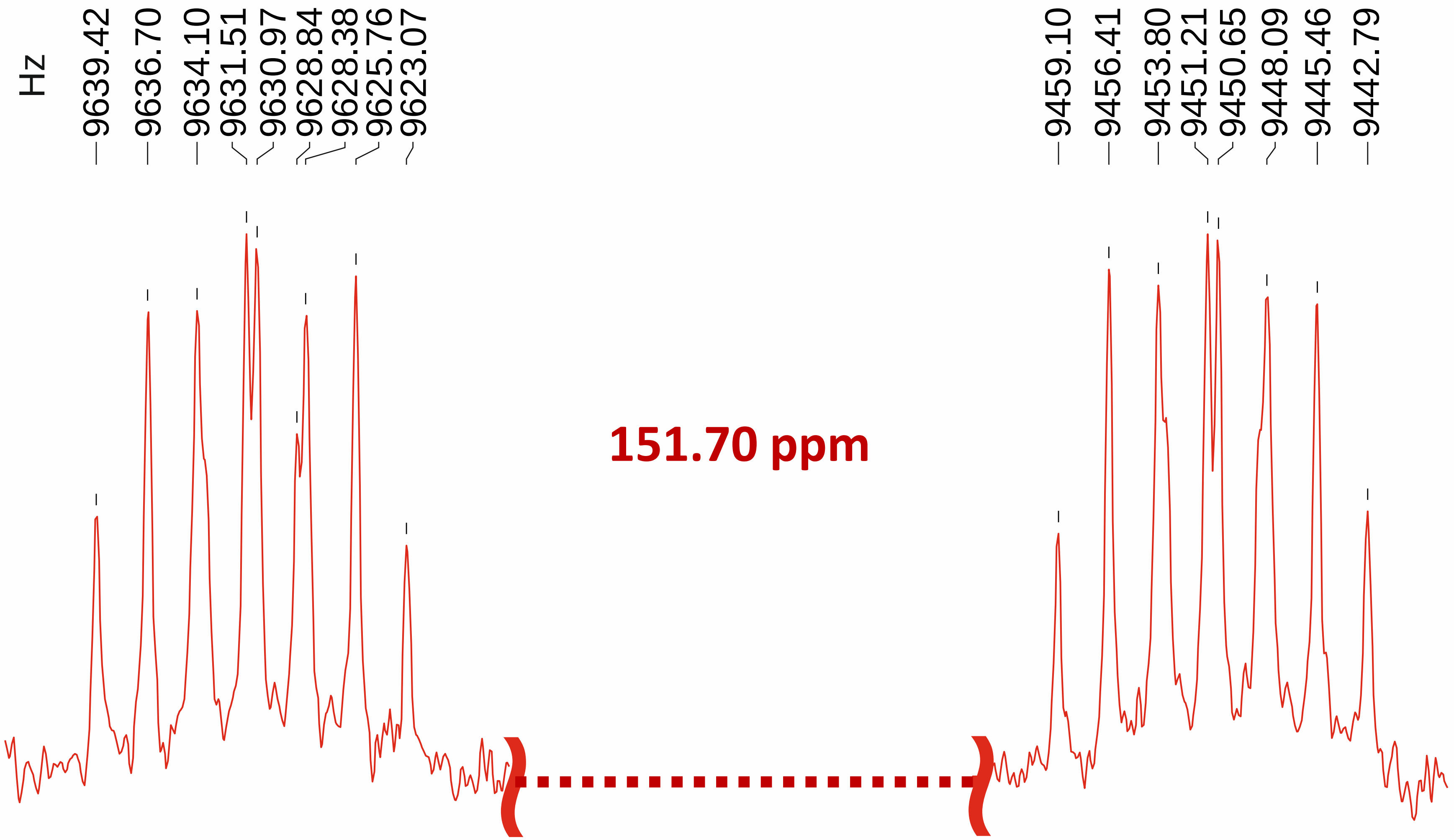
C_4H_8O measured in $CDCl_3$

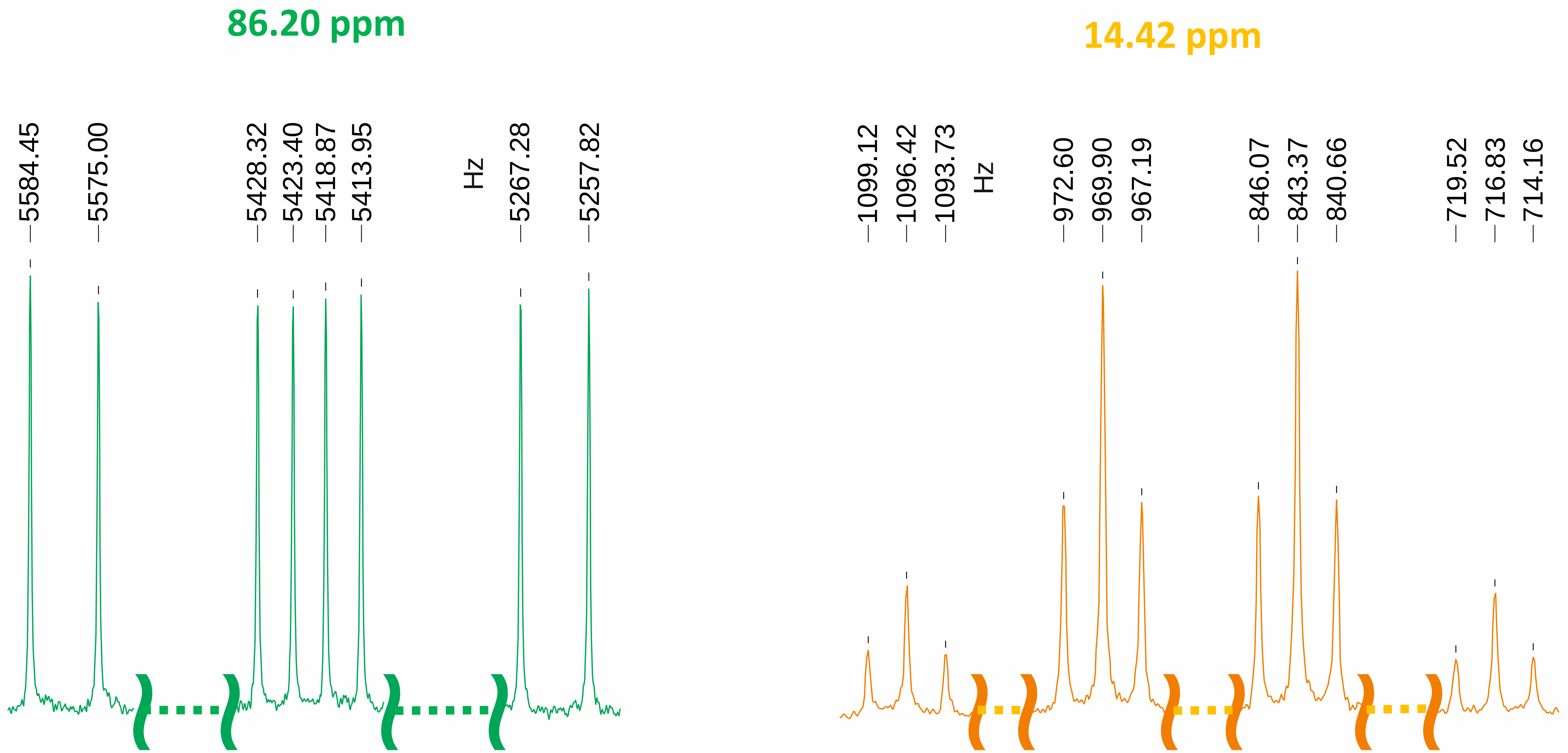
Deduce both constitution and configuration, analyze each multiplet and extract both all homonuclear and heteronuclear coupling constants!

To see the coloured multiplets in higher resolution, please visit the next pages.



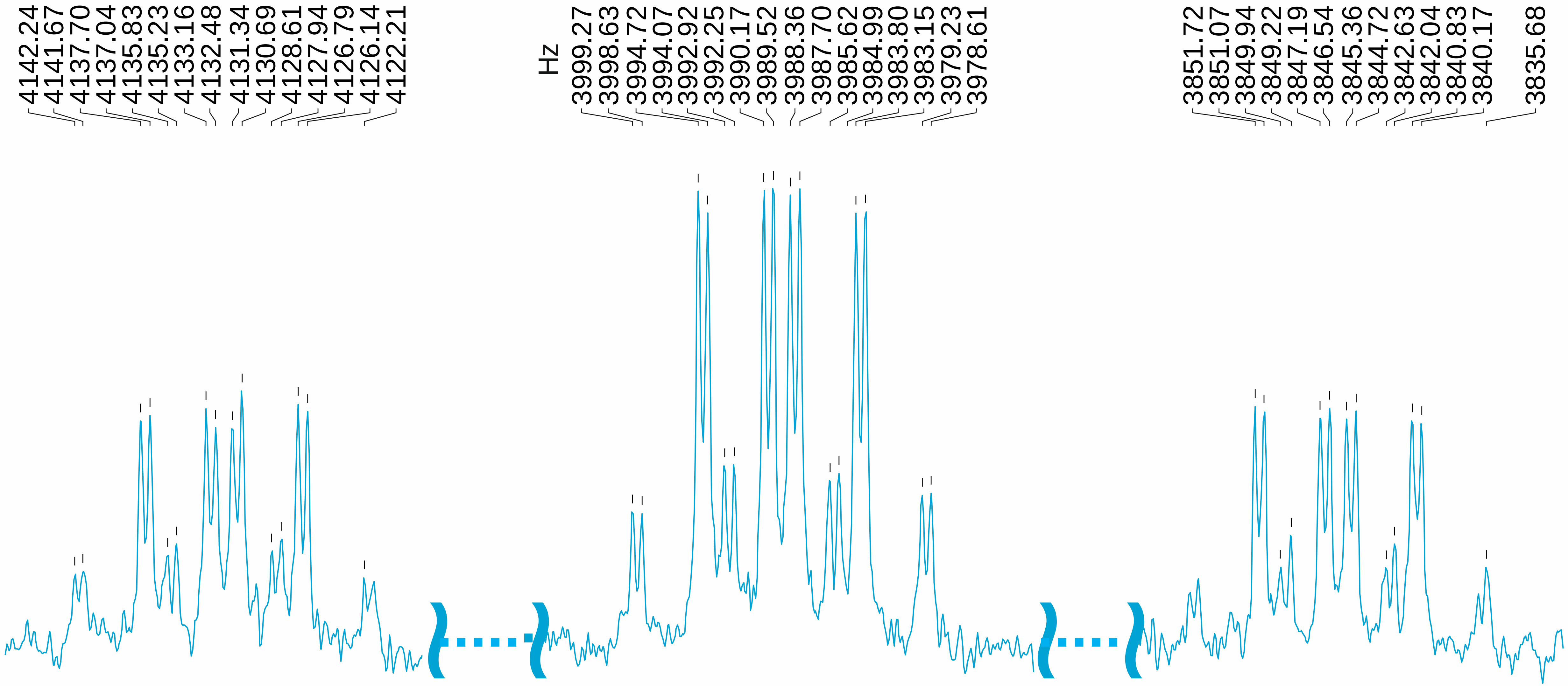
To make optimal use of the available space, parts of the multiplets were replaced by the symbol <--->. This area contains baseline and noise only about 100 Hz each.

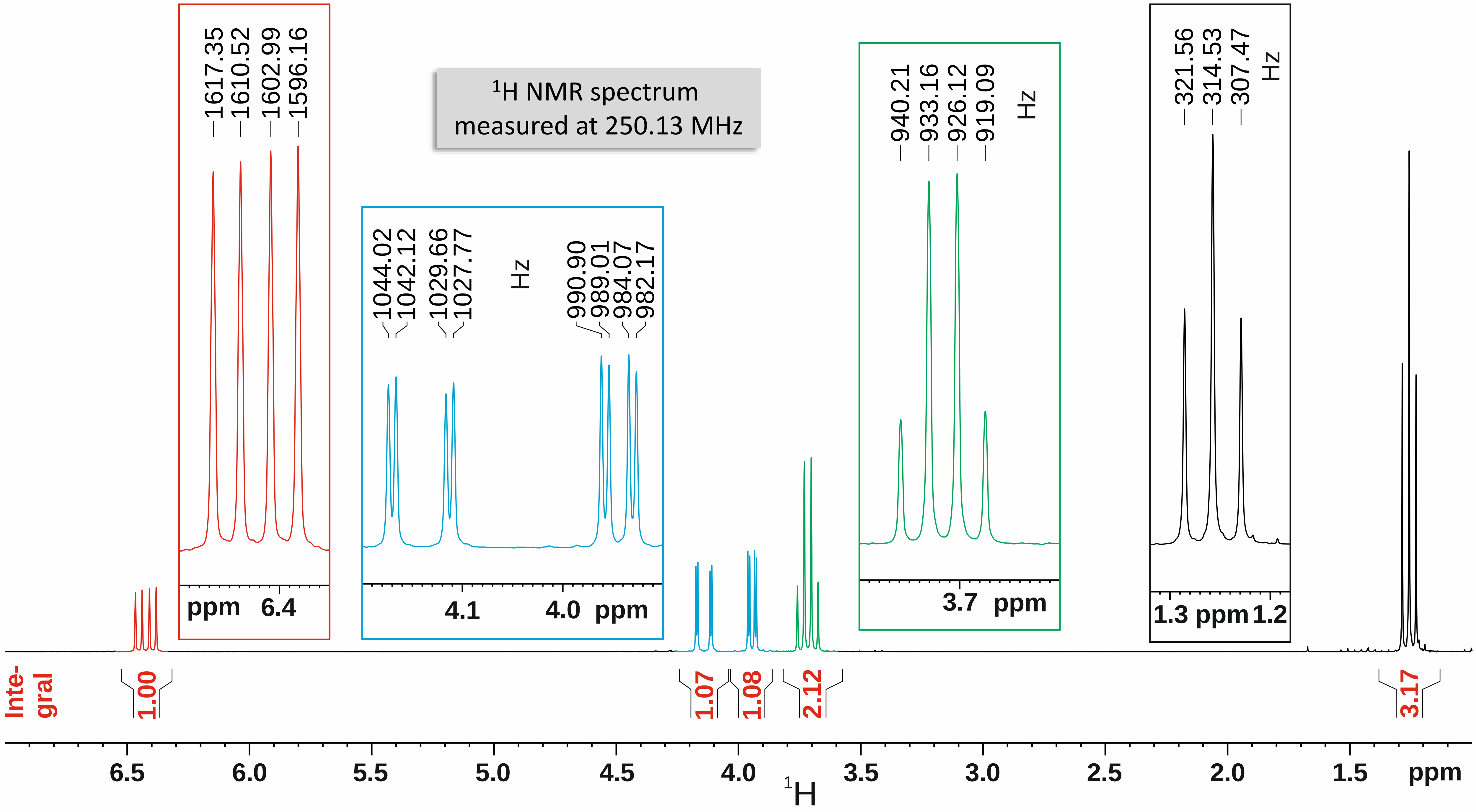




86.20 ppm
5584.45
5575.00
5428.32
5423.40
5418.87
5413.95
Hz
5267.28
5257.82
14.42 ppm
1099.12
1096.42
1093.73
Hz
972.60
969.90
967.19
846.07
843.37
840.66
719.52
716.83
714.16

63.43 ppm


4142.24
4141.67
4137.70
4137.04
4135.83
4135.23
4133.16
4132.48
4131.34
4130.69
4128.61
4127.94
4126.79
4126.14
4122.21
Hz
3999.27
3998.63
3994.72
3994.07
3992.92
3992.25
3990.17
3989.52
3988.36
3987.70
3985.62
3984.99
3983.80
3983.15
3979.23
3978.61
3851.72
3851.07
3849.94
3849.22
3847.19
3846.54
3845.36
3844.72
3842.63
3842.04
3840.83
3840.17
3835.68



1617.35
1610.52
1602.99
1596.16
ppm 6.4
1044.02
1042.12
1029.66
1027.77
Hz
990.90
989.01
984.07
982.17
4.1
4.0 ppm
¹H NMR spectrum
measured at 250.13 MHz
940.21
933.16
926.12
919.09
Hz
3.7 ppm
321.56
314.53
307.47
Hz
1.3 ppm 1.2
Inte-
gral
1.00
1.07
1.08
2.12
3.17
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
¹H

First pieces of information

Let us first try to determine the constitution and configuration from the clearly laid out proton spectrum.

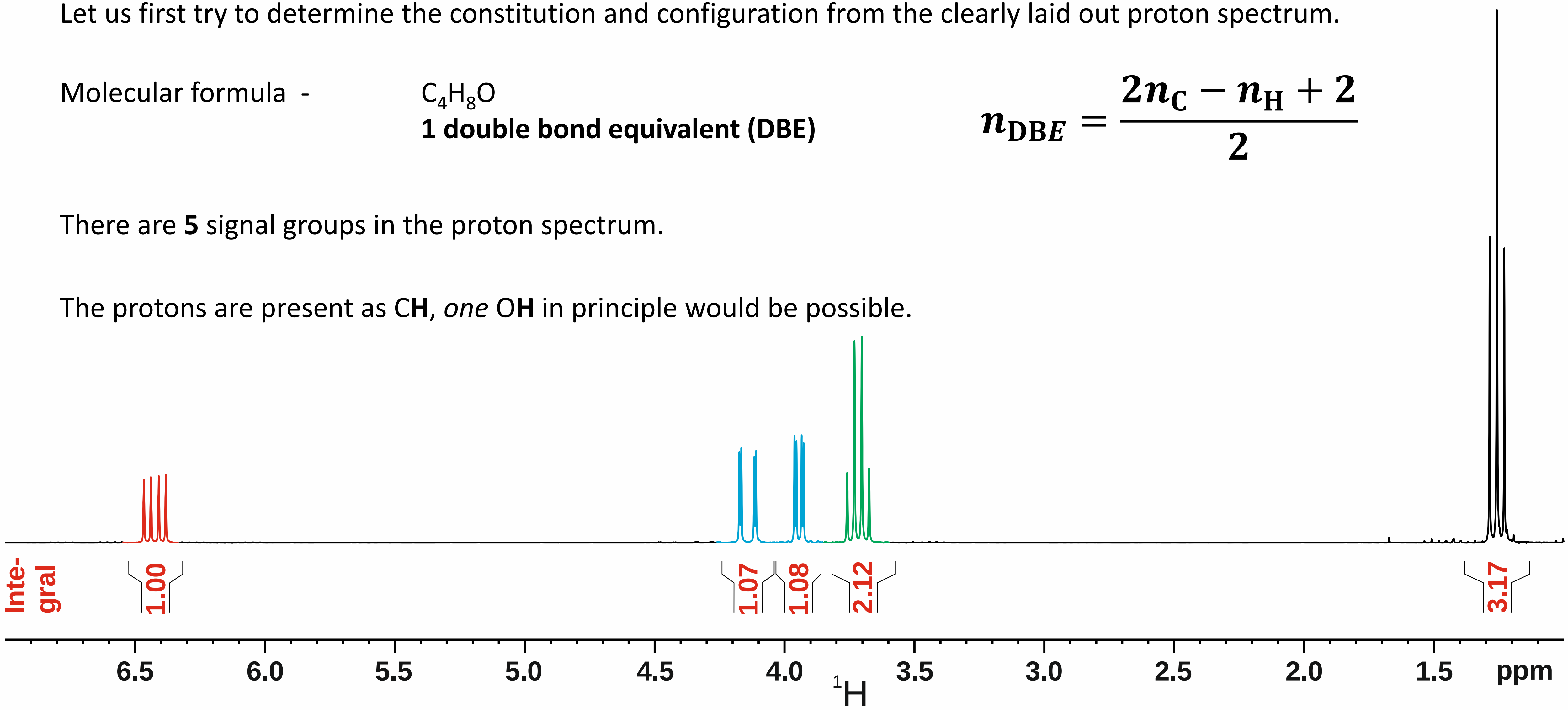
Molecular formula - C_4H_8O

1 double bond equivalent (DBE)

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

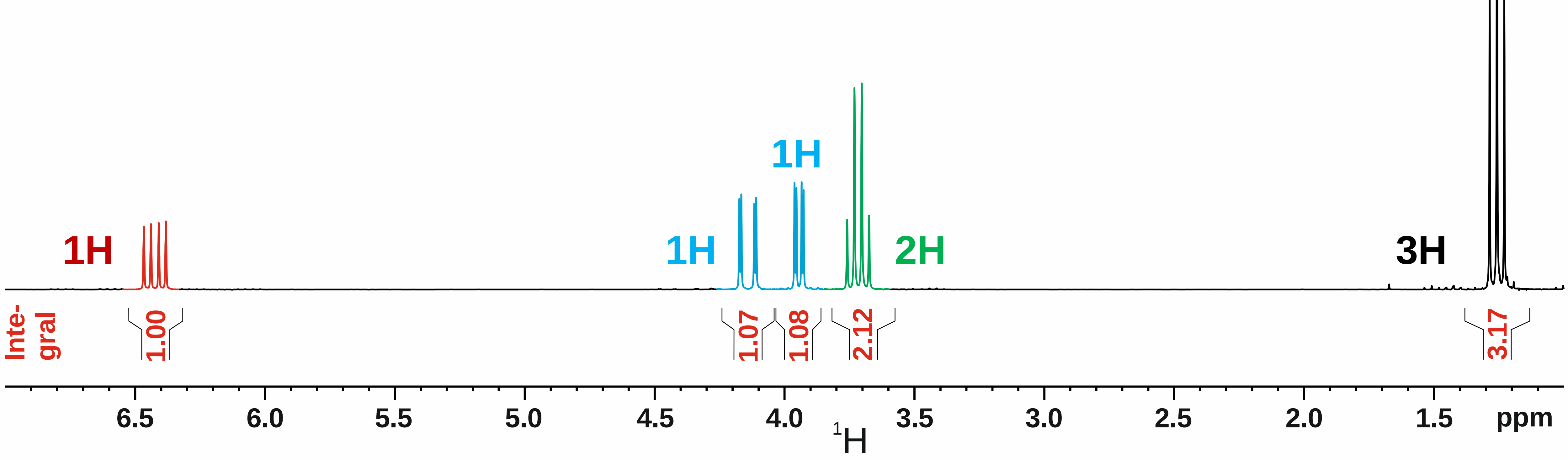
There are **5** signal groups in the proton spectrum.

The protons are present as C**H**, *one* O**H** in principle would be possible.

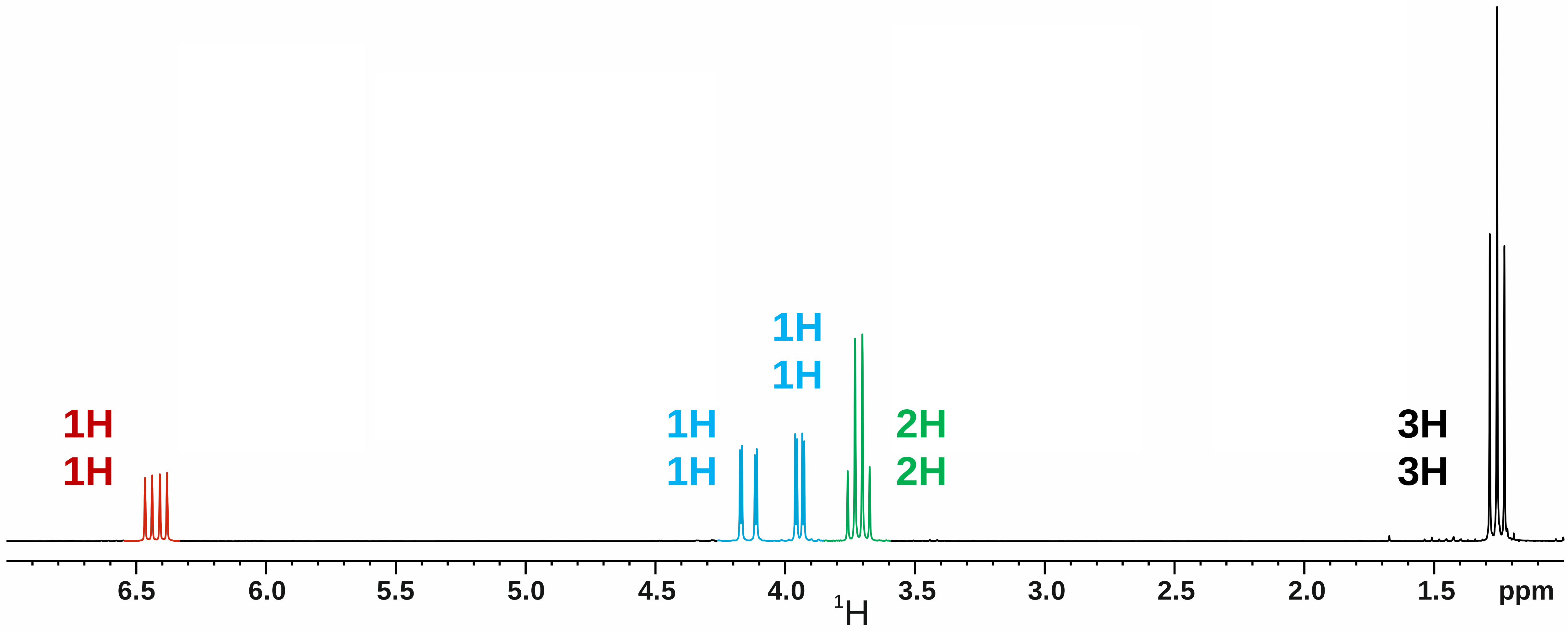


Integration

measured integrals of the five signal groups	**1.00**	**1.07**	**1.08**	**2.12**	**3.17**
sum of all integrals			**8.44**		
number of protons according to molecular formula			**8**		
coefficient of proportionality			**0.95** (8 / 8.44)		
number of protons within each signal group	0.95	1.01	1.02	2.01	3.01

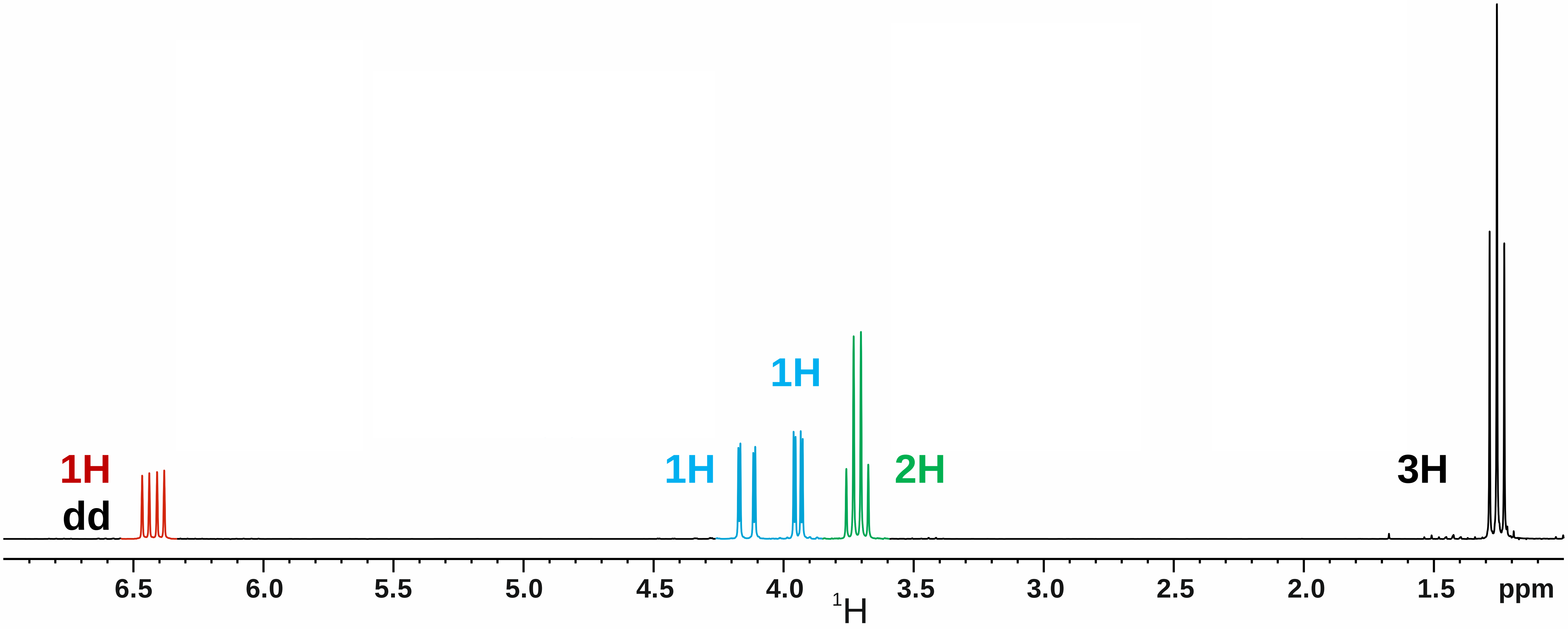


Multiplet structure



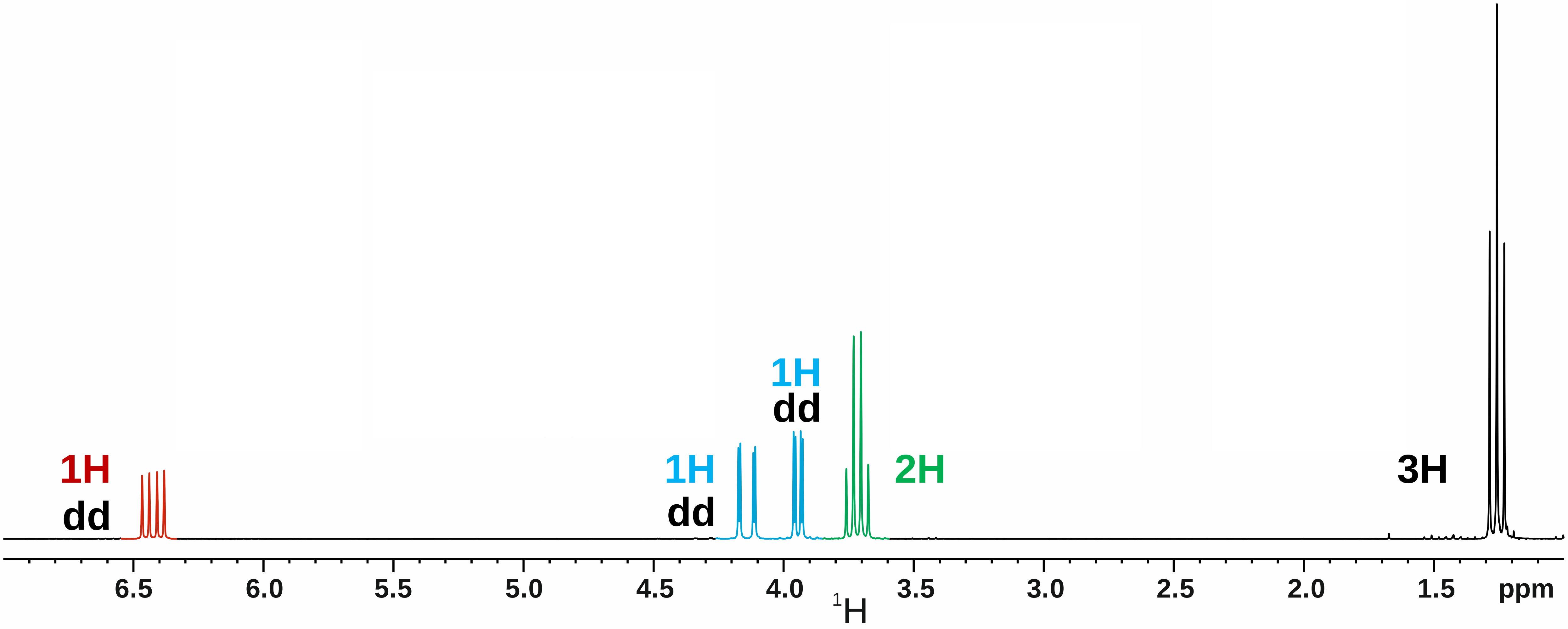
Multiplet structure

The multiplet at about 6.4 ppm is a doublet of doublets (**dd**). For four lines with almost identical intensity there is no other possibility if only nuclei with *I* = ½ are available as coupling partners.



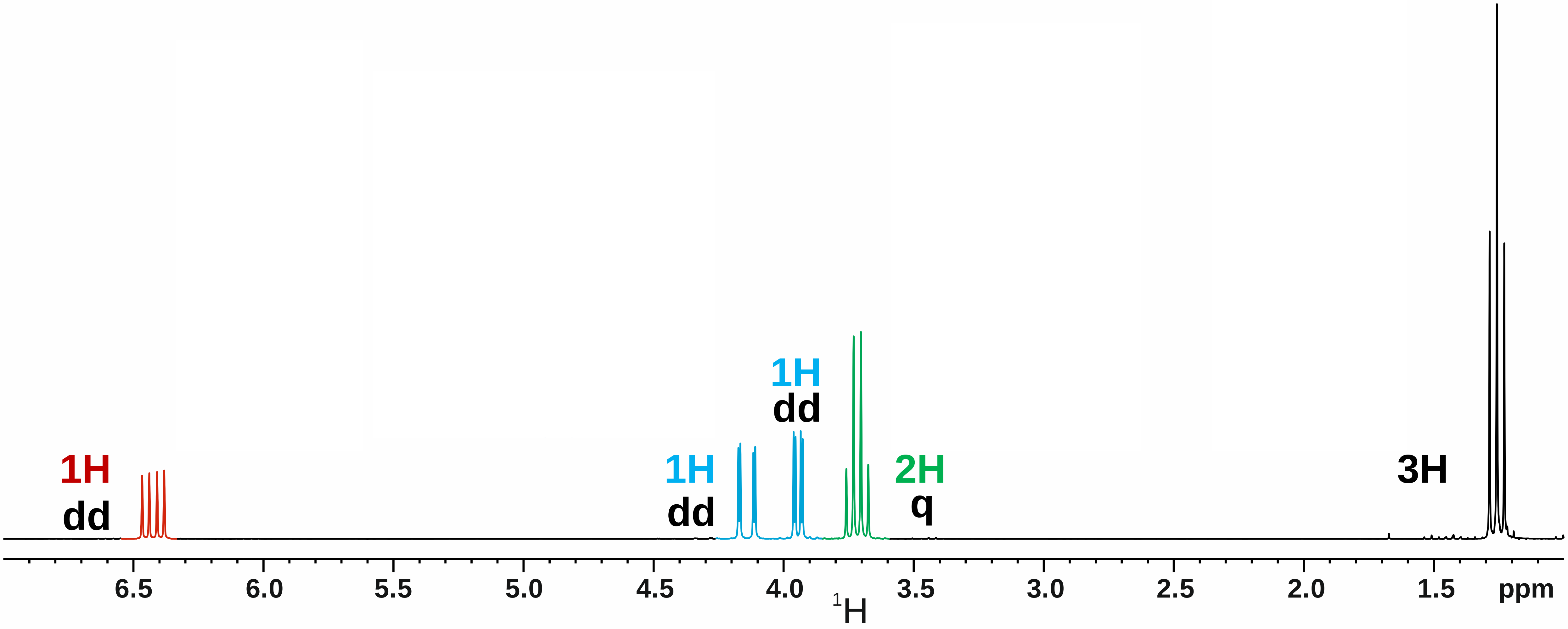
Multiplet structure

At about 4.15 ppm and 3.95 ppm there is also a doublet of doublets (**dd**) in each case. The same reasoning applies.



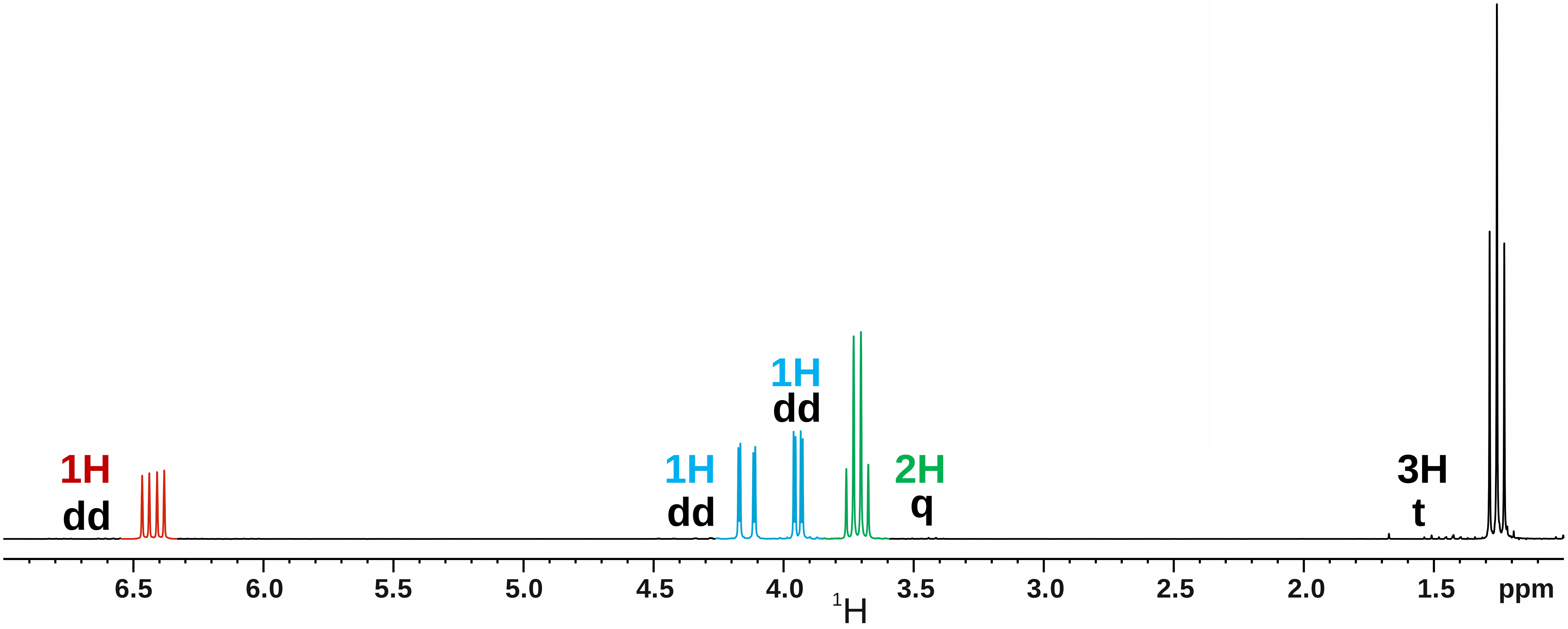
Multiplet structure

At about 3.8 ppm, there is a pure quartet (**q**) in the intensity ratio of the individual lines of **1** : **3** : **3** : **1**. In the case of pure multiplets, the ratio of the intensity of the individual lines to each other obeys a binomial distribution as long as coupling partners with *I* = ½ are involved.



Multiplet structure

Finally there is a triplet (**t**) with three individual lines in an intensity ratio of **1** : **2** : **1** at approx. 1.3 ppm.



Multiplet analysis

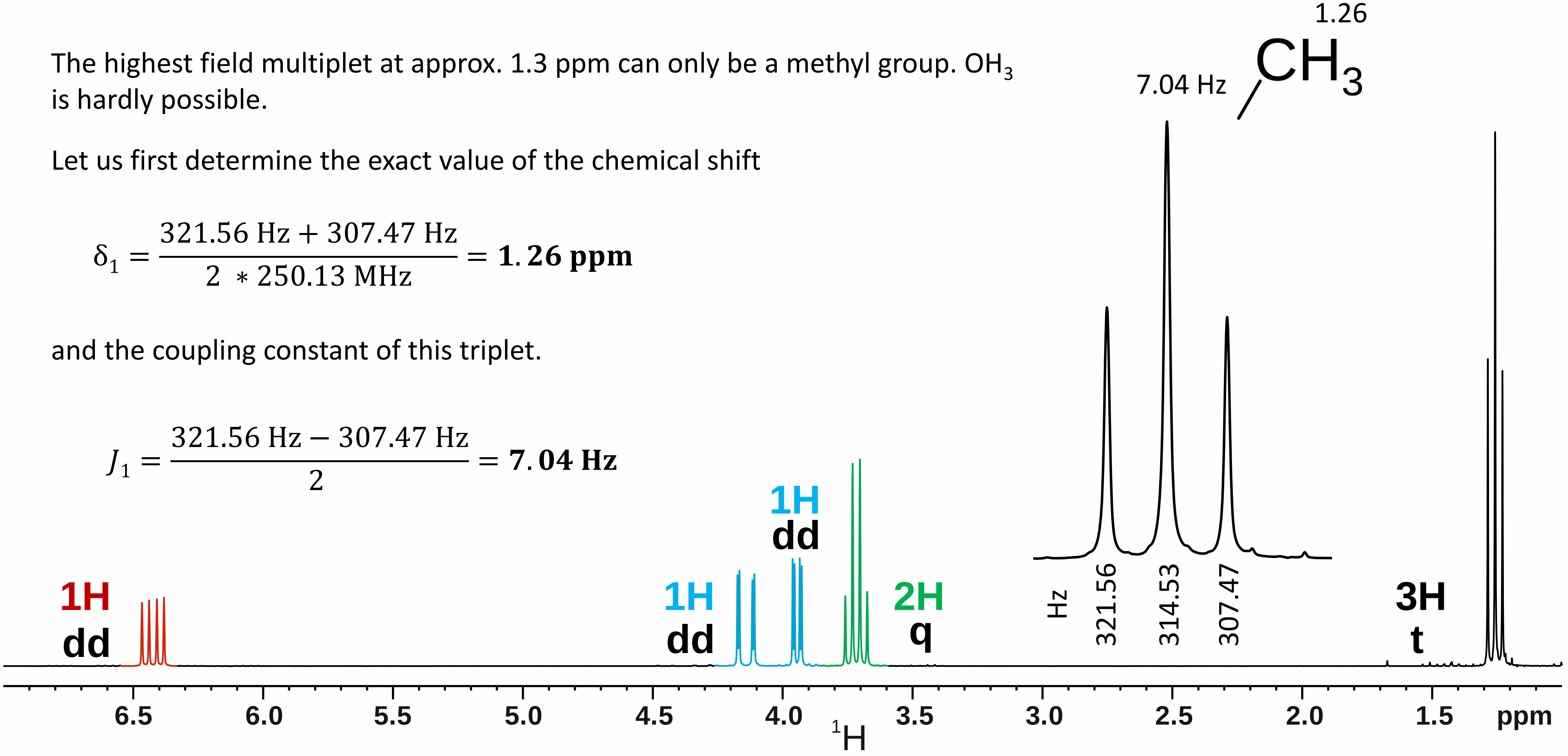
The highest field multiplet at approx. 1.3 ppm can only be a methyl group. OH_3 is hardly possible.

Let us first determine the exact value of the chemical shift

$$\delta_1 = \frac{321.56\ \text{Hz} + 307.47\ \text{Hz}}{2\ * 250.13\ \text{MHz}} = \mathbf{1.26\ ppm}$$

and the coupling constant of this triplet.

$$J_1 = \frac{321.56\ \text{Hz} - 307.47\ \text{Hz}}{2} = \mathbf{7.04\ Hz}$$

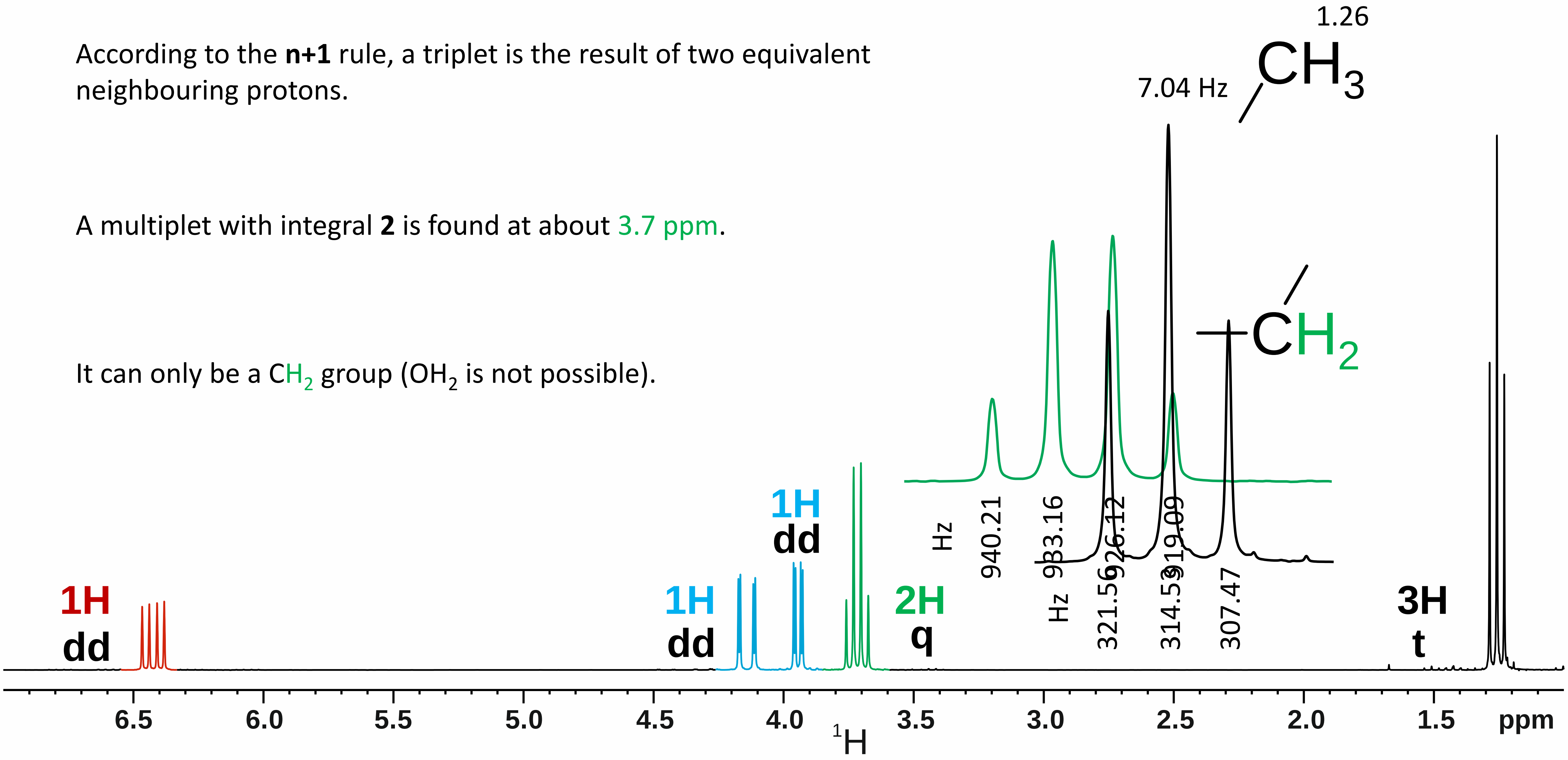


Multiplet analysis

According to the **n+1** rule, a triplet is the result of two equivalent neighbouring protons.

A multiplet with integral **2** is found at about 3.7 ppm.

It can only be a CH_2 group (OH_2 is not possible).



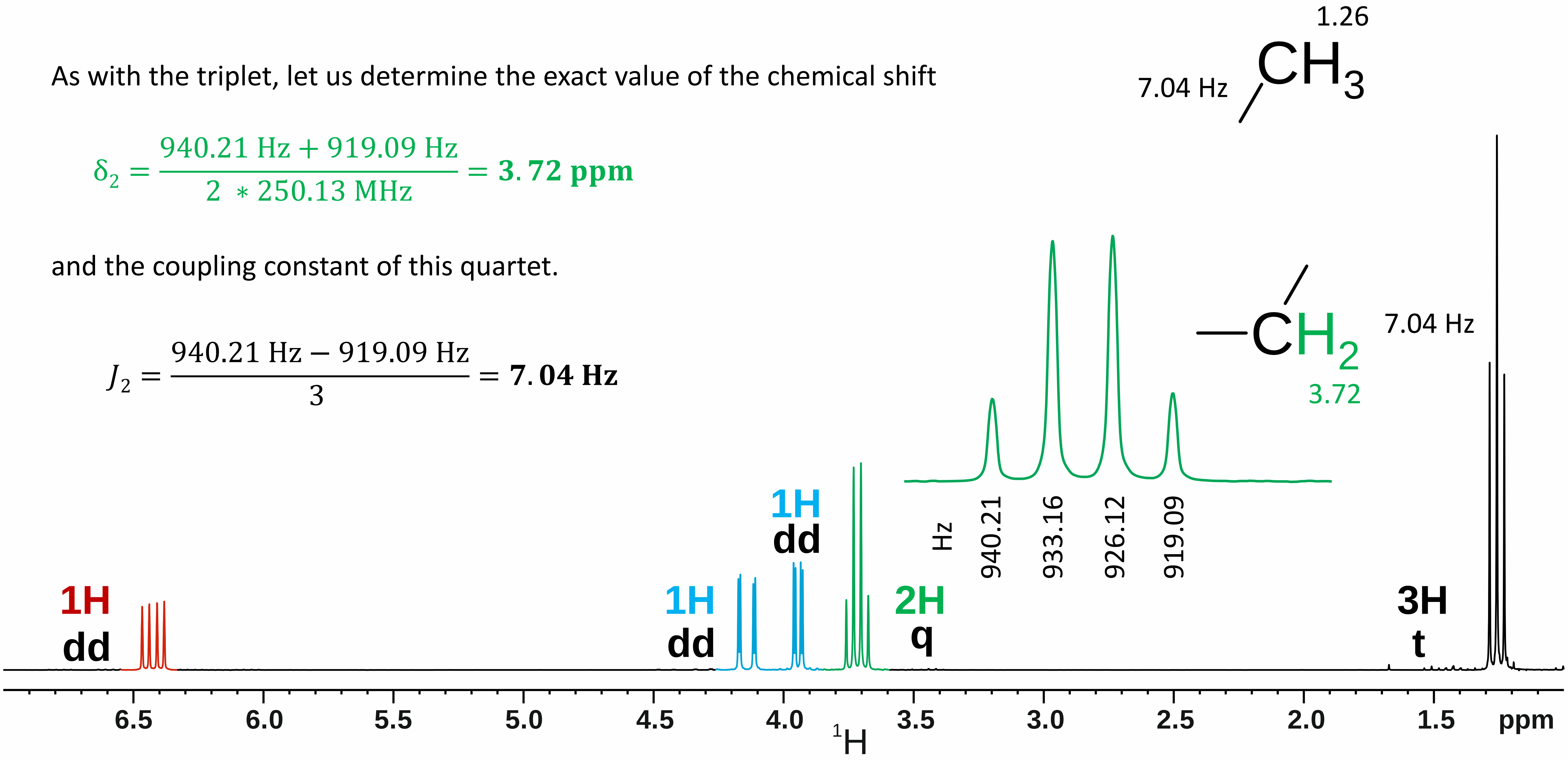
Multiplet analysis

As with the triplet, let us determine the exact value of the chemical shift

$$\delta_2 = \frac{940.21\ \text{Hz} + 919.09\ \text{Hz}}{2\ *\ 250.13\ \text{MHz}} = \mathbf{3.72\ ppm}$$

and the coupling constant of this quartet.

$$J_2 = \frac{940.21\ \text{Hz} - 919.09\ \text{Hz}}{3} = \mathbf{7.04\ Hz}$$

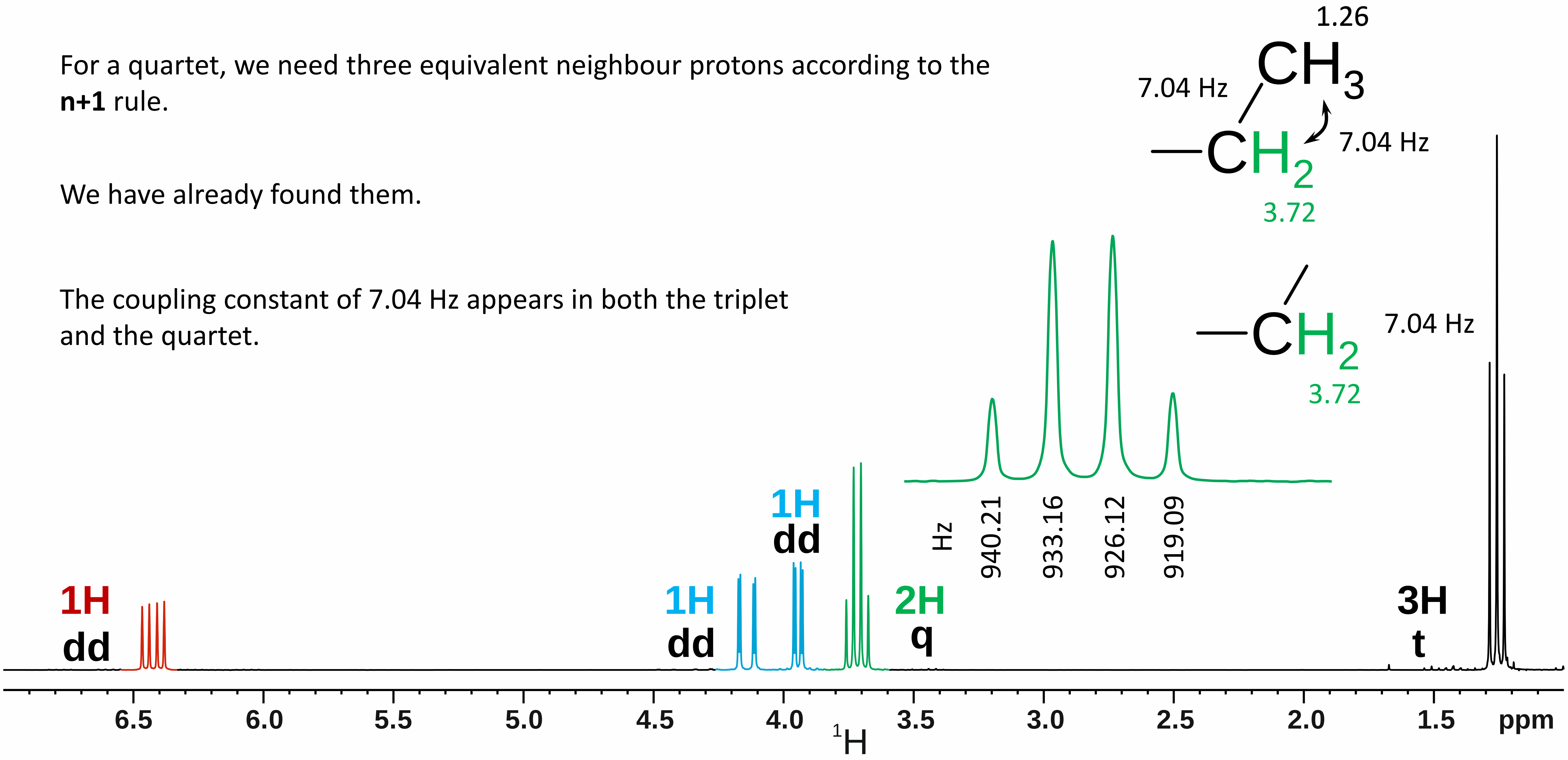


Multiplet analysis

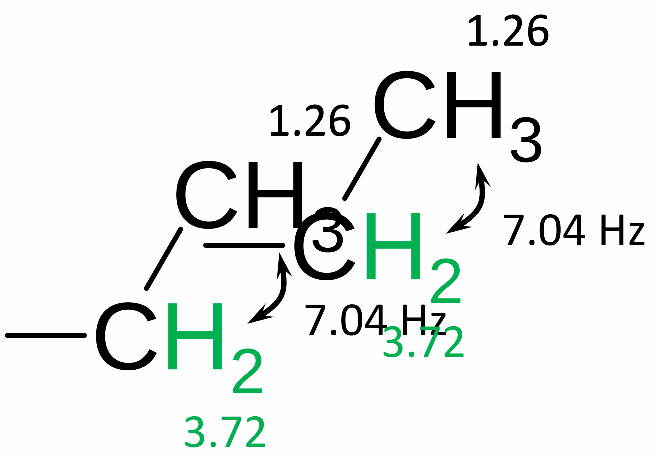
For a quartet, we need three equivalent neighbour protons according to the **n+1** rule.

We have already found them.

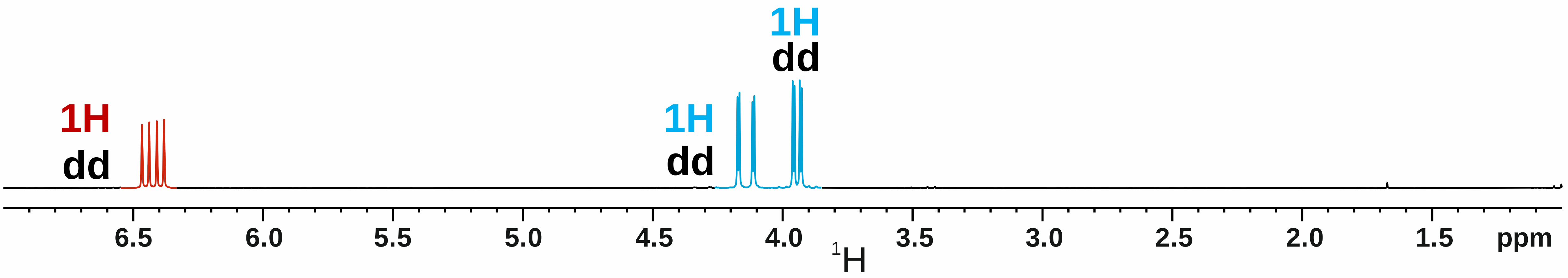
The coupling constant of 7.04 Hz appears in both the triplet and the quartet.



Multiplet analysis



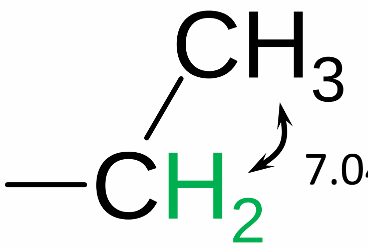
For further analysis, we no longer need the two multipletts of the ethyl group. In order to focus on the remaining multiplets, the signals of the two multipletts were removed from the ^{1}H NMR spectrum.



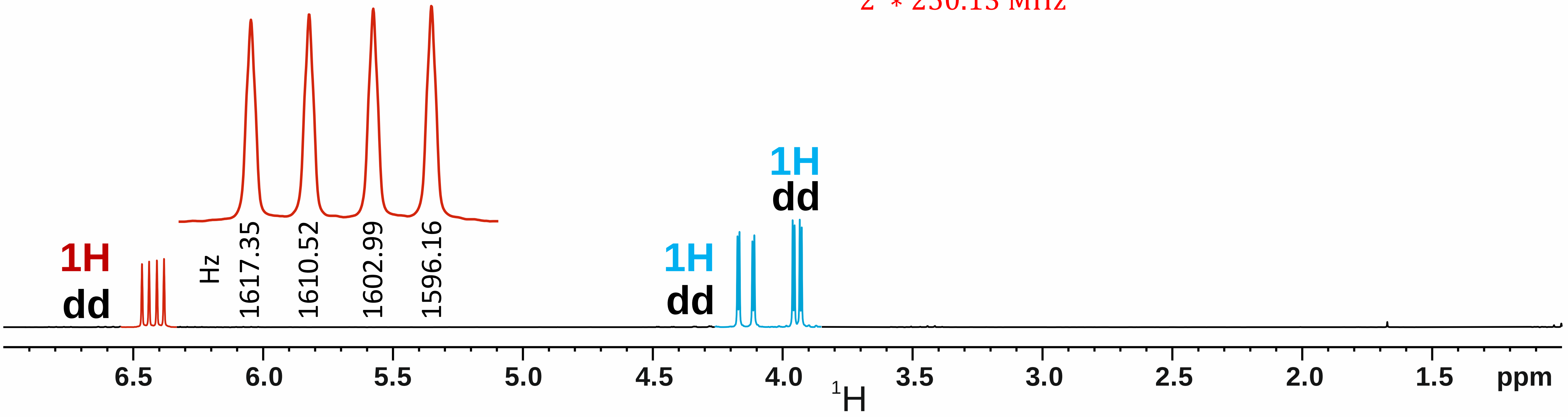
Multiplet analysis

6.42 ppm

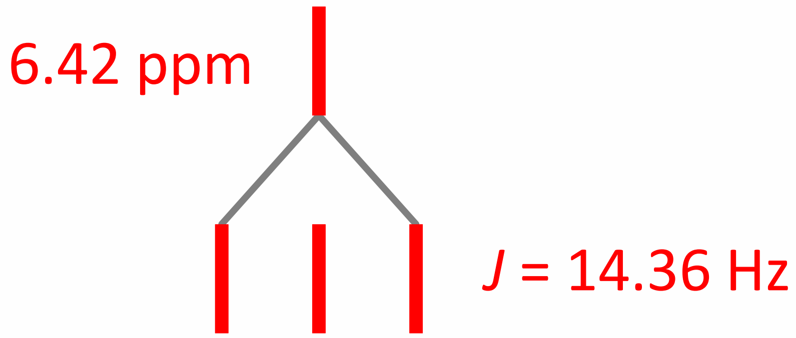
The three doublets of doublets can each be analysed according to the same scheme. Let's start with the exact value of the chemical shift of the lowest field multiplet.



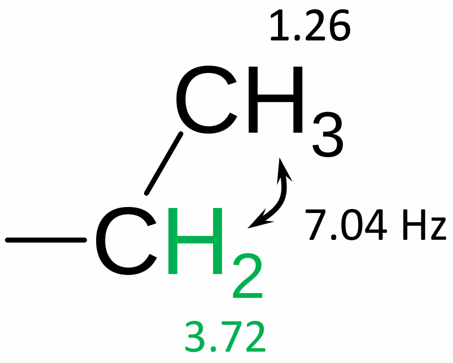
$$\delta_3 = \frac{1617.35\ \text{Hz} + 1596.16\ \text{Hz}}{2 * 250.13\ \text{MHz}} = \mathbf{6.42\ ppm}$$



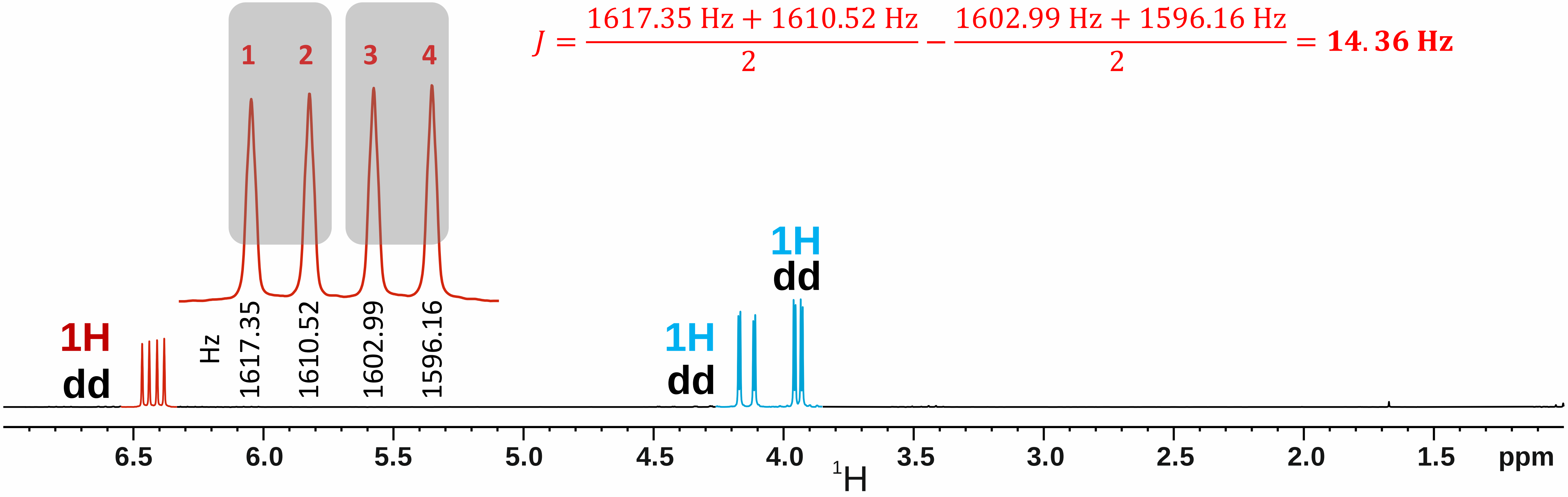
Multiplet analysis



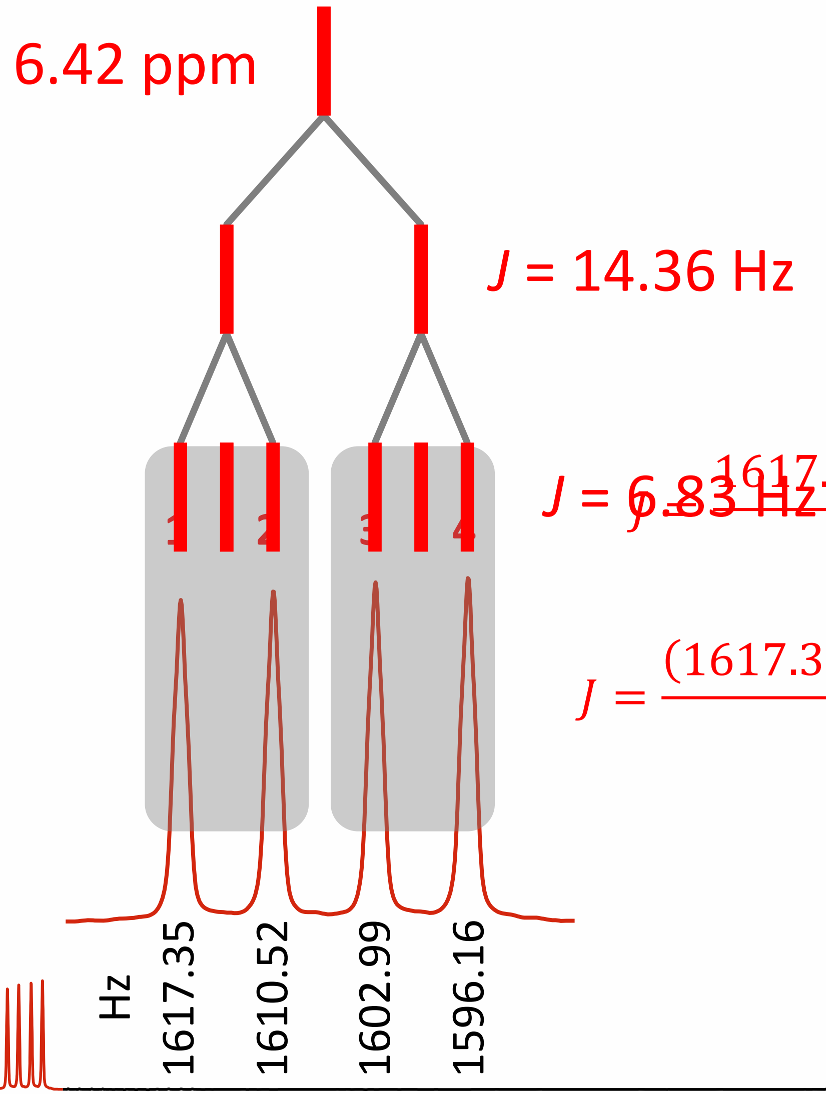
The larger of the two coupling constants is obtained by subtracting the mean value of lines **3** and **4** from the mean value of lines **1** and **2** (counting from left to right).

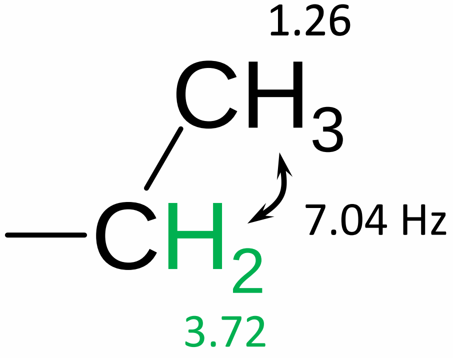


$$J = \frac{1617.35\ \mathrm{Hz} + 1610.52\ \mathrm{Hz}}{2} - \frac{1602.99\ \mathrm{Hz} + 1596.16\ \mathrm{Hz}}{2} = \mathbf{14.36\ Hz}$$



Multiplet analysis

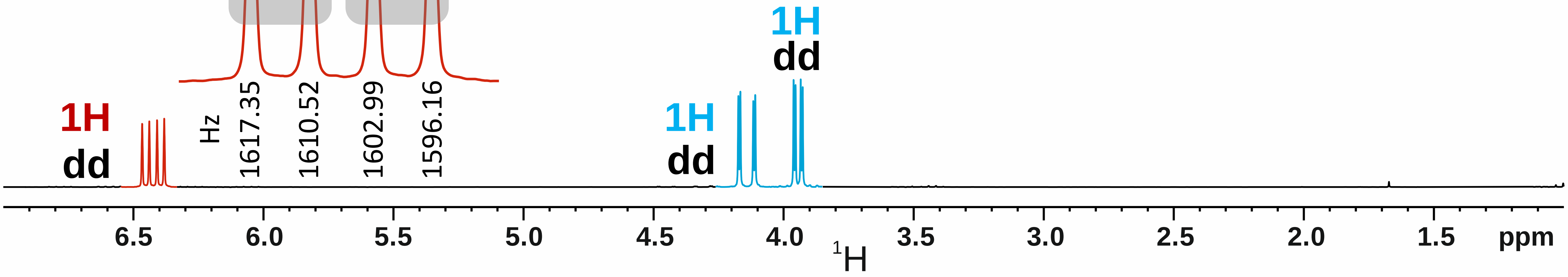




The smaller of the two coupling constants results from the difference of lines **3** and **4** or lines **1** and **2**, or for improved accuracy from the mean value of both differences.

$$J = \frac{1617.35\ \text{Hz} + 1610.52\ \text{Hz}}{2} - \frac{1602.99\ \text{Hz} + 1596.16\ \text{Hz}}{2} = \mathbf{14.36\ Hz}$$

$$J = \frac{(1617.35\ \text{Hz} - 1610.52\ \text{Hz}) + (1602.99\ \text{Hz} - 1596.16\ \text{Hz})}{2} = \mathbf{6.83\ Hz}$$



Multiplet analysis

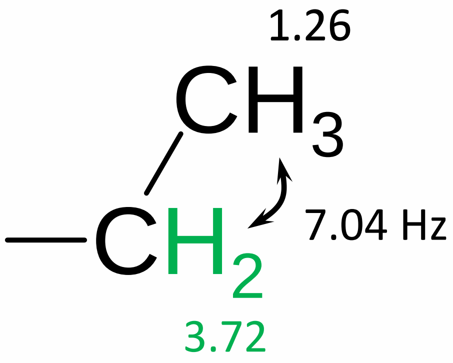
6.42 ppm

J = 14.36 Hz

J = 6.83 Hz

We temporarily note the chemical shift and the two coupling constants next to the corresponding multiplet.

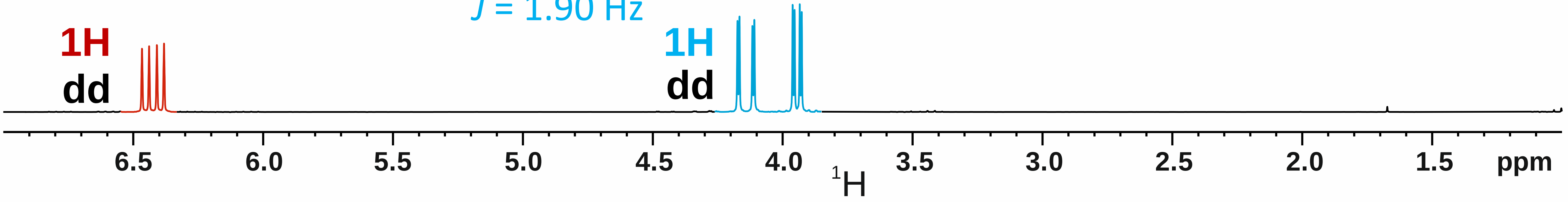
In the analogous analysis of the two further doublets of doublets, one chemical shift and two coupling constants each are also obtained.



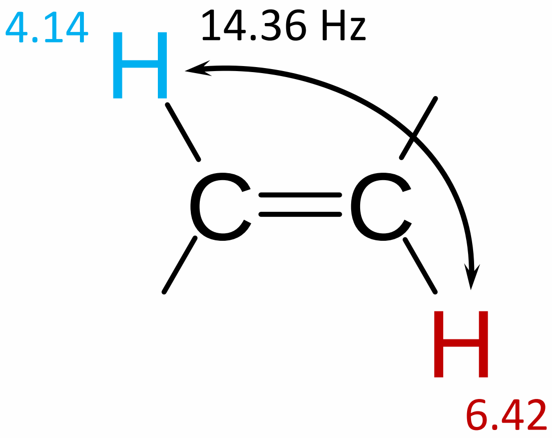
6.42 ppm
J = 14.36 Hz
J = 6.83 Hz

4.14 ppm
J = 14.36 Hz
J = 1.90 Hz

3.94 ppm
J = 6.83 Hz
J = 1.90 Hz



First structure fragment

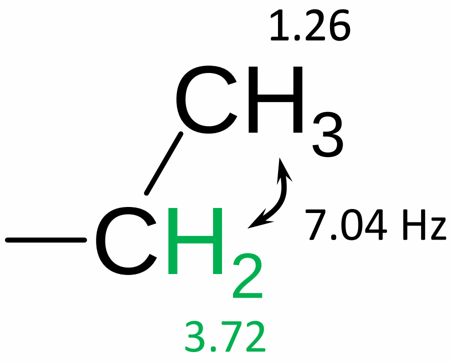


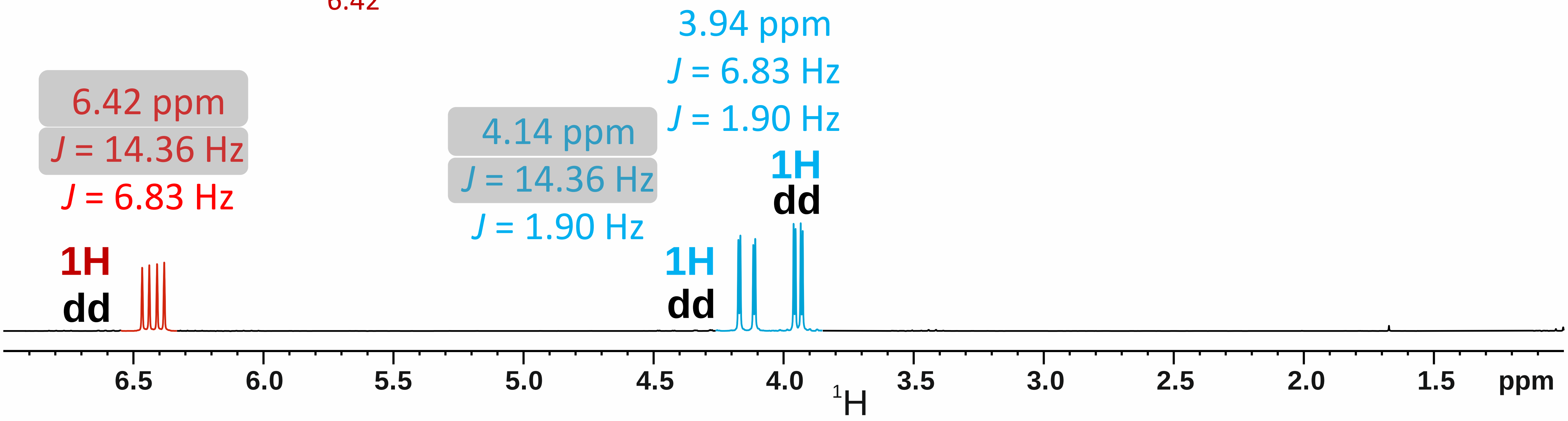
A chemical shift of 6.42 ppm fits a proton bonded to an sp^2 hybridised carbon atom.

A coupling constant of 14.36 Hz is very characteristic for two protons in the **E position** on an ethene fragment.

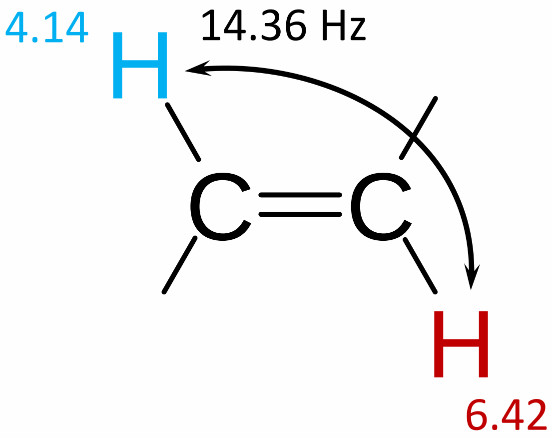
The missing coupling partner with a coupling constant of 14.36 Hz has a chemical shift of 4.14 ppm.

We expect the following structural fragment.



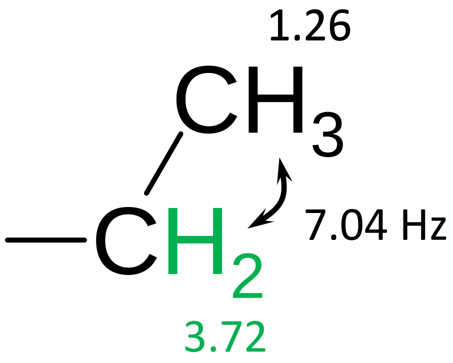


First structure fragment



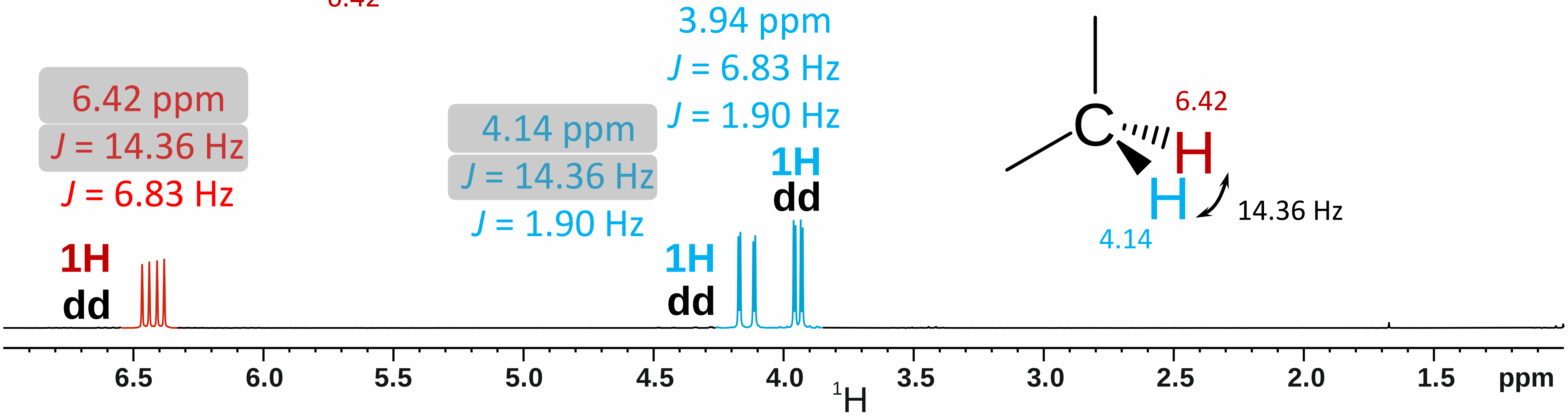
But …

4.14 ppm for a proton bound to an sp2-hybridised carbon?

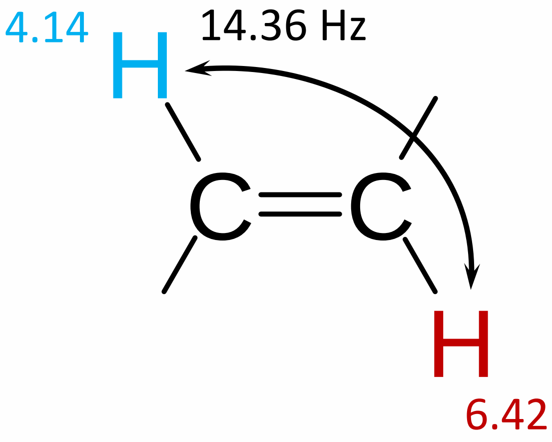


14.36 Hz could also correspond to a geminal coupling constant between two diastereotopic protons on an sp^3 hybridised carbon atom.

In this case, the 6.42 ppm would be very strange. Let's stay with the ethene derivative and try to understand later. Some pieces of information are no longe necessary.

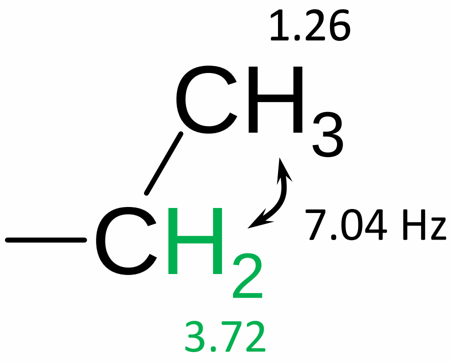


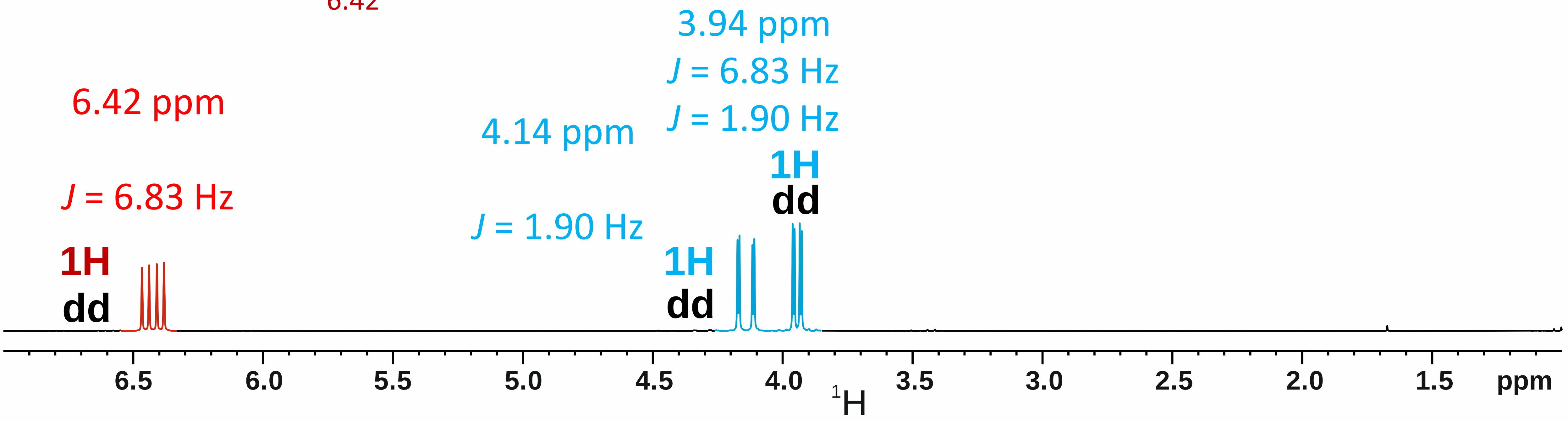
First structure fragment



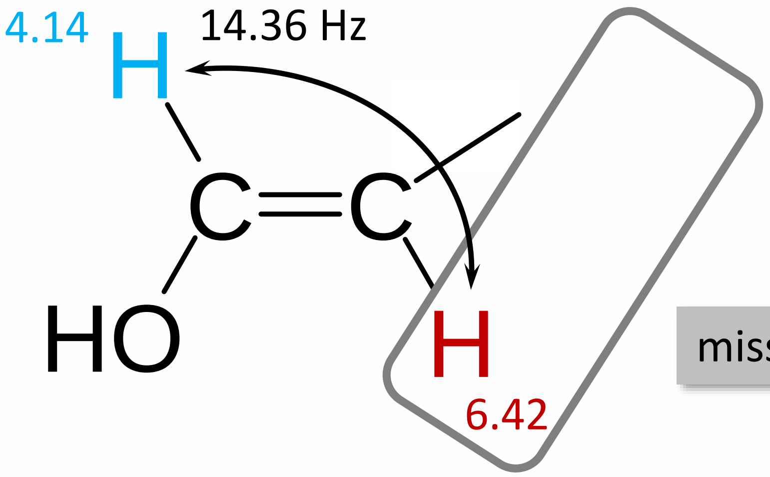
What is actually missing?

molecular formula	–	C_4H_8O
known fragments	–	C_4H_7
missing	–	**OH**

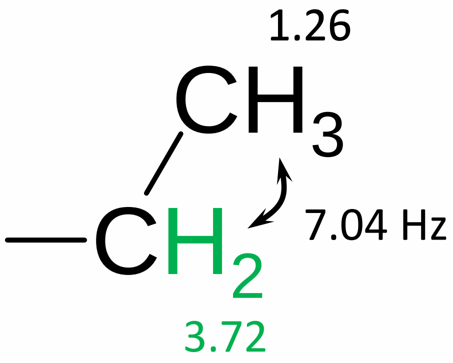




First structure fragment



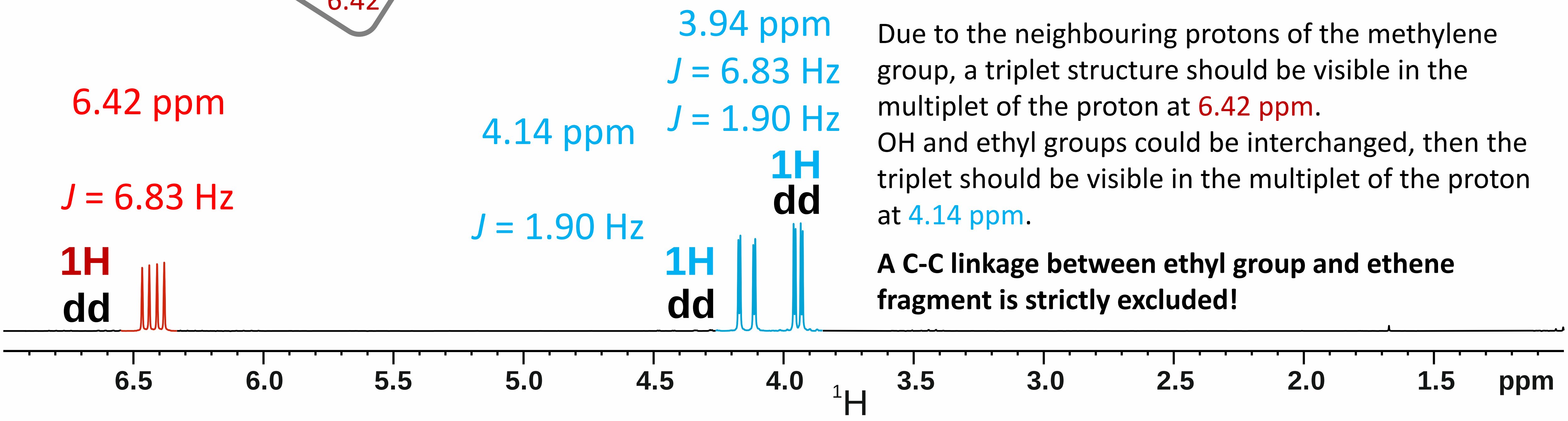
missing – OH



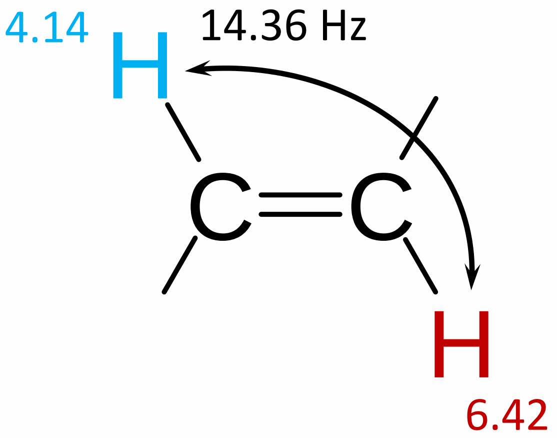
This way?

Due to the neighbouring protons of the methylene group, a triplet structure should be visible in the multiplet of the proton at 6.42 ppm.
OH and ethyl groups could be interchanged, then the triplet should be visible in the multiplet of the proton at 4.14 ppm.

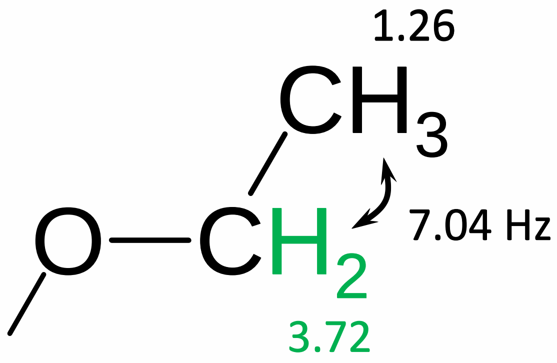
A C-C linkage between ethyl group and ethene fragment is strictly excluded!



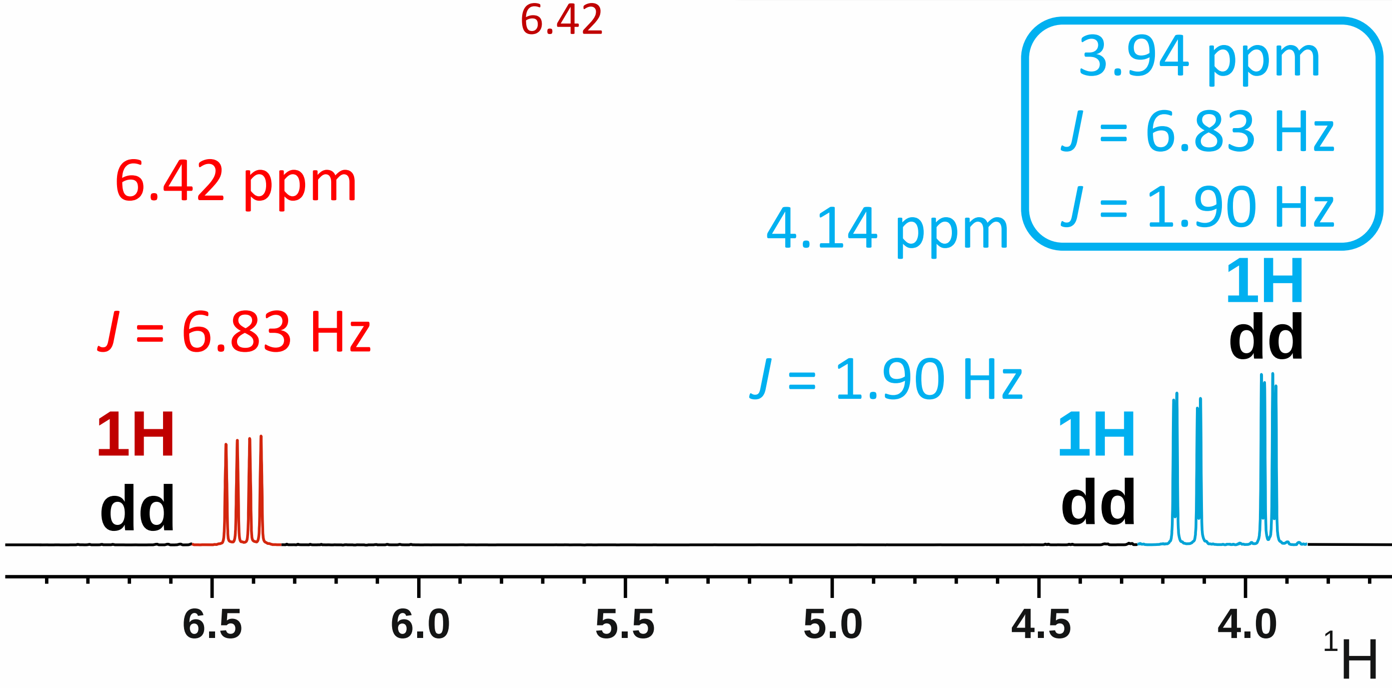
First structure fragment



Is there another choice?



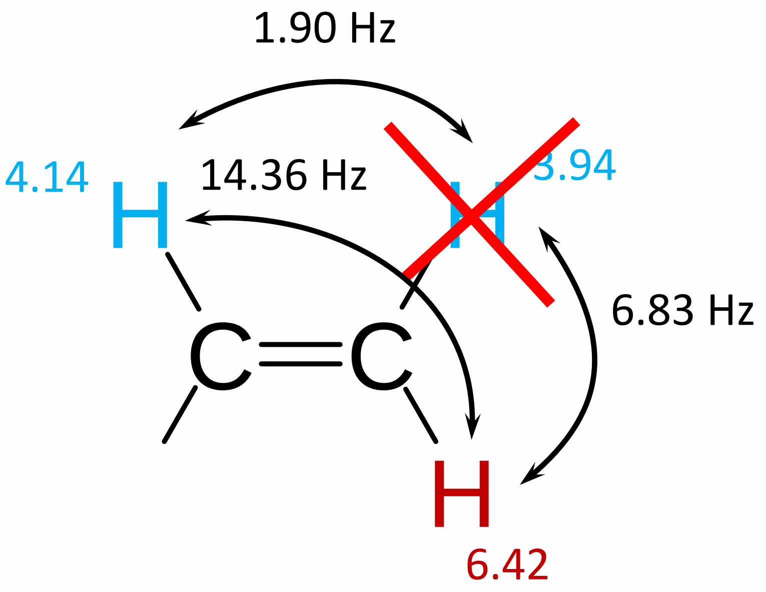
missing	–	OH

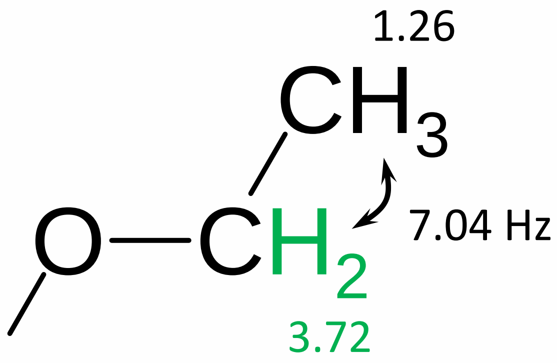


A direct C-C linkage can only be prevented with the two atoms still available by an oxygen atom **next to the methylene group**.

The last remaining building block is the proton with the chemical shift of 3.94 ppm. Two positions are possible.

First structure fragment

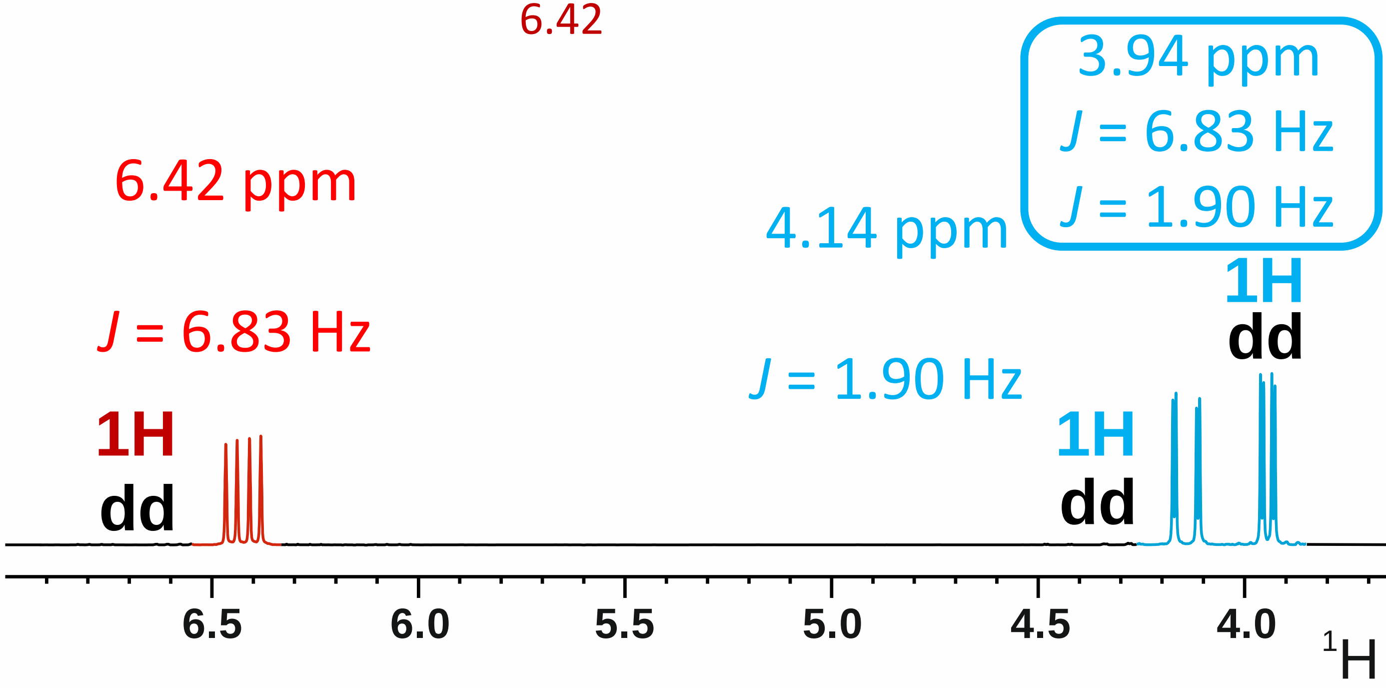




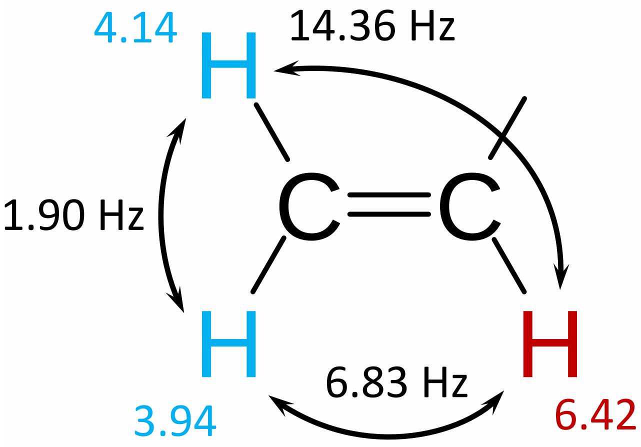
Let's just try one of the two possibilities.

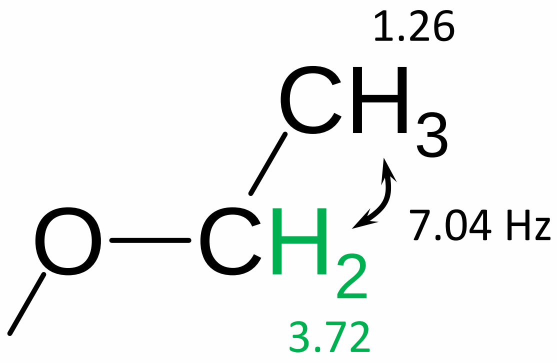
A vicinal coupling constant of **1.90 Hz** between the Z-site protons with the chemical shift of 3.94 ppm and 4.14 ppm is much too small. A rough estimate for this coupling constant is **8 Hz**.

On the other hand, the typical geminal coupling constant between the two protons of a $=CH_2$ group is roughly **-1 Hz**. **6.83 Hz** (the sign is not known) is much too large..



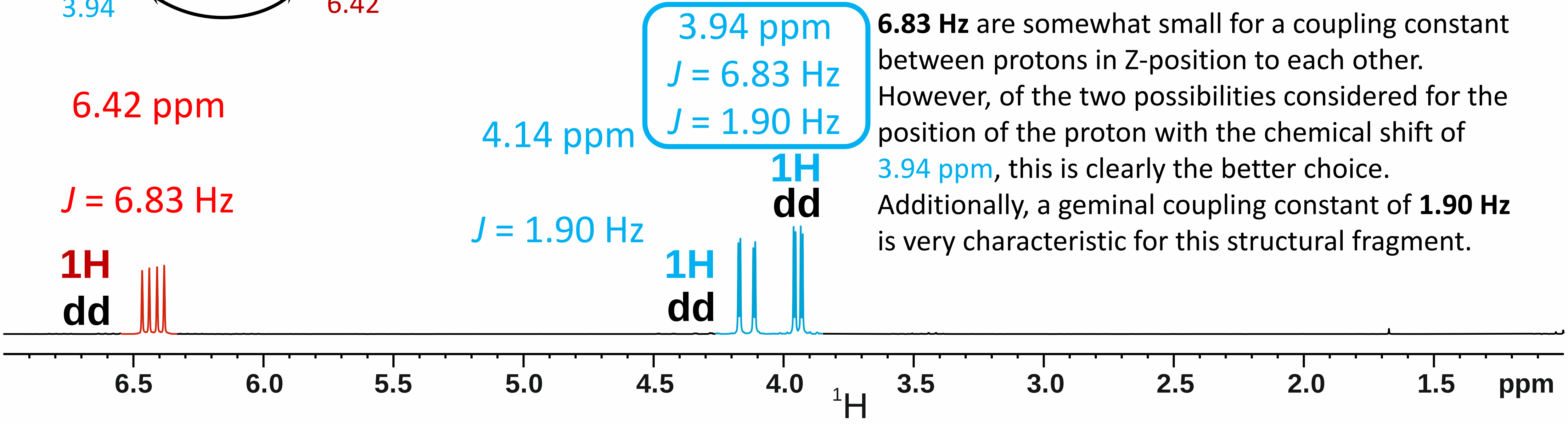
First structure fragment



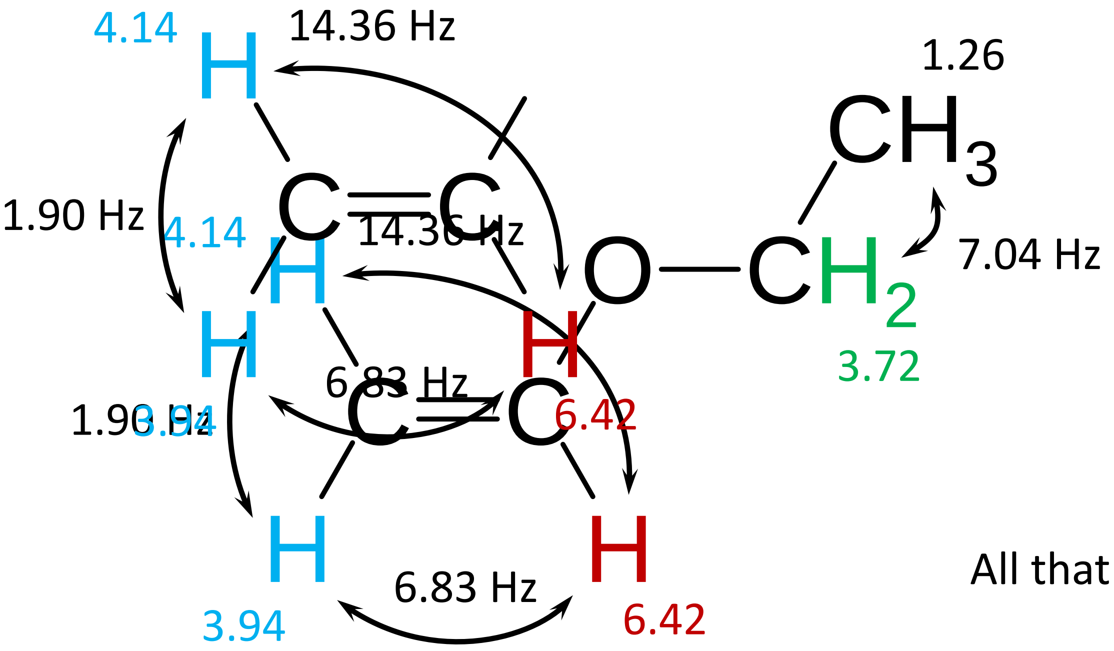


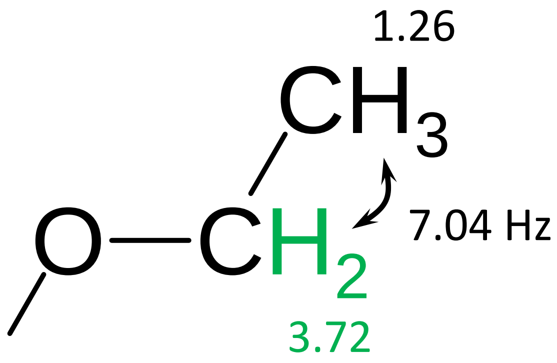
What about the alternative position of the proton?

6.83 Hz are somewhat small for a coupling constant between protons in Z-position to each other. However, of the two possibilities considered for the position of the proton with the chemical shift of 3.94 ppm, this is clearly the better choice. Additionally, a geminal coupling constant of **1.90 Hz** is very characteristic for this structural fragment.



Final structure

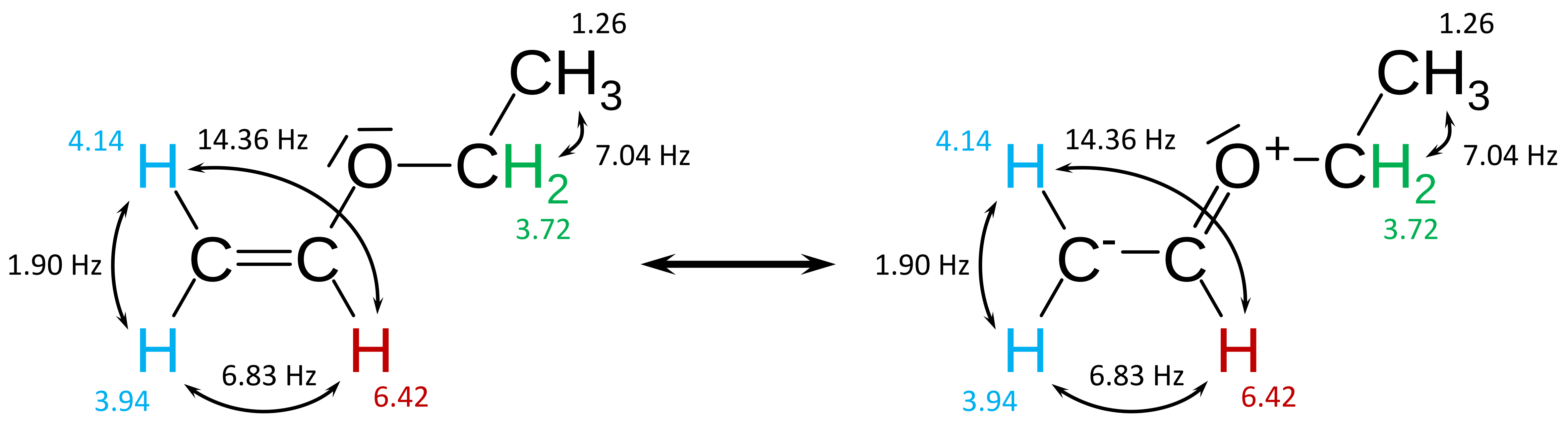




All that remains to be done is to combine the two existing building blocks.

But what is the reasonfor these somewhat strange chemical shifts of 4.14 and 3.94 ppm?

Mesomerism in ethyl vinyl ether



The oxygen has two free electron pairs.

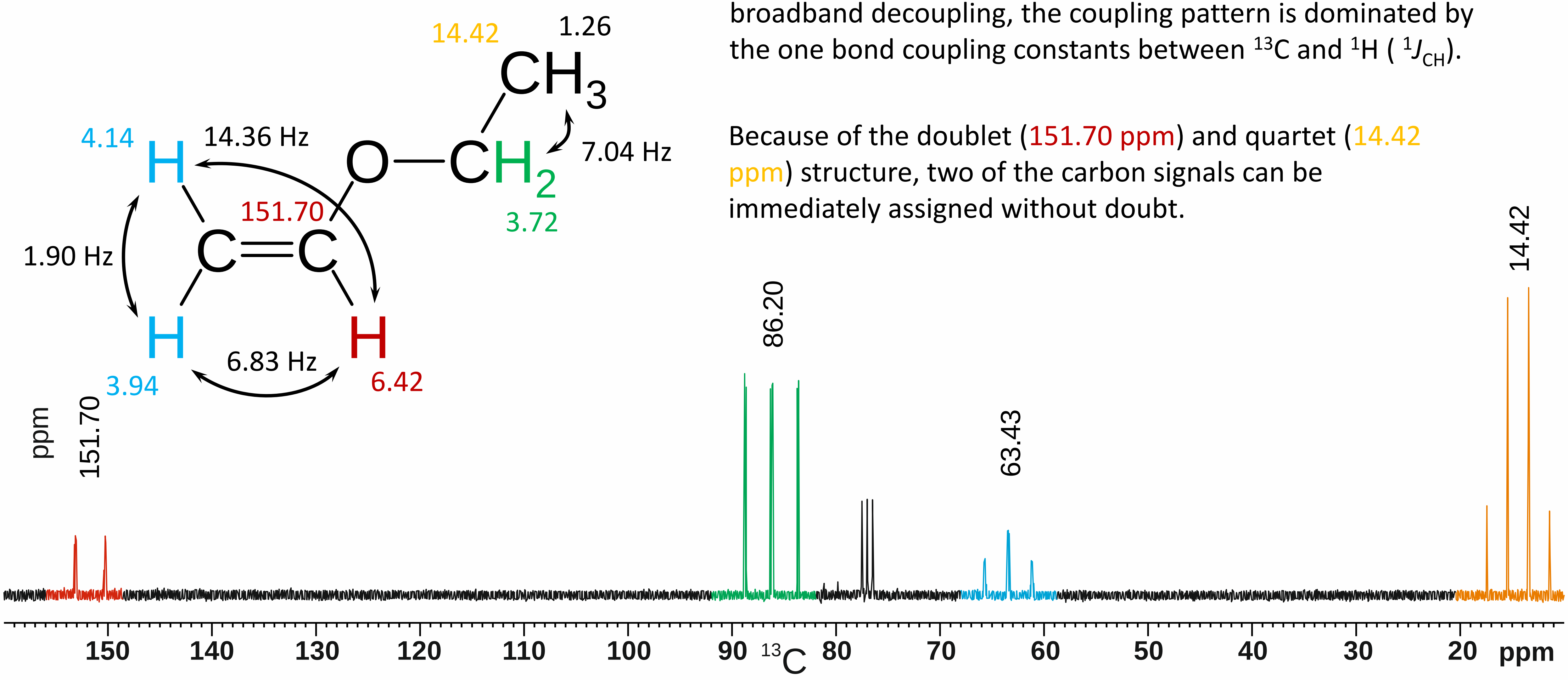
Using one of the two electron pairs, it is easy to set up a mesomeric structure with a negative electric charge next to the two $=CH_2$ protons.

This electron causes a slight additional shielding at the two protons bound to the carbon atom, resulting in a high-field shift of their signals.
The same effect is found with the **o** and **p** protons in phenol or its derivatives.

Assignment of the carbon signals

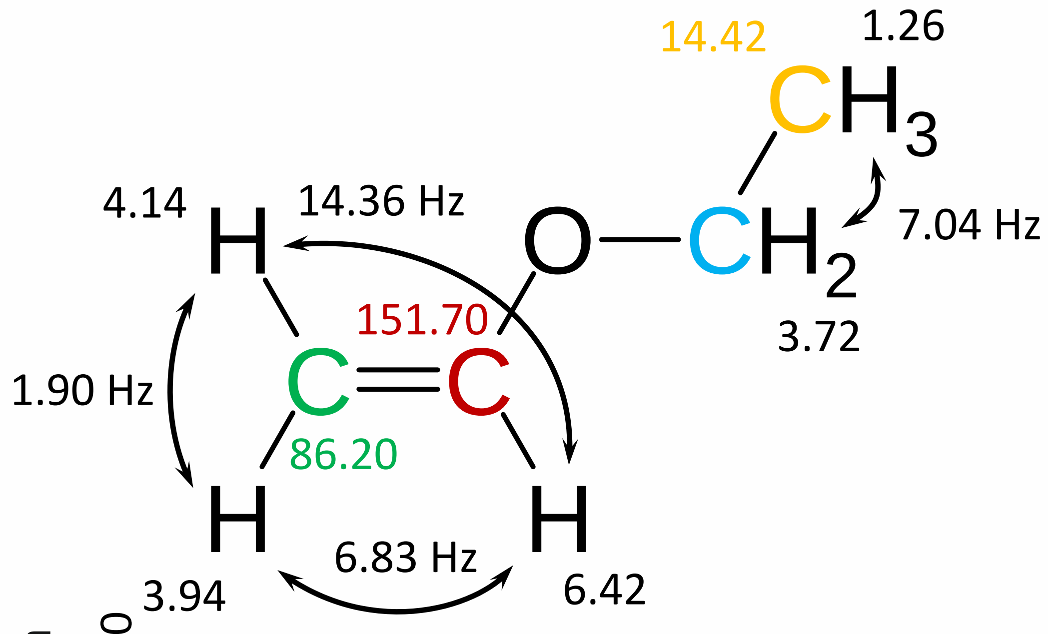
If the carbon spectrum is measured without the usual proton broadband decoupling, the coupling pattern is dominated by the one bond coupling constants between ^{13}C and ^{1}H ($^{1}J_{CH}$).

Because of the doublet (151.70 ppm) and quartet (14.42 ppm) structure, two of the carbon signals can be immediately assigned without doubt.



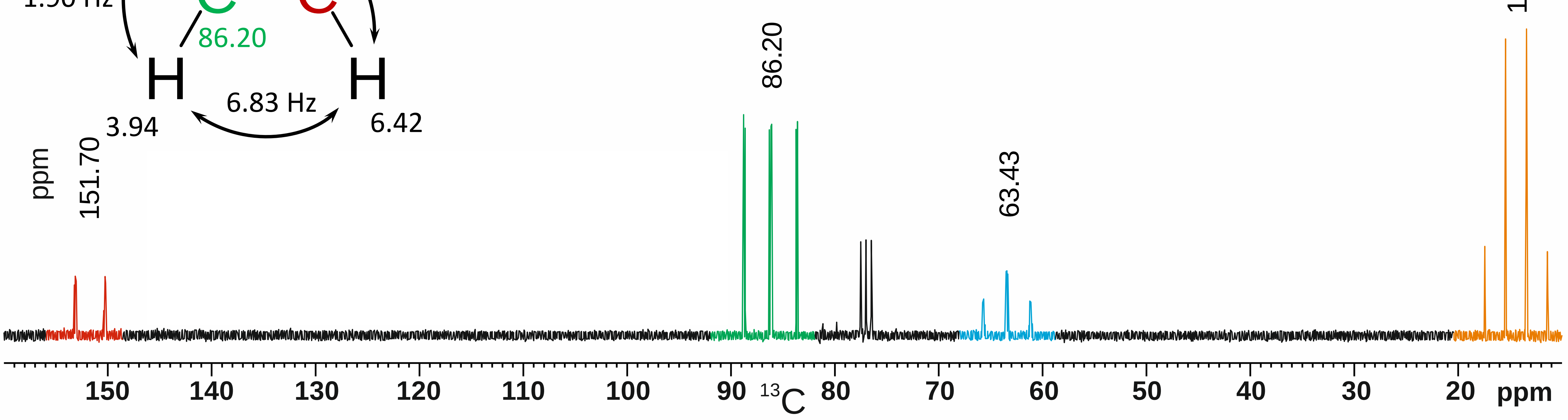
Assignment of the carbon signals

(The colour coding has been changed to focus on carbon assignment.)



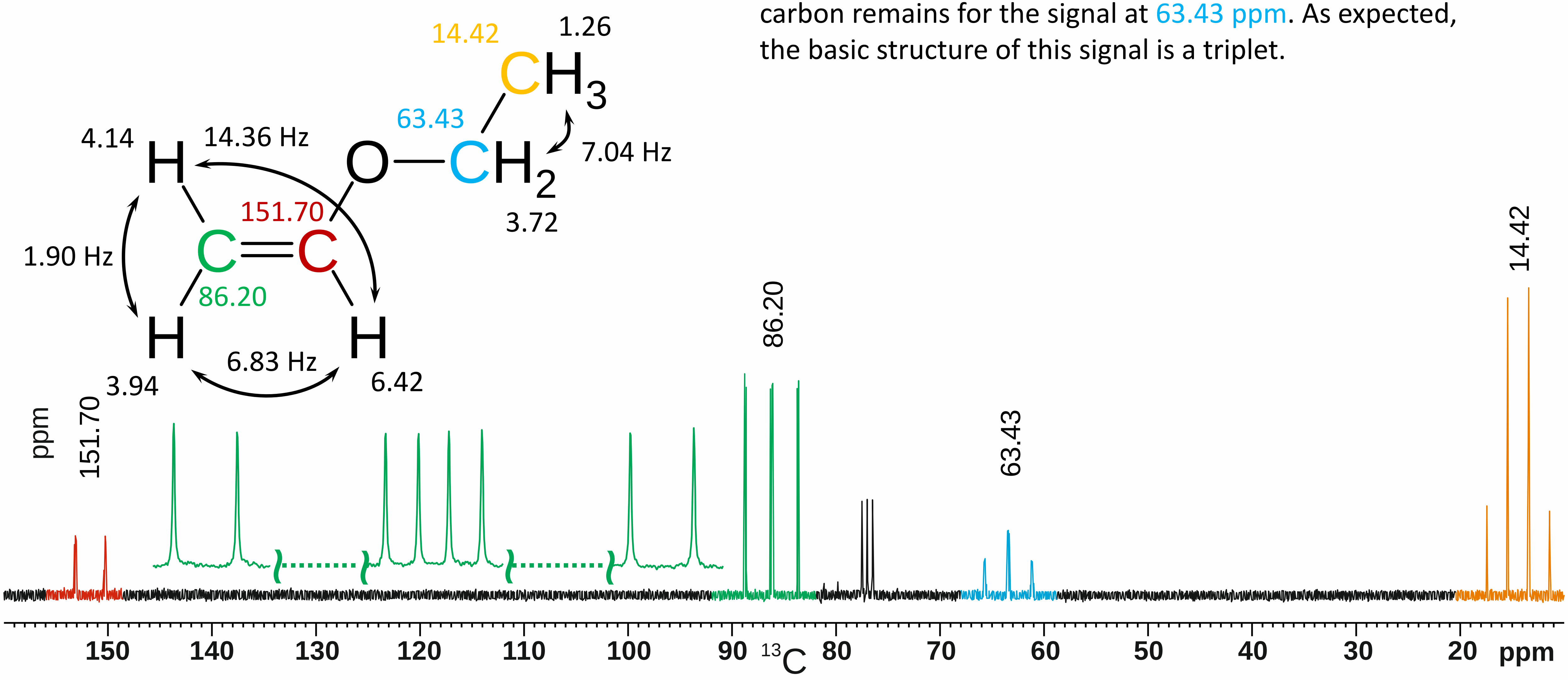
Although of the two remaining carbon atoms, one is sp^2 and the other sp^3 hybridised, their chemical shifts are not too different.

On closer inspection, the signal at 86.2 ppm consists of eight lines of equal intensity, a **doublet** of **doublets** of **doublets**. There are no two chemically equivalent neighbours. The CH_2 carbon atom with two equivalent neighbour protons is thus ruled out.

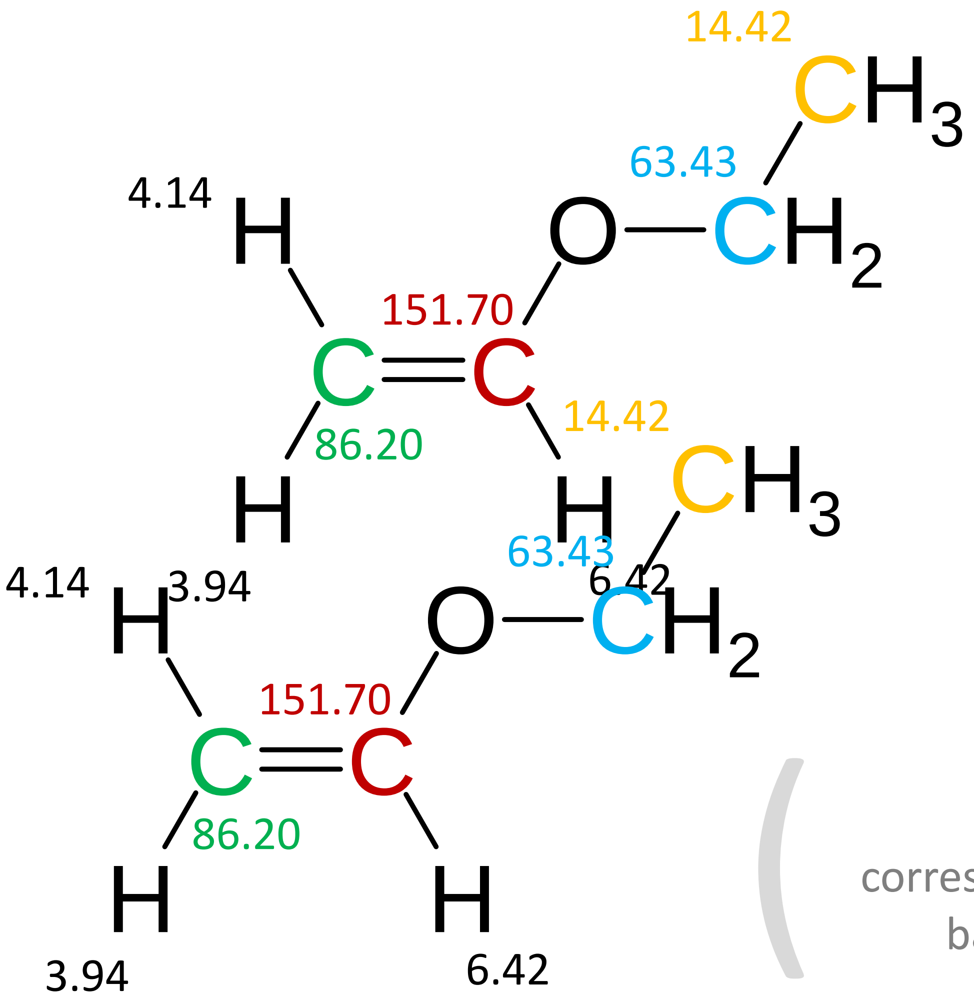


Assignment of the carbon signals

After excluding the assignments already done, only the CH_2 carbon remains for the signal at 63.43 ppm. As expected, the basic structure of this signal is a triplet.



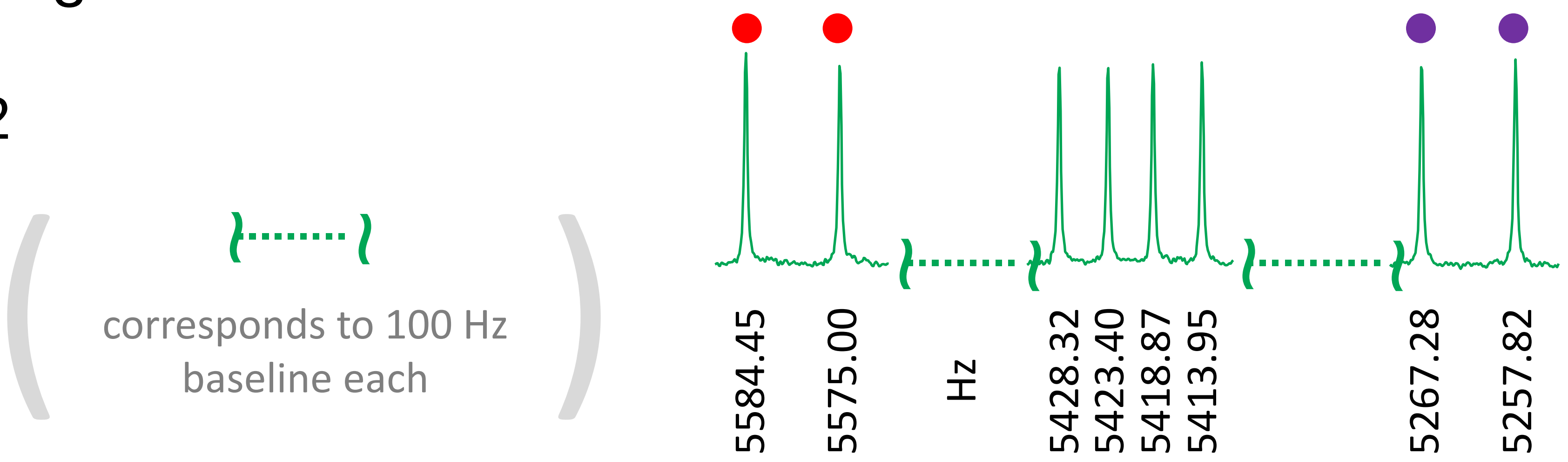
Carbon multiplet detailed analysis



The structure of the multiplet of the carbon signal at 86.20 ppm seems to be the easiest to solve.

It is clearly a **doublet of doublets of doublets**. there should be three chemically different protons in the neighbourhood of this carbon atom. Only the protons at **3.94**, **4.14** and **6.42 ppm** can be considered for this.

Two doublets are easy to recognise, the coupling constant of these two doublets should be observed four times in total. Let us mark both doublets using different colours.



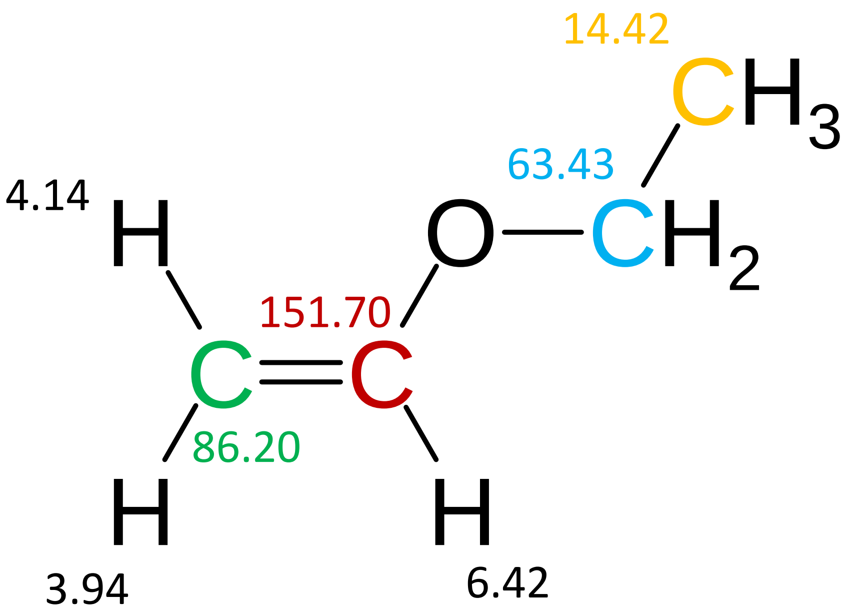
Carbon multiplet detailed analysis

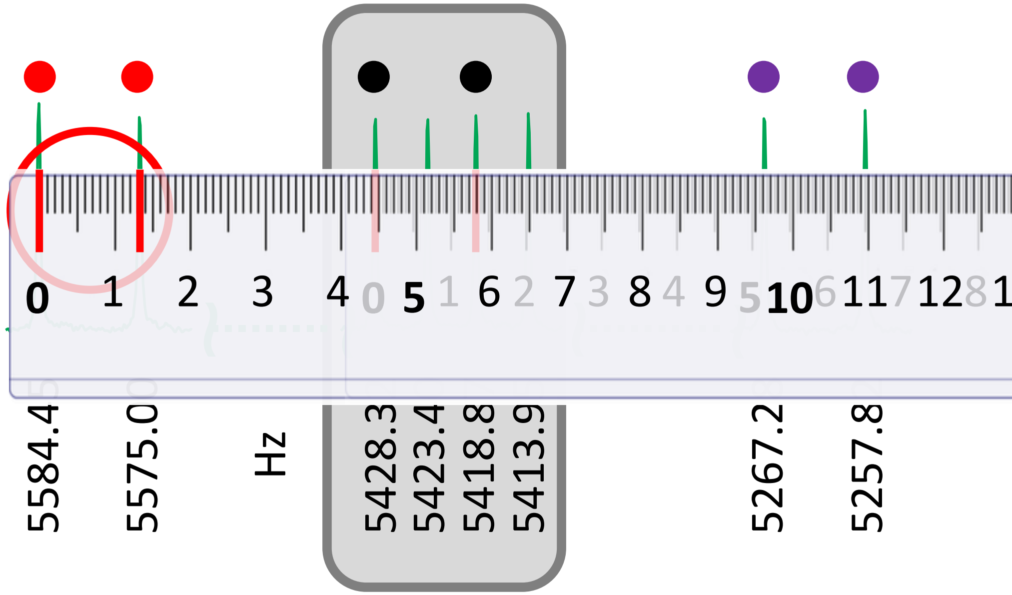
The other two doublets must be hidden in the middle of the composite multiplet.
Howe can we locate them?

Let us first mark on a ruler a doublet that has been identified without any doubt..

Using this pattern we can now try to find the doublet one more time.

We label the two lines having exactly the right distance.

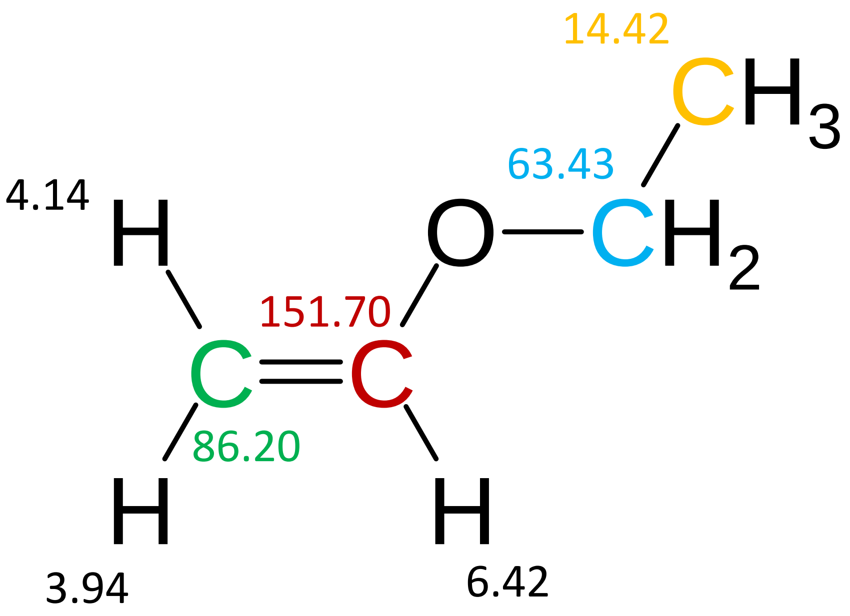


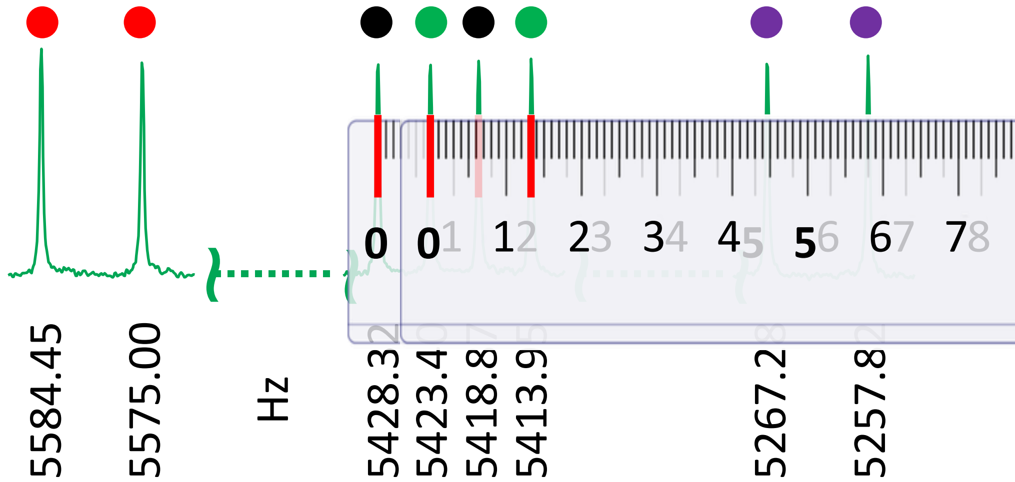


Carbon multiplet detailed analysis

The wo lines remain have to be the still missing fourth doublet that is still missing.
Let us check.

We now have four different coloured doublets.



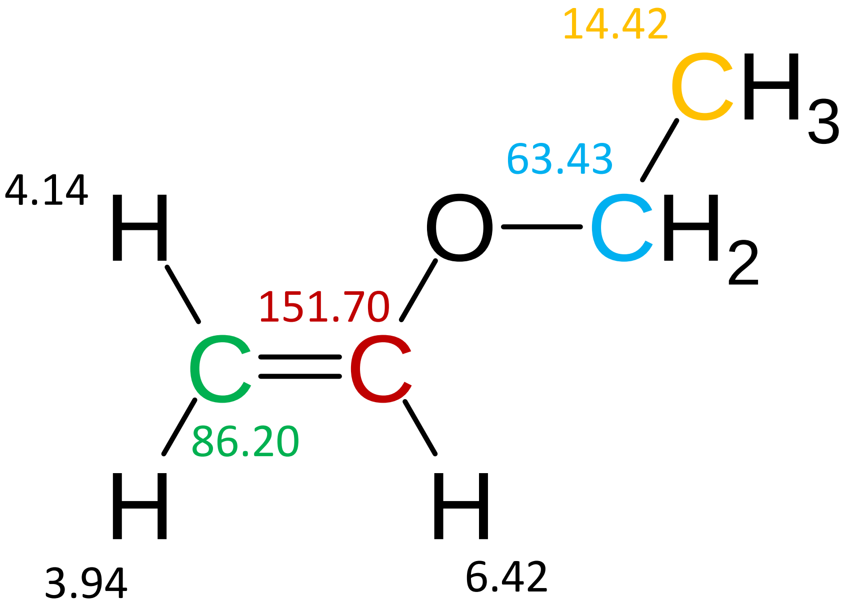


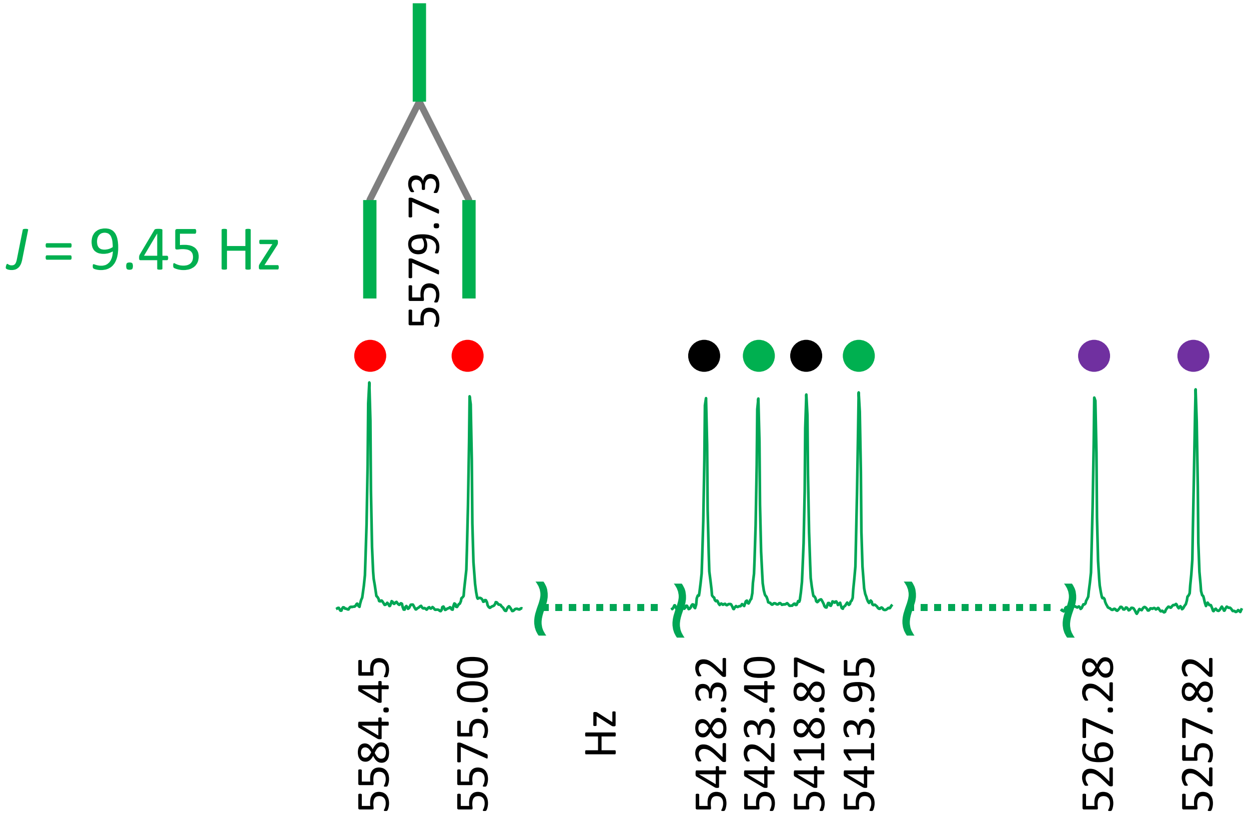
Carbon multiplet detailed analysis

$$J = (5584.45\ \text{Hz} - 5575.00\ \text{Hz}) = \mathbf{9.45\ Hz}$$

$$\delta = \frac{(5584.45\ \text{Hz} + 5575.00\ \text{Hz})}{2} = \mathbf{5579.73\ Hz}$$

Analysis of one of the doublets provides a coupling constant and the chemical shift of the signal from which the doublet comes from.





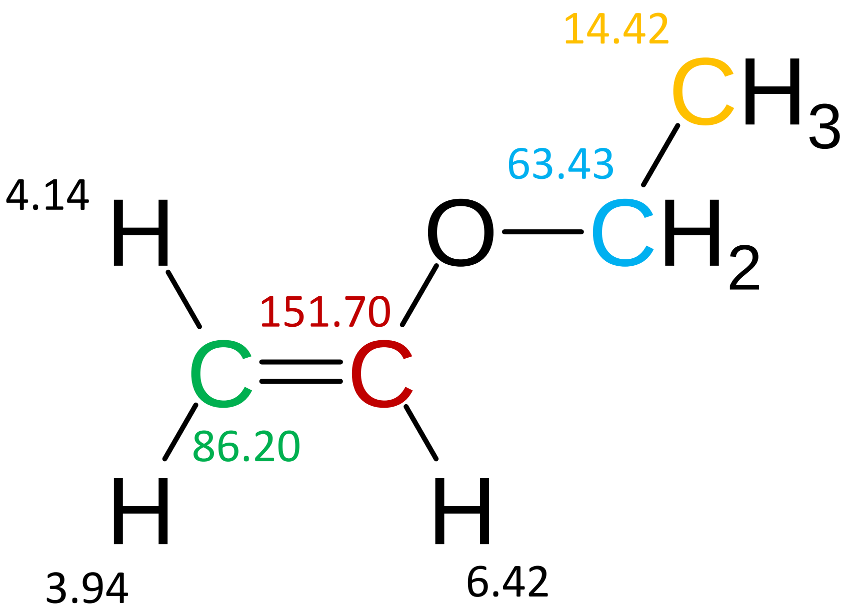
Carbon multiplet detailed analysis

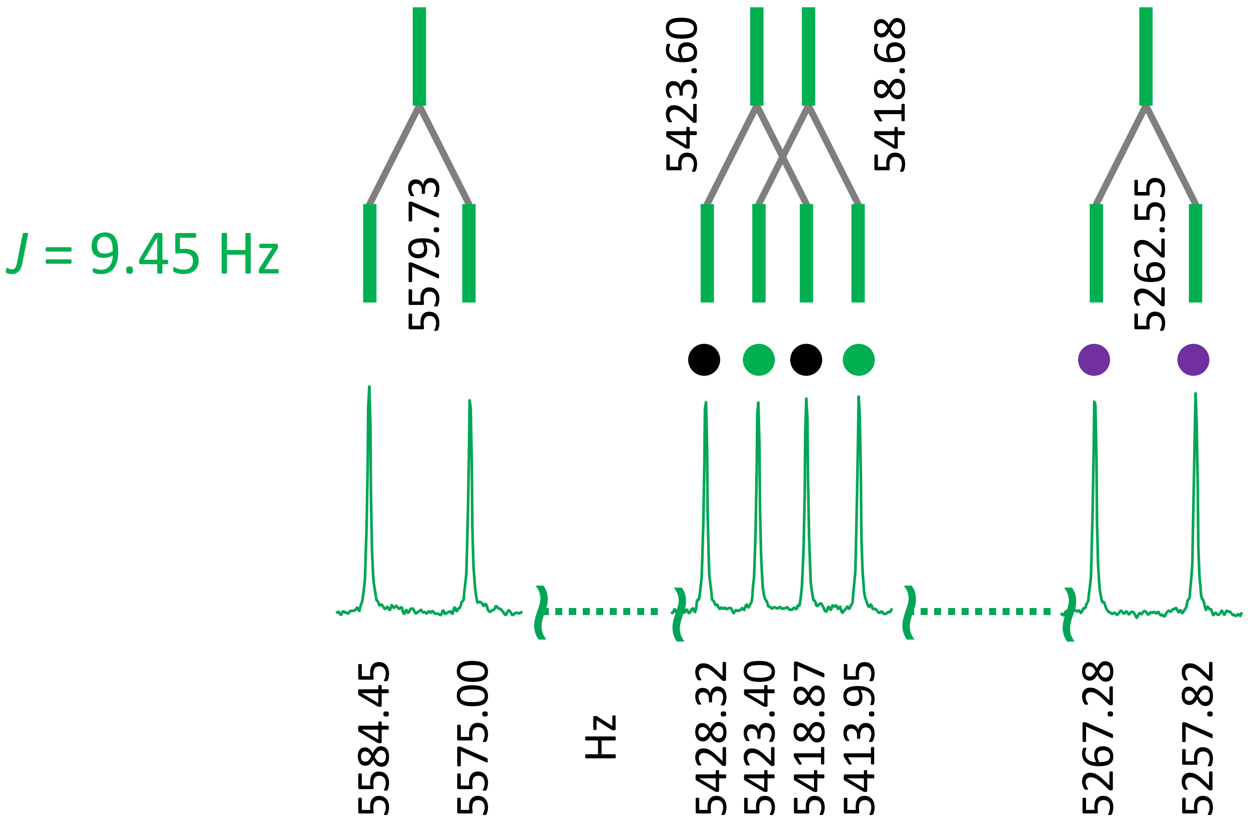
$$J = (5428.32\ \text{Hz} - 5418.84\ \text{Hz}) = \mathbf{9.45\ Hz}$$

$$\delta = \frac{(5428.32\ \text{Hz} + 5418.87\ \text{Hz})}{2} = \mathbf{5423.60\ Hz}$$

The three other labelled doublets are evaluated in the same way.

It is best to wait with the assignment of the coupling constant until the analysis of this multiplet is completely finished.

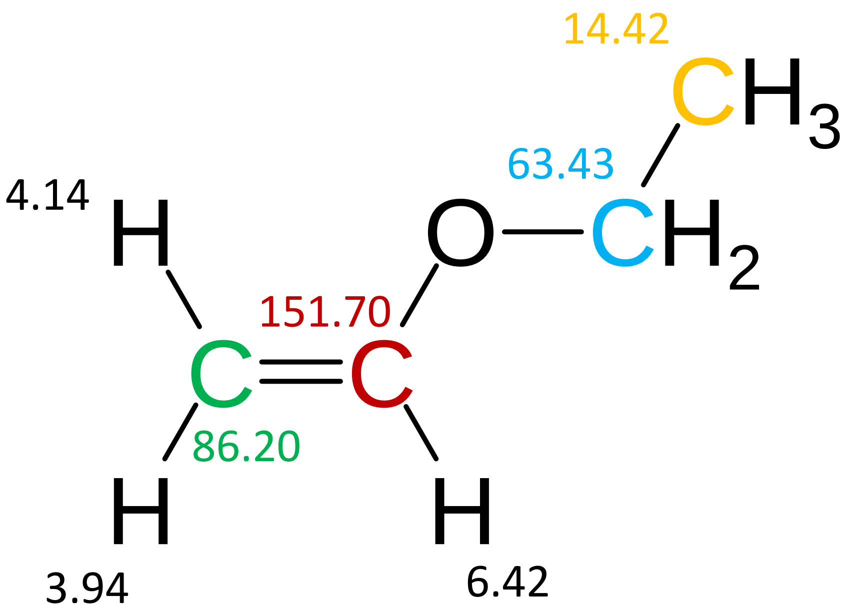




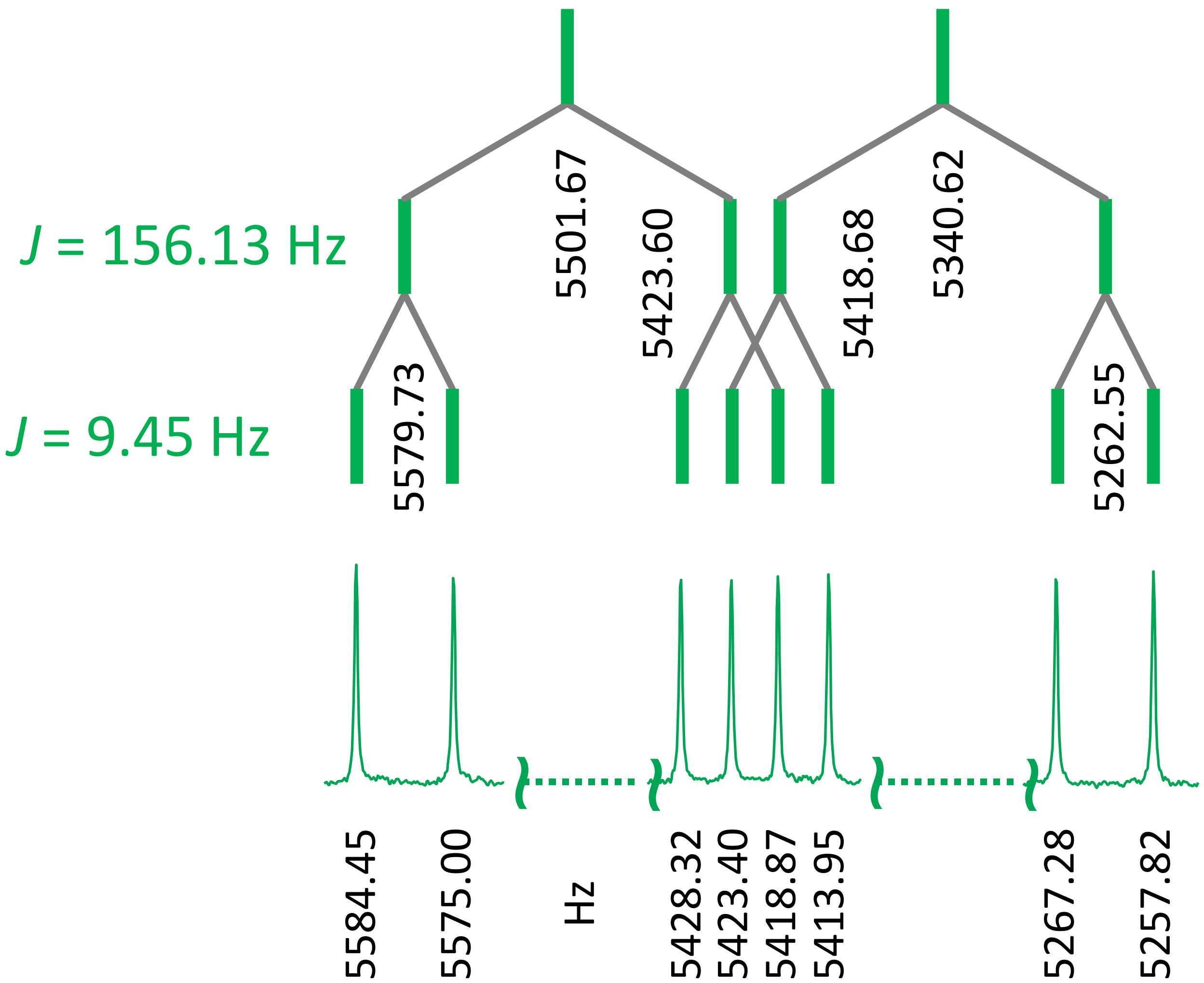
Carbon multiplet detailed analysis

$$J = (5579.73\ \text{Hz} - 5423.60\ \text{Hz}) = \mathbf{156.13\ Hz}$$

$$\delta = \frac{(5579.73\ \text{Hz} + 5423.60\ \text{Hz})}{2} = \mathbf{5501.67\ Hz}$$



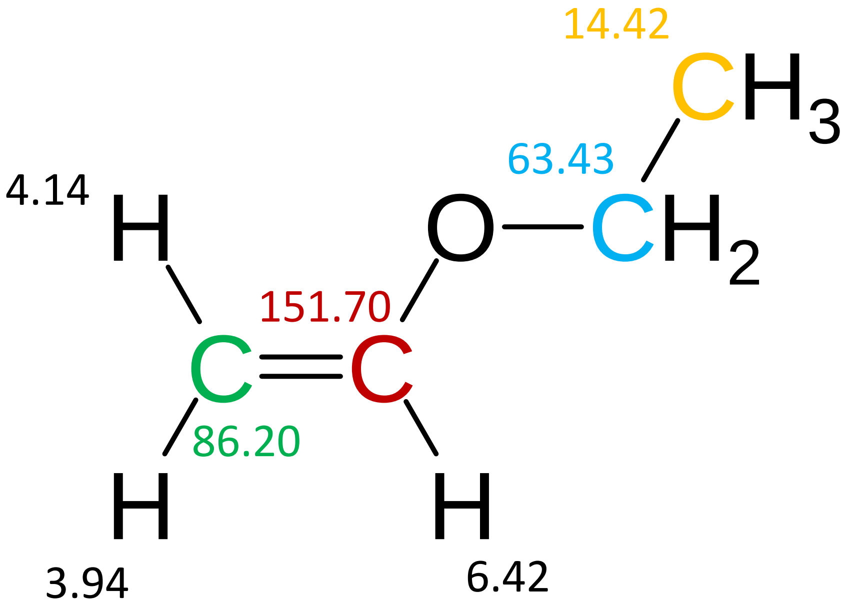
The remaining doublet of doublets is easy to decompose.

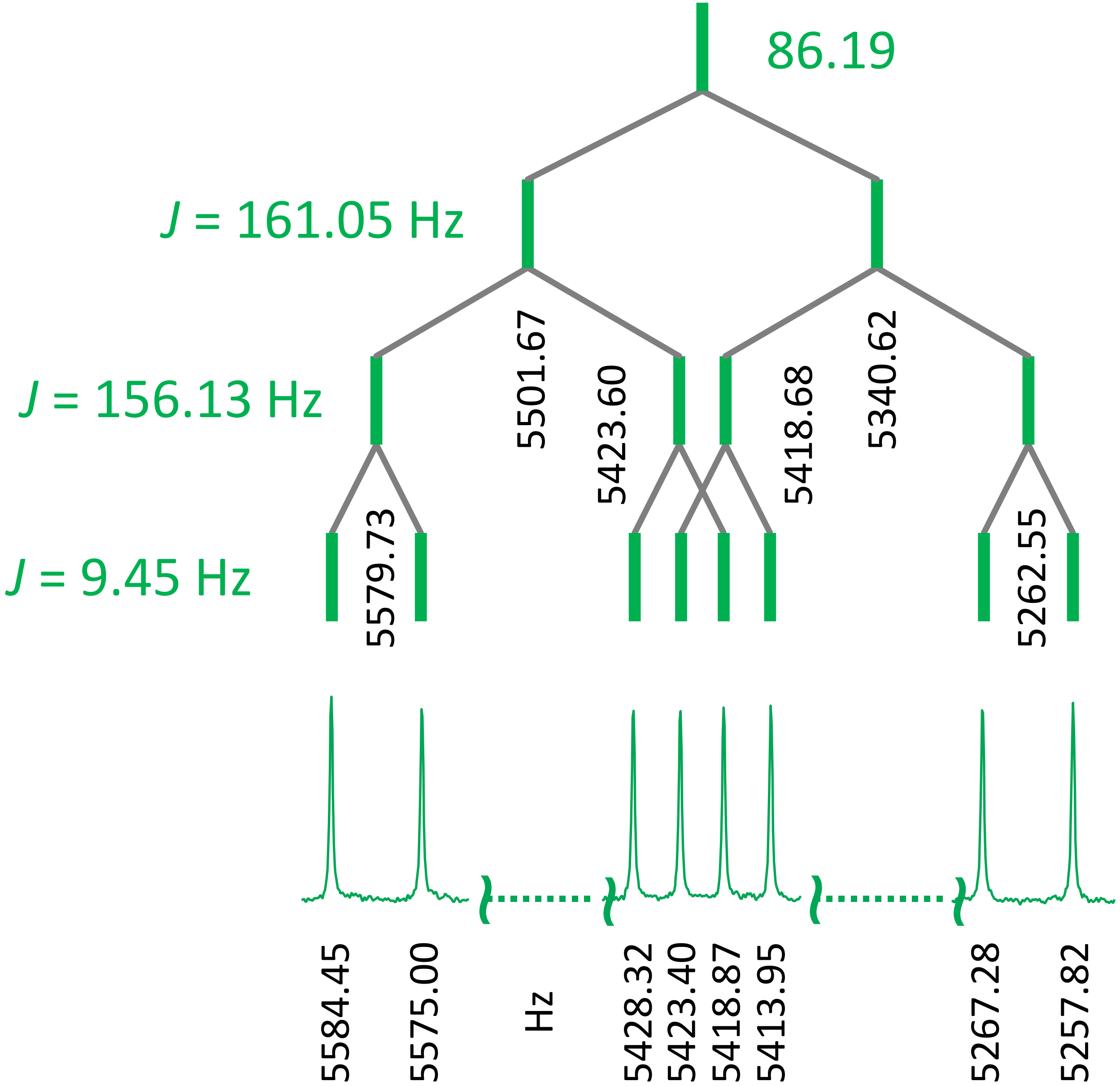


Carbon multiplet detailed analysis

$$J = (5501.67\ \text{Hz} - 5340.62\ \text{Hz}) = \mathbf{161.05\ Hz}$$

$$\delta = \frac{(5501.67\ \text{Hz} + 5340.62\ \text{Hz})}{2 \ * 62.90\ \text{MHz}} = \mathbf{86.19\ ppm}$$





Carbon multiplet detailed analysis

We still have to assign the coupling constants.

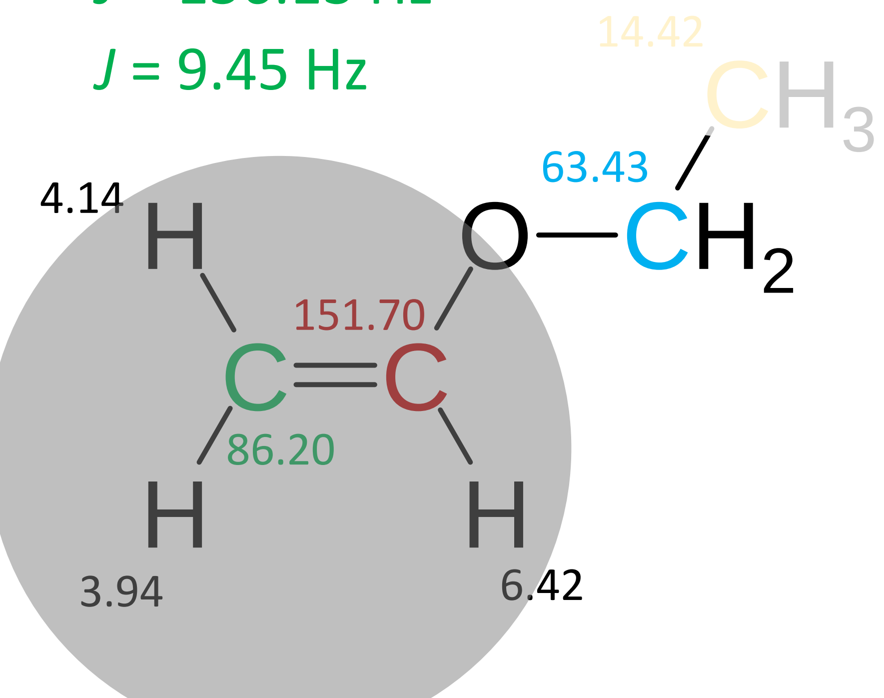
$$J = (5501.67\ \text{Hz} - 5340.62\ \text{Hz}) = \mathbf{161.05\ Hz}$$

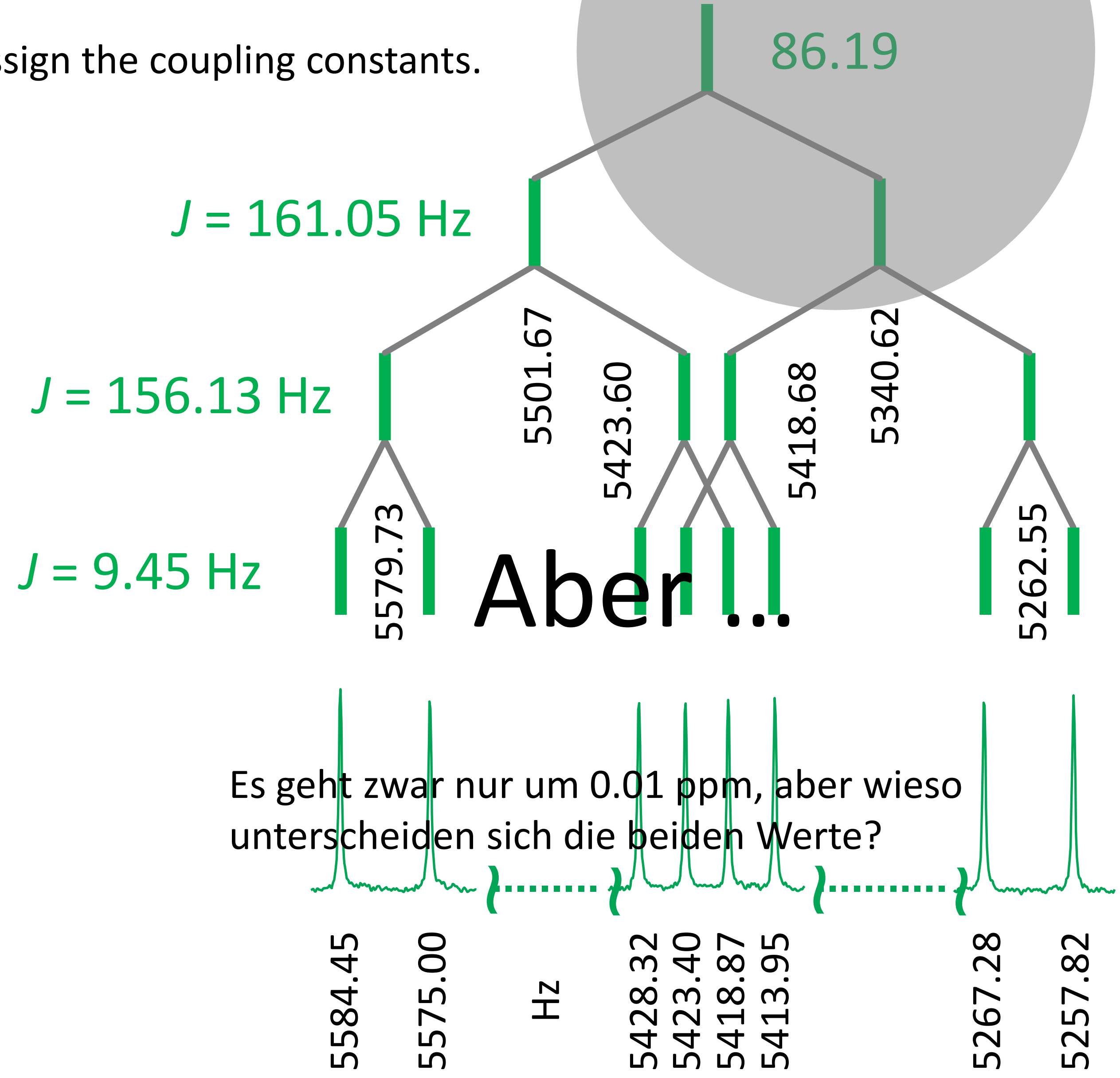
$$\delta = \frac{(5501.67\ \text{Hz} + 5340.62\ \text{Hz})}{2 \ * 62.90\ \text{MHz}} = \mathbf{86.19\ ppm}$$

J = 161.05 Hz

J = 156.13 Hz

J = 9.45 Hz





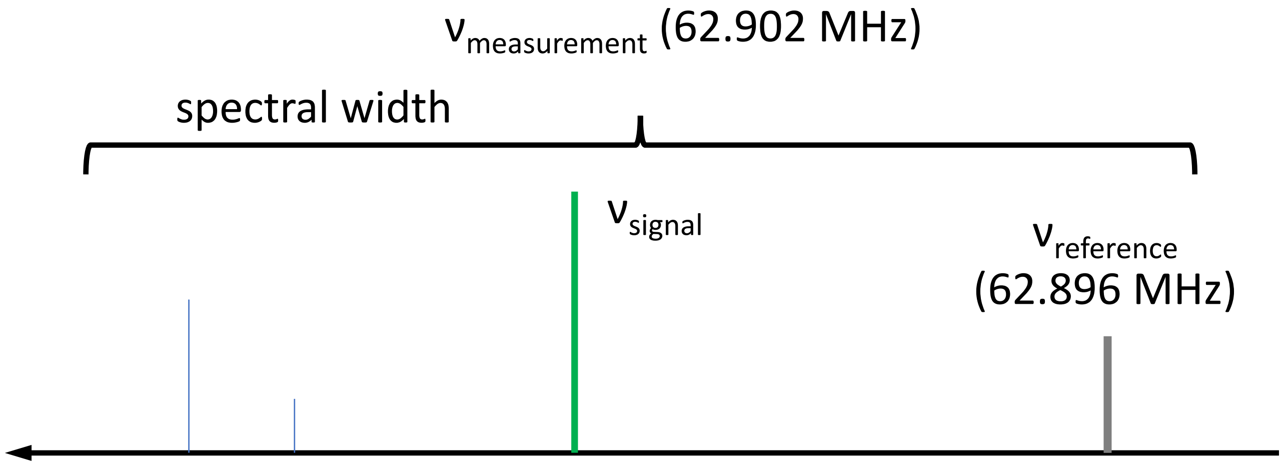
Aber ...

Es geht zwar nur um 0.01 ppm, aber wieso unterscheiden sich die beiden Werte?

Carbon multiplet detailed analysis

86.19

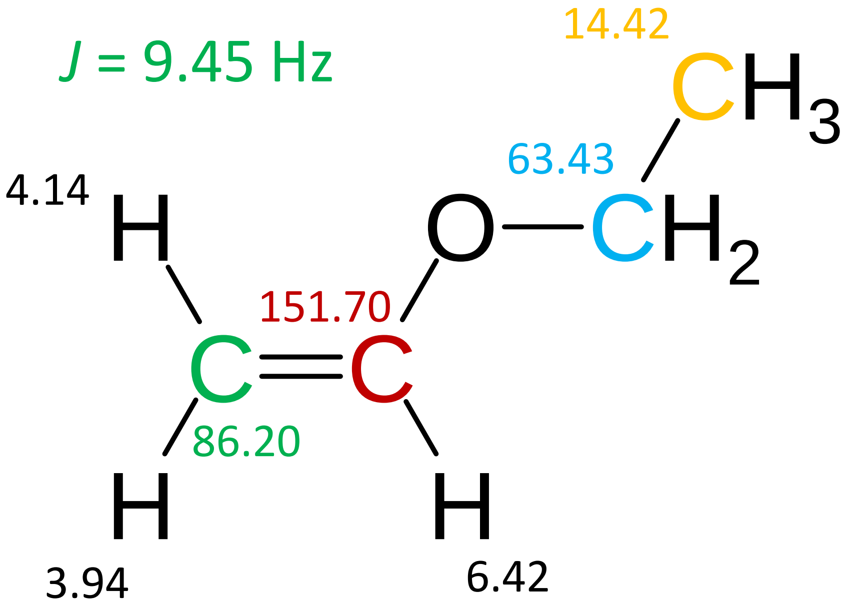
It is not necessary for the evaluation of this spectroscopic challenge, but at this point a more detailed explanation might be a reasonale idea.



J = 161.05 Hz

J = 156.13 Hz

J = 9.45 Hz



Measurements are made with a fixed frequency and a spectrum width determined by the dwell time.

Within the spectrum width are the observed signal and a reference signal, from which according to the known formula

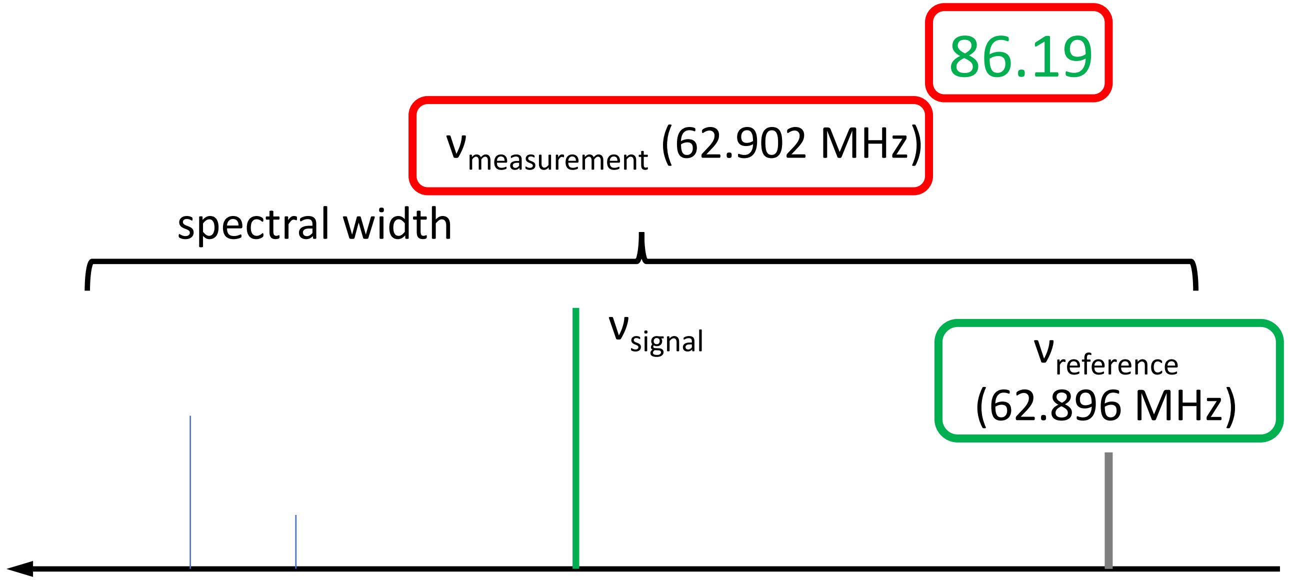
$$\delta = \frac{\nu_{\mathrm{Signal}} - \nu_{\mathrm{Referenz}}}{\nu_{\mathrm{Referenz}}}$$

the chemical shift is determined.

The frequency of the reference signal has nothing to do with the measuring frequency. In this example the two frequencies differ by about 6 kHz.

Carbon multiplet detailed analysis

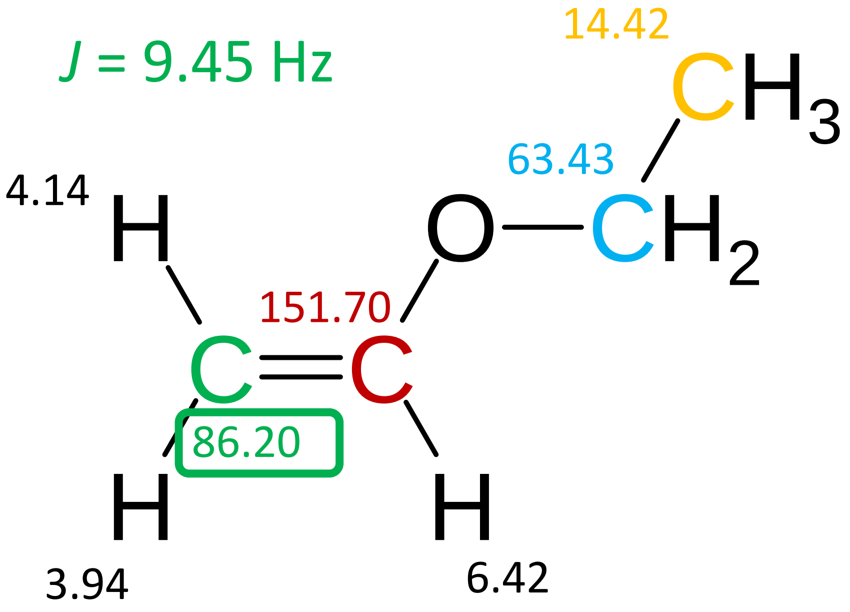
It is not necessary for the evaluation of this spectroscopic challenge, but at this point a more detailed explanation might be a reasonale idea.



J = 161.05 Hz

J = 156.13 Hz

J = 9.45 Hz



The difference of about 0.01 ppm here is due to the fact that the processing software correctly converts from **Hz** to **ppm** with $\nu_{reference}$, but when publishing spectra (as done here), the measurement frequency is usually specified.

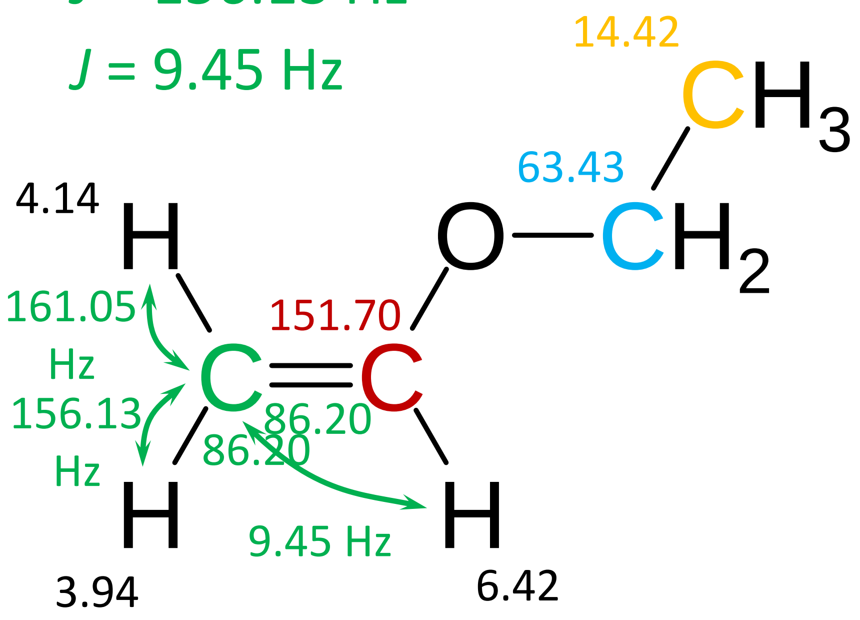
For nuclei with a very wide range of chemical shift (e.g. platinum), this can result in significantly larger errors than 0.01 ppm.

Carbon multiplet detailed analysis

J = 161.05 Hz

J = 156.13 Hz

J = 9.45 Hz



There remains some ambiguity assigning the coupling constant.

A typical value for $^1J_{CH}$ (with sp^2 hybridised carbon) is about 165 Hz.

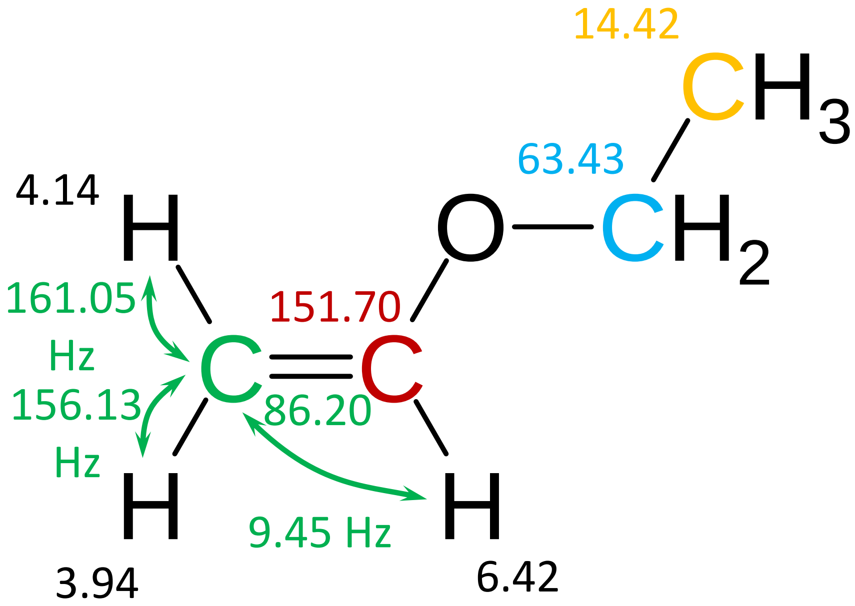
A clear assignment of the two values would only be possible by selectively decoupling one of the two protons. Technically, this is not quite trivial because of the multiplet structure and the slight difference in the chemical shift between the two protons.

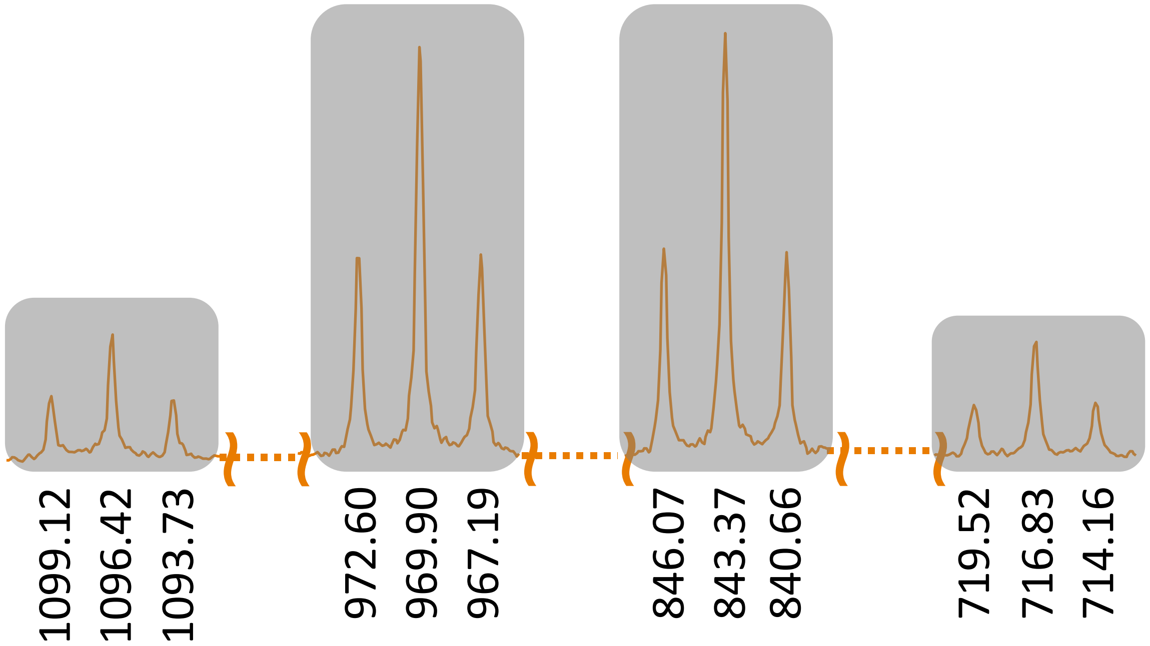
The last copulation constant is easy to assign.

Carbon multiplet detailed analysis

The multiplet of the carbon atom at 14.42 ppm is much easier to decompose.

A triplet structure occurs a total of four times, the intensity distribution of the four blocks with triplet structure is about **1 : 3 : 3 : 1**.



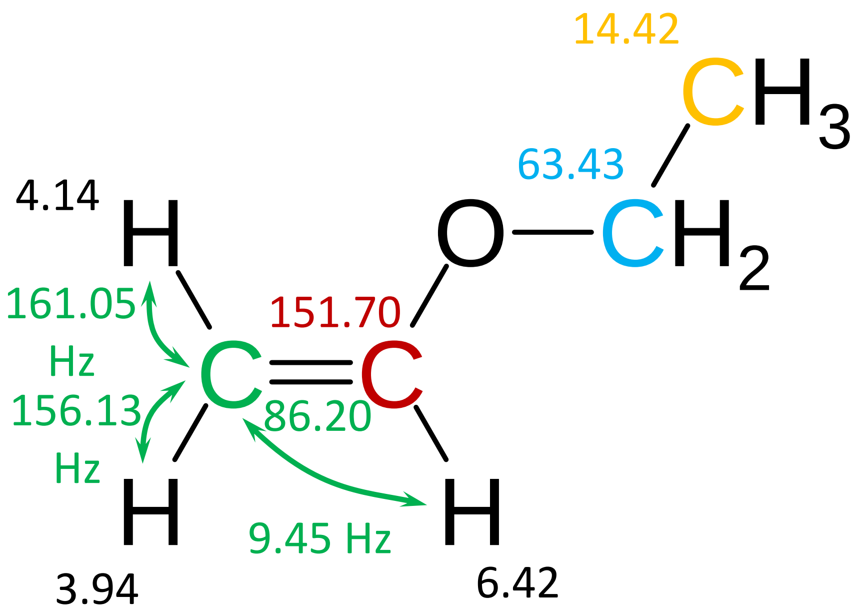


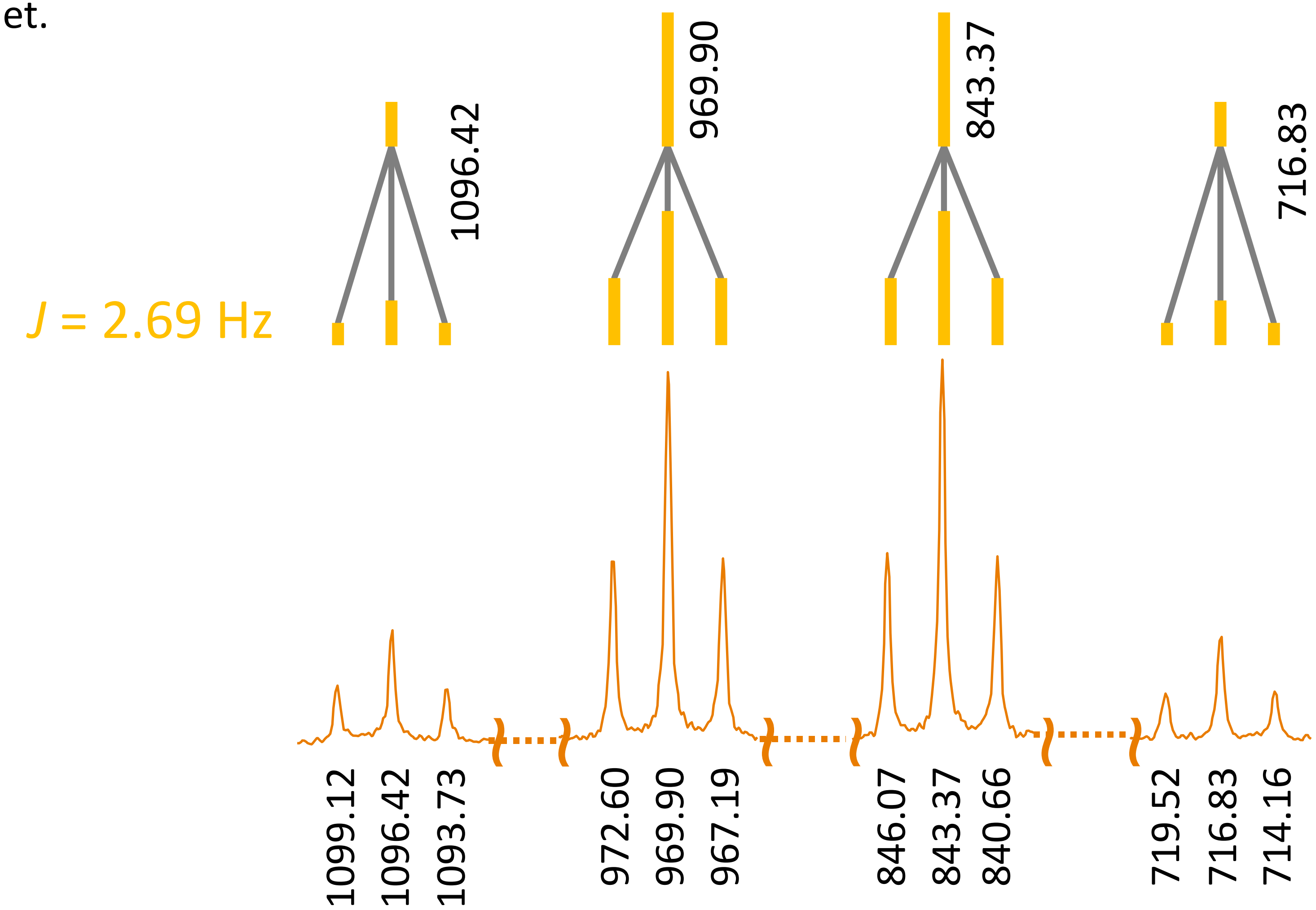
Carbon multiplet detailed analysis

For the detailed analysis, the coupling constants of the triplets are extracted first.

The chemical shift for the analysis of the parent multiplet is simply taken from the middle line of each triplet.

$$J = \frac{(1099.12\ \text{Hz} - 1093.73\ \text{Hz})}{2} = \mathbf{2.69\ Hz}$$





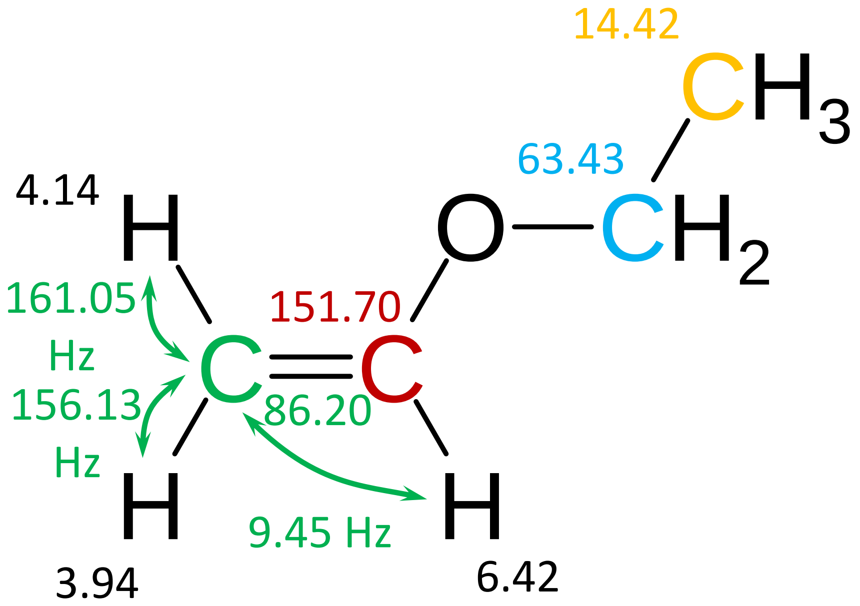
Carbon multiplet detailed analysis

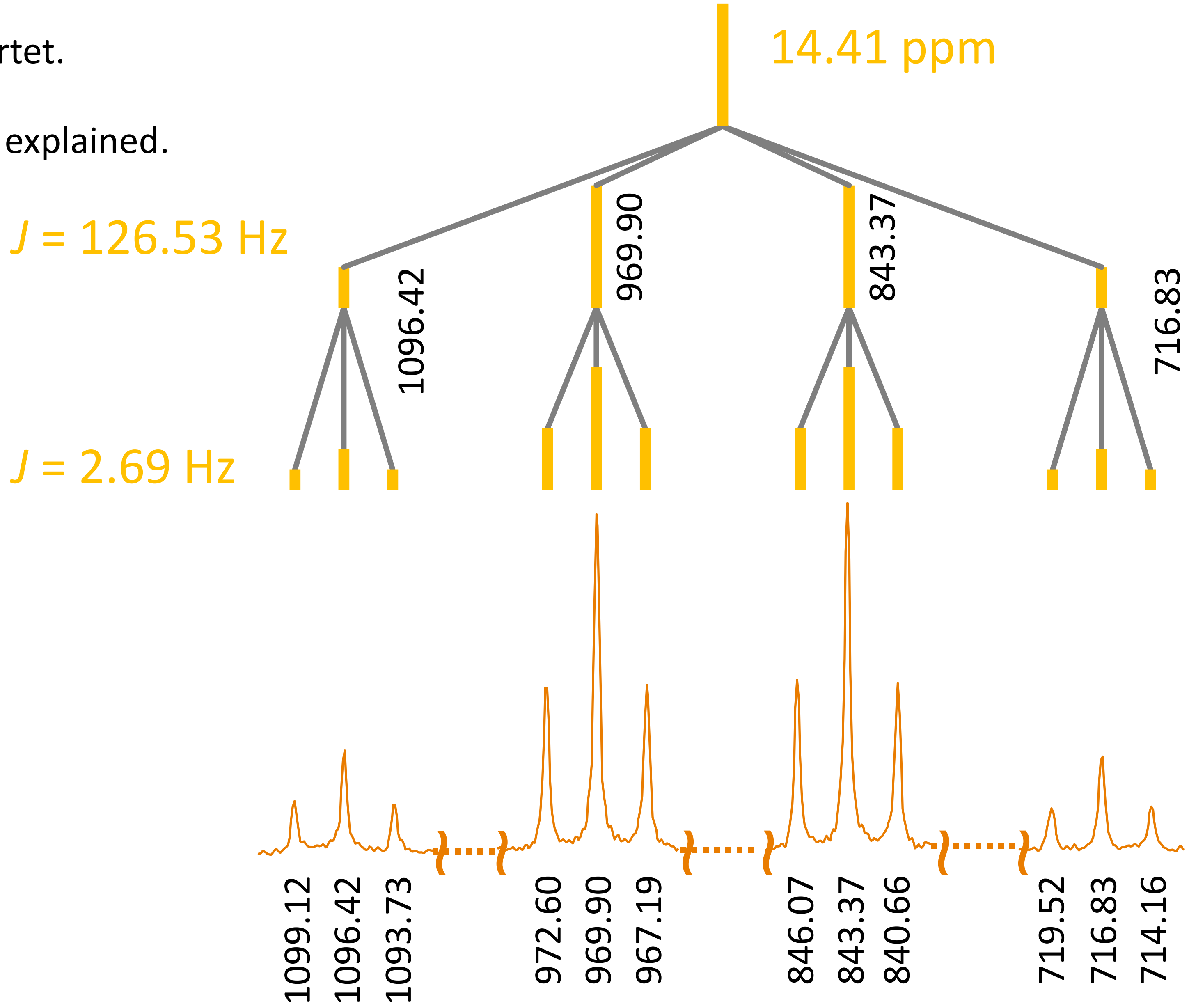
What remains is the simple analysis of the quartet.

The discrepancy of 0.01 ppm has already been explained.

$$J = \frac{(1096.42\ \text{Hz} - 716.83\ \text{Hz})}{3} = \mathbf{126.53\ Hz}$$

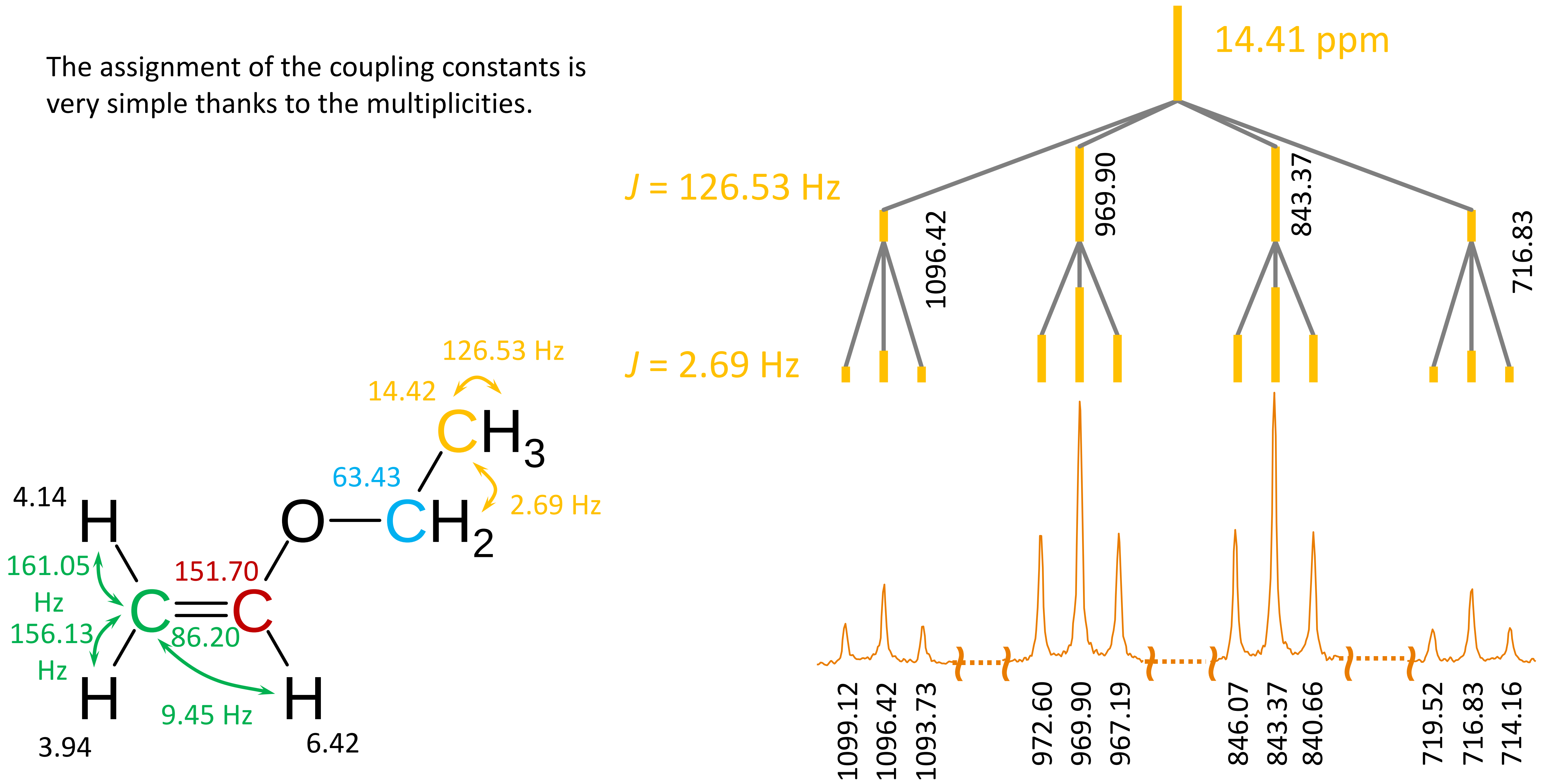
$$\delta = \frac{(1096.42\ \text{Hz} + 716.83\ \text{Hz})}{2 * 62.90\ \text{MHz}} = \mathbf{14.41\ ppm}$$



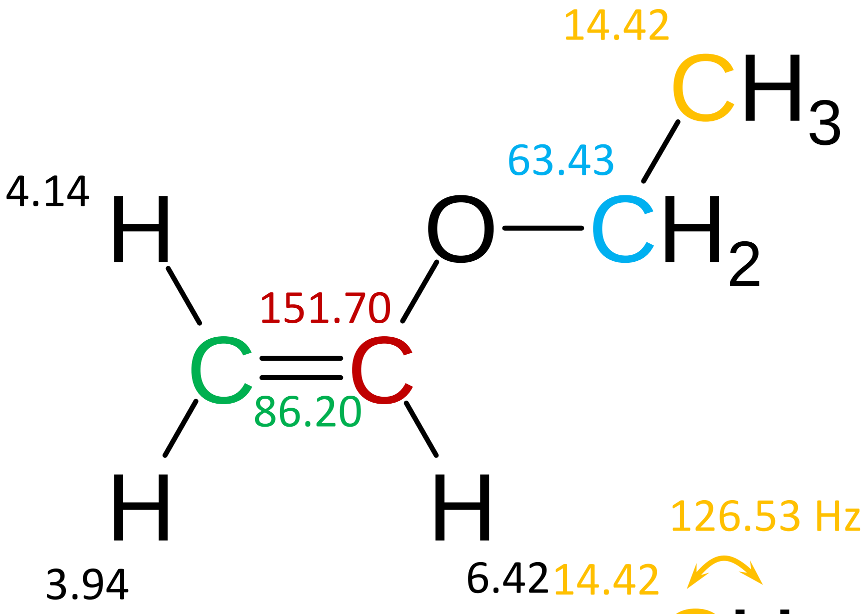


Carbon multiplet detailed analysis

The assignment of the coupling constants is very simple thanks to the multiplicities.

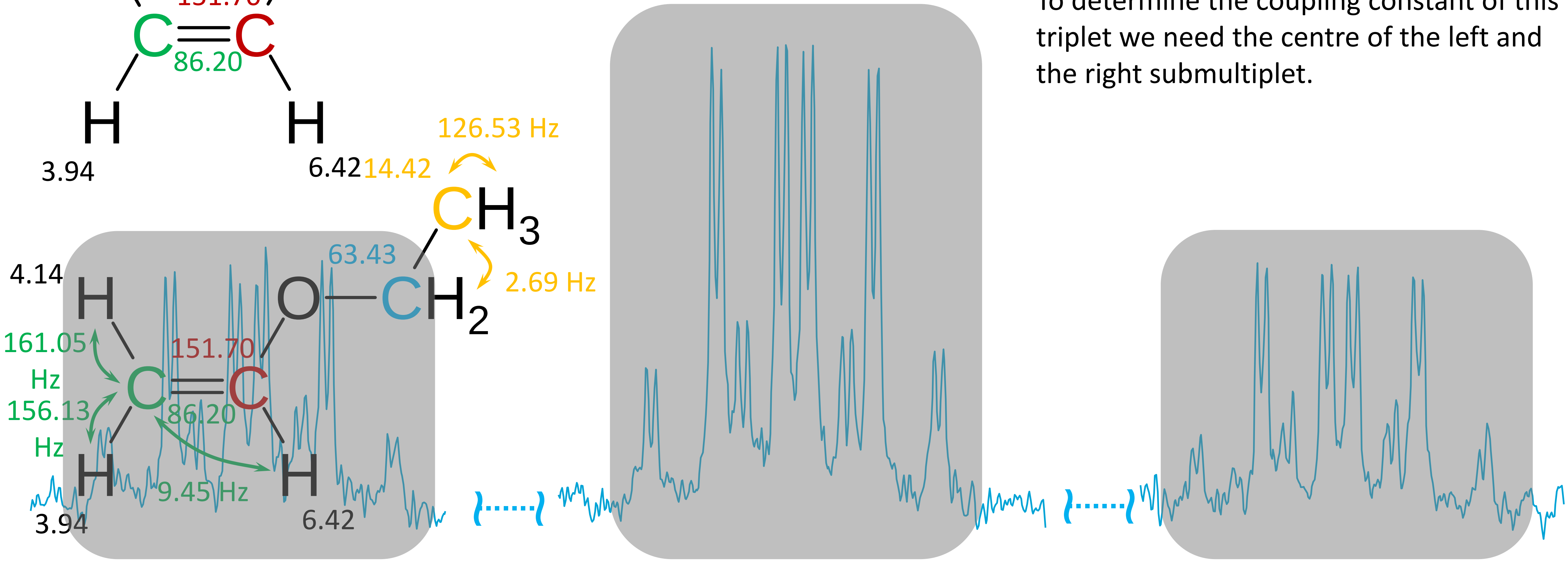


Carbon multiplet detailed analysis

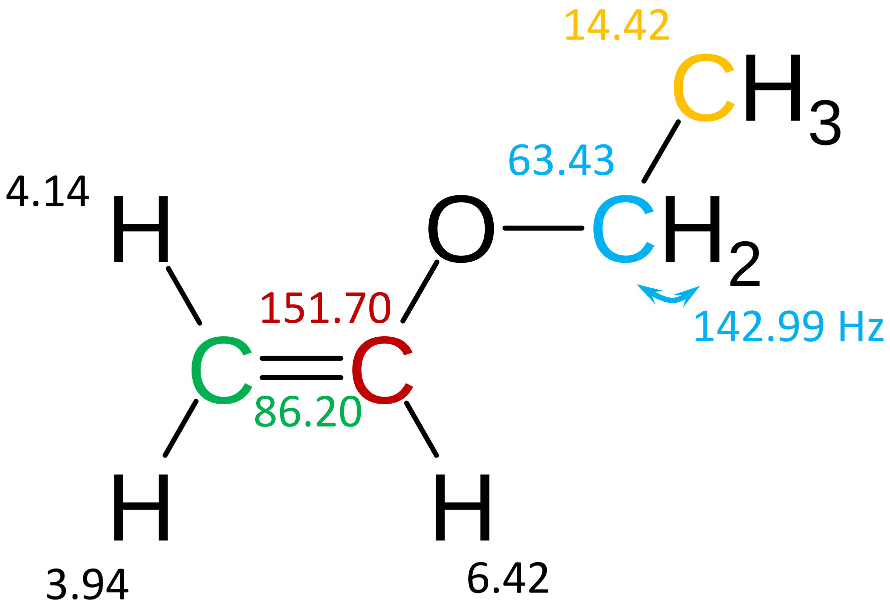


The underlying structure of the carbon signal at 63.43 ppm must be a triplet with a coupling constant of about **130 Hz** because there are two chemically equivalent methylene protons separated by one bond.

To determine the coupling constant of this triplet we need the centre of the left and the right submultiplet.

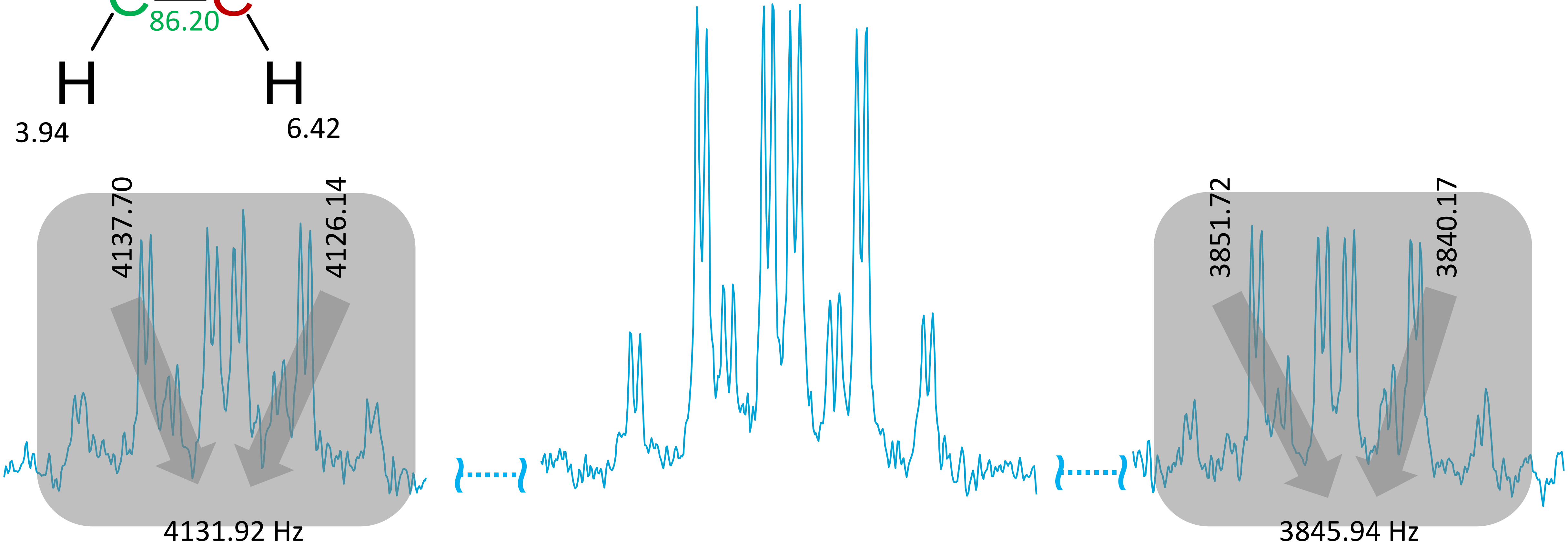


Carbon multiplet detailed analysis

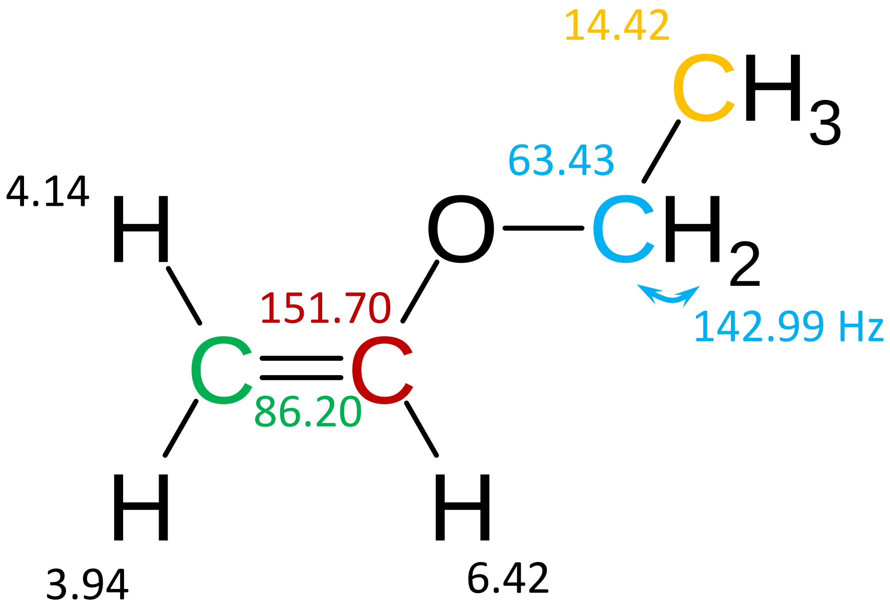


We only need the frequencies of a few selected peaks.

$$J = \frac{(4131.92\ \text{Hz} - 3845.94\ \text{Hz})}{2} = \mathbf{142.99\ Hz}$$

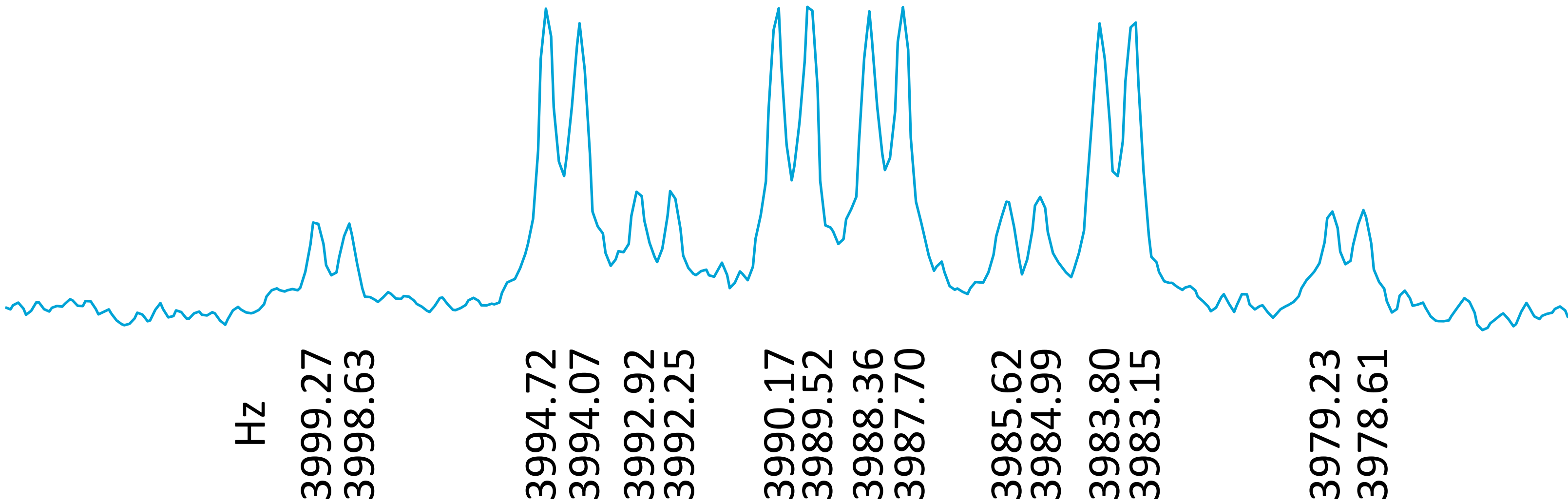


Carbon multiplet detailed analysis

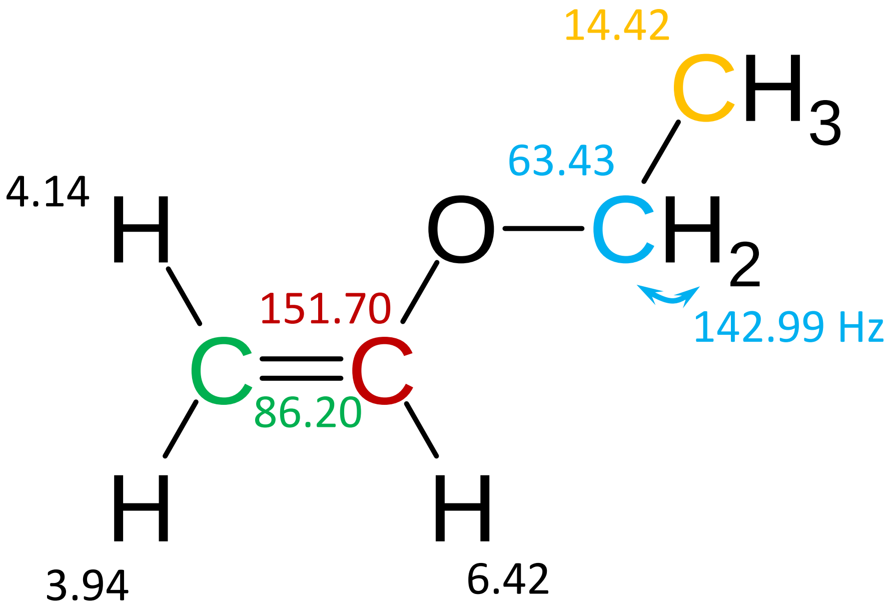


The three submultiplets each have an identical fine structure.

For further analysis, one of the three partial multiplets is sufficient; of course, the one with the best signal-to-noise ratio is used..



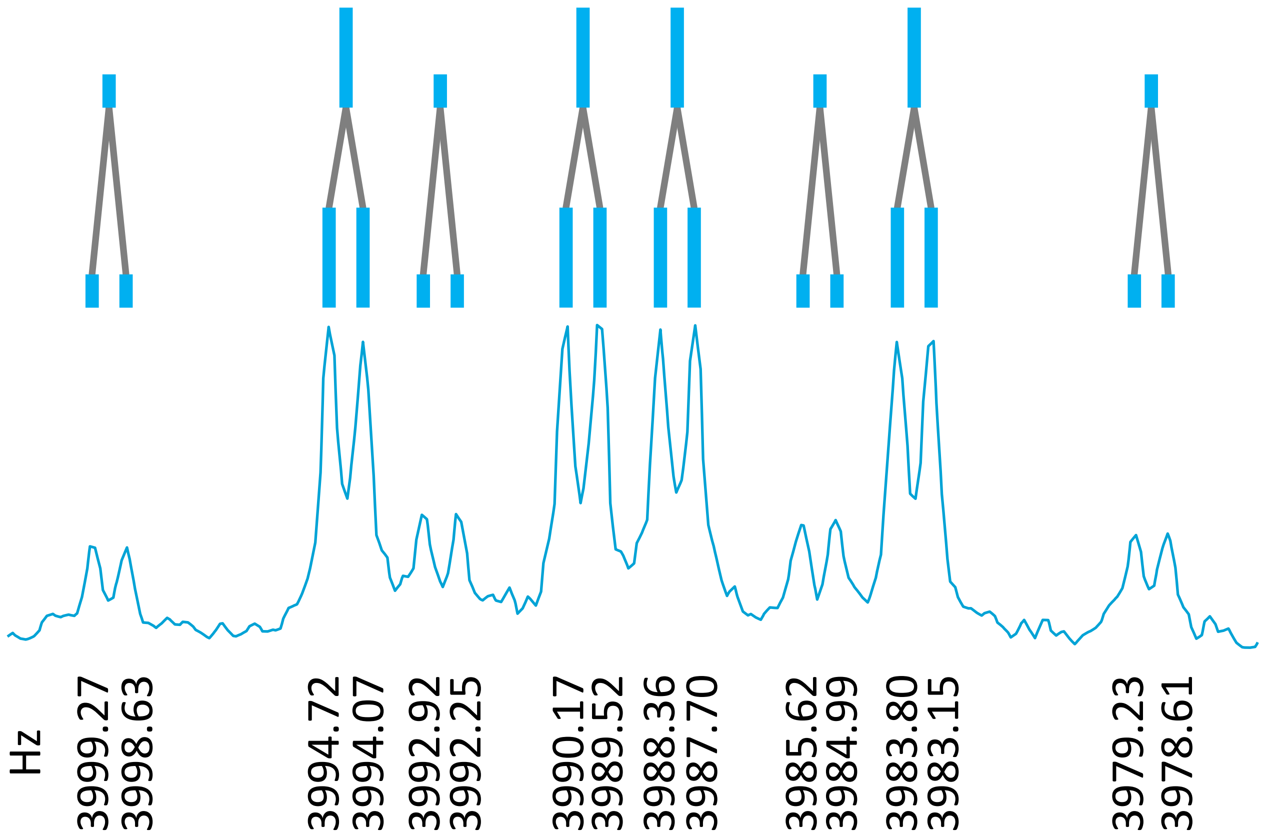
Carbon multiplet detailed analysisis



In the very confusing multiplet, one immediately notices that all lines appear twice.

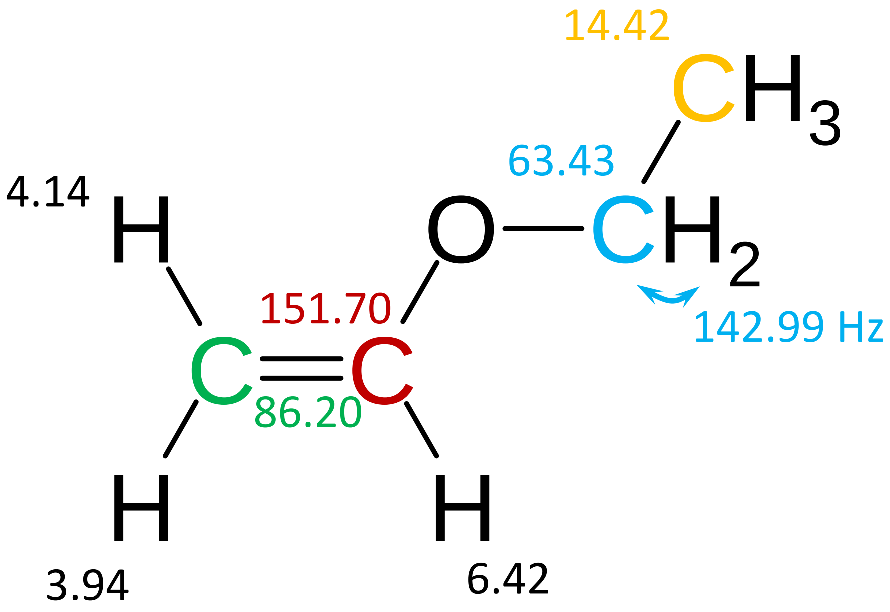
After reduction of all 8 doublets to one line each (the coupling constant determined as an example for one pair of lines can also be averaged over all 8 doublets), a no less clear multiplet of 8 lines in the intensity ratio **1** : **3** : **1** : **3** : **3** : **1** : **3** : **1** remains.

J = 0.65 Hz



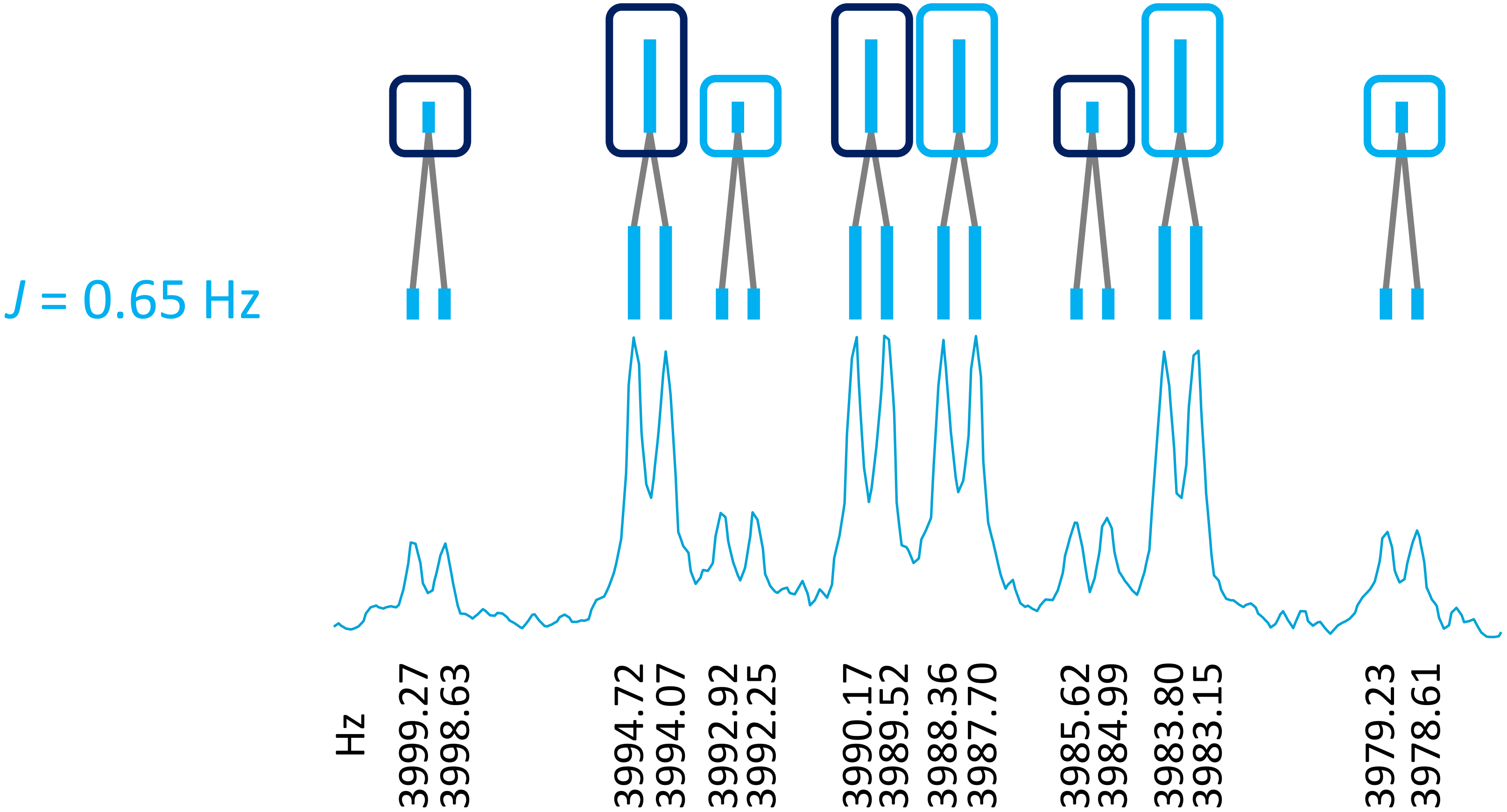
$$J = (3990.17\text{ Hz} - 3989.52\text{ Hz}) = \mathbf{0.65\ Hz}$$

Carbon multiplet detailed analysis

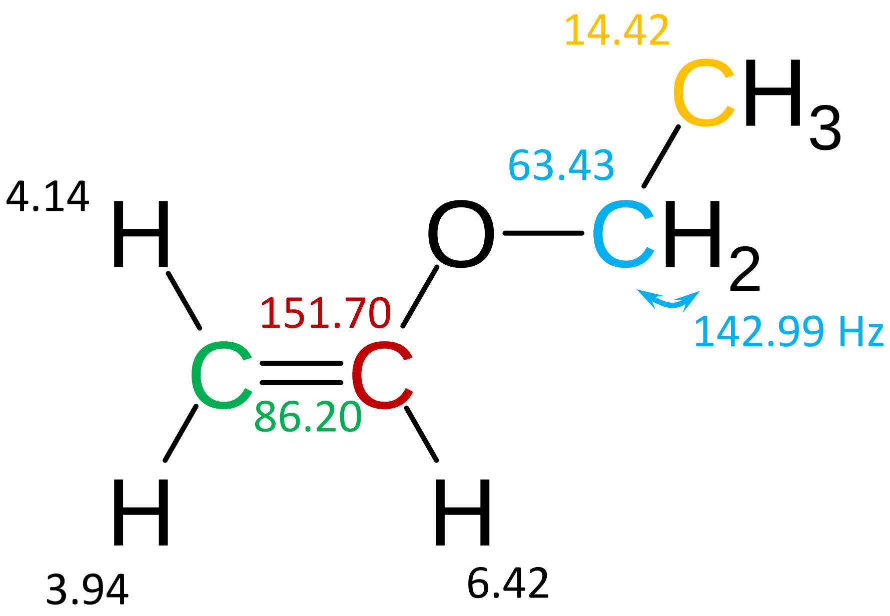


With the "ruler method" already used before, one finds four equidistant lines.

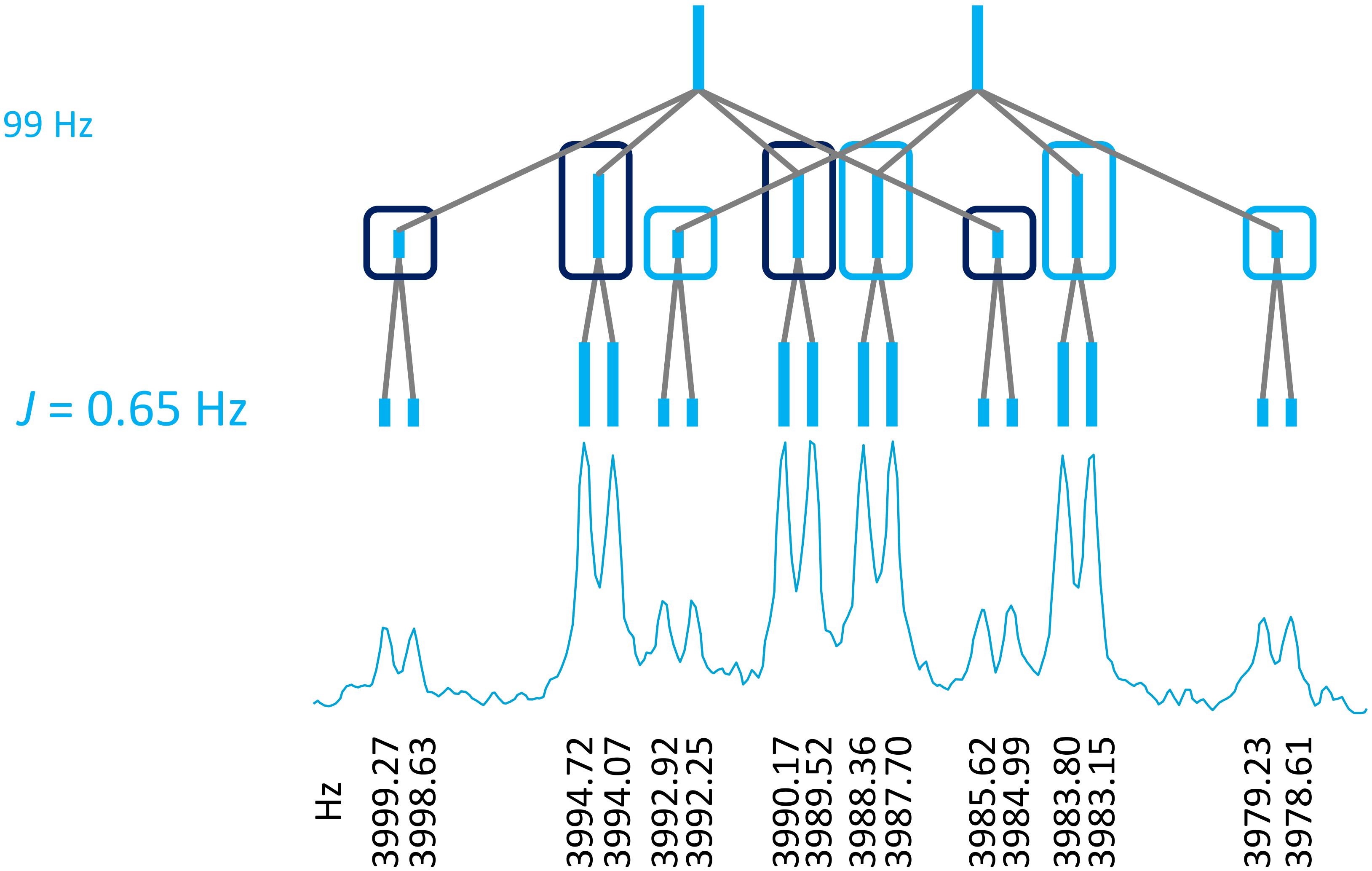
It is a quartet. A second quartet is now quite easy to recognise.



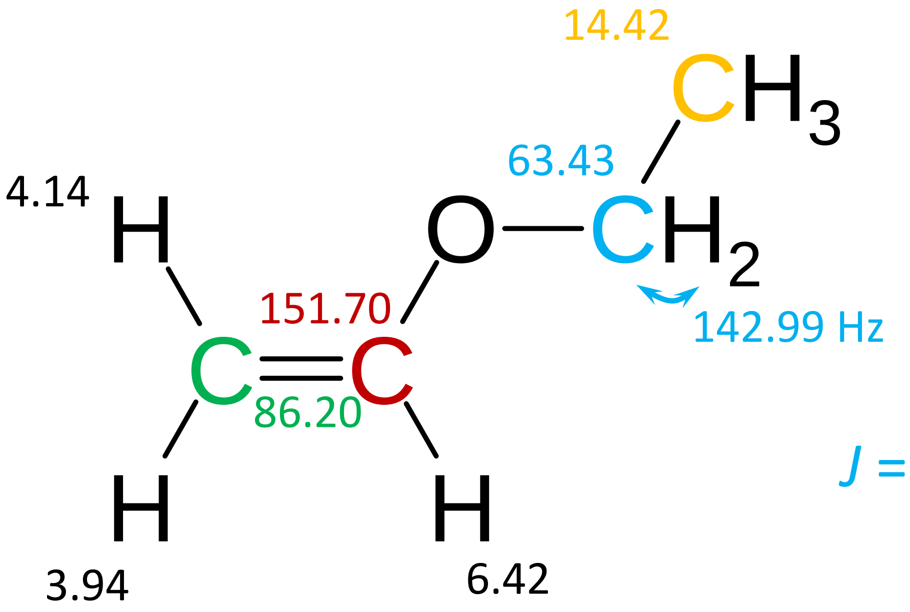
Carbon multiplet detailed analysis



The base of the quartets are two lines of equal intensity.

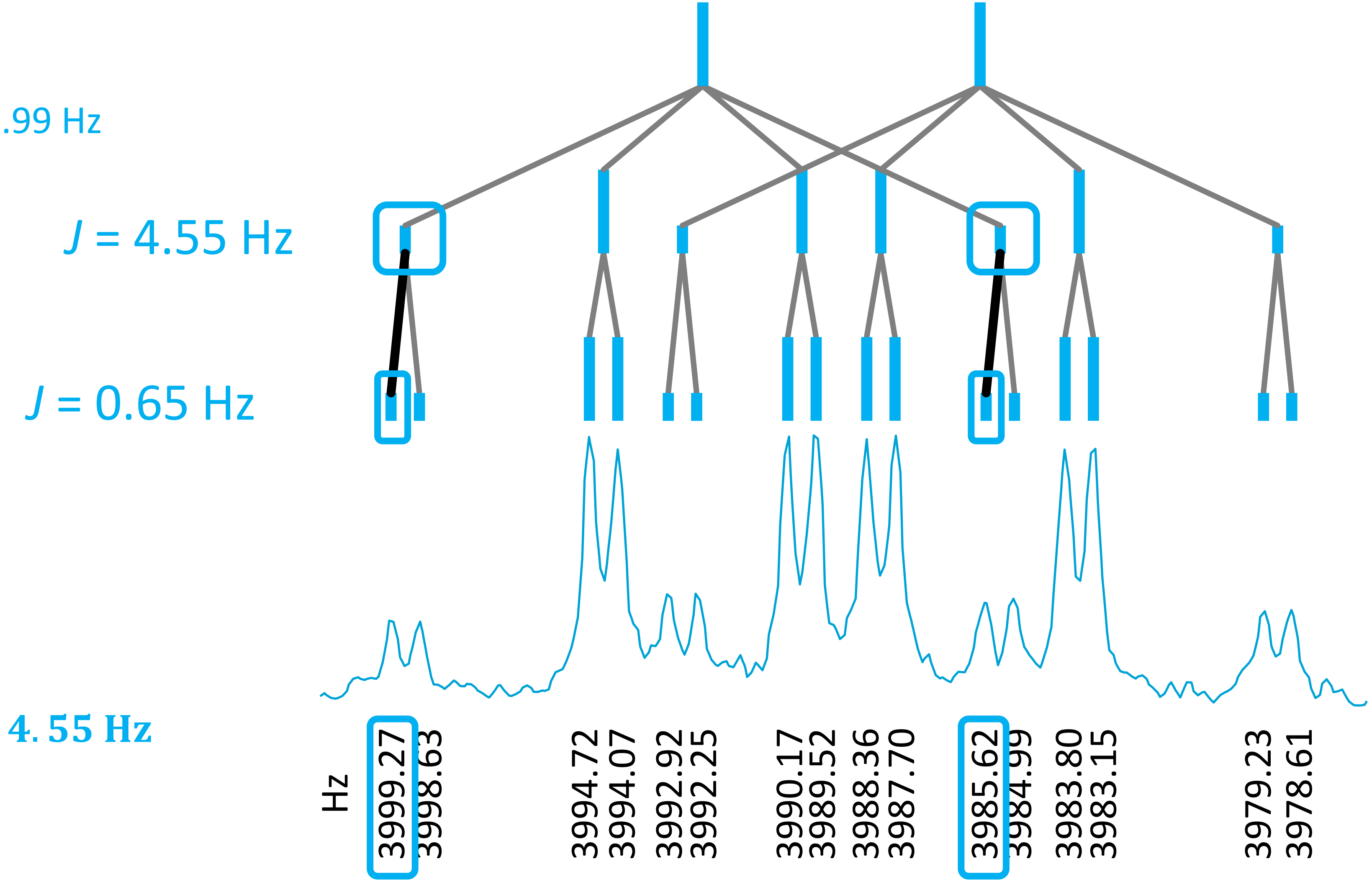


Carbon multiplet detailed analysis



The coupling constant of the quartet is three times the distance between these two lines.

We can read off the numeric values here, for example.

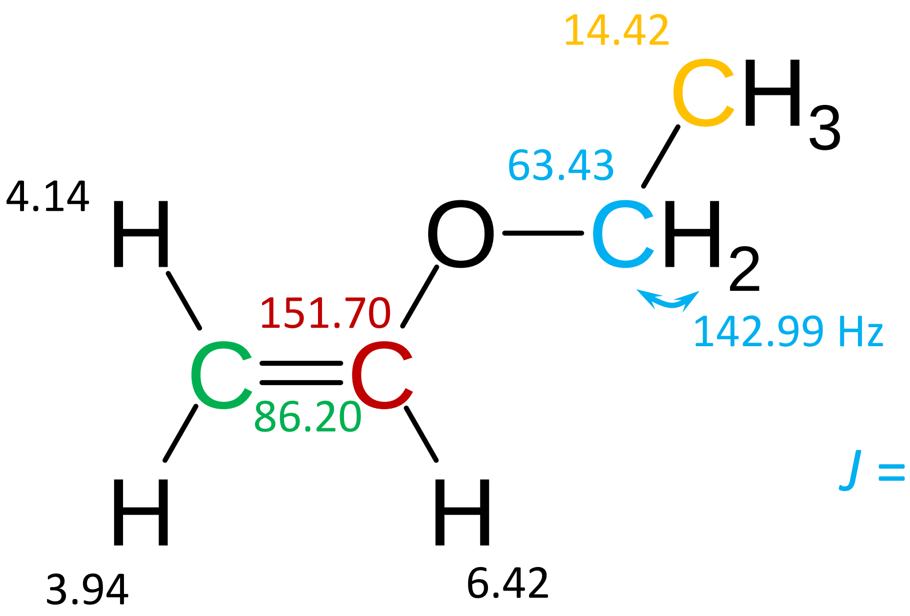


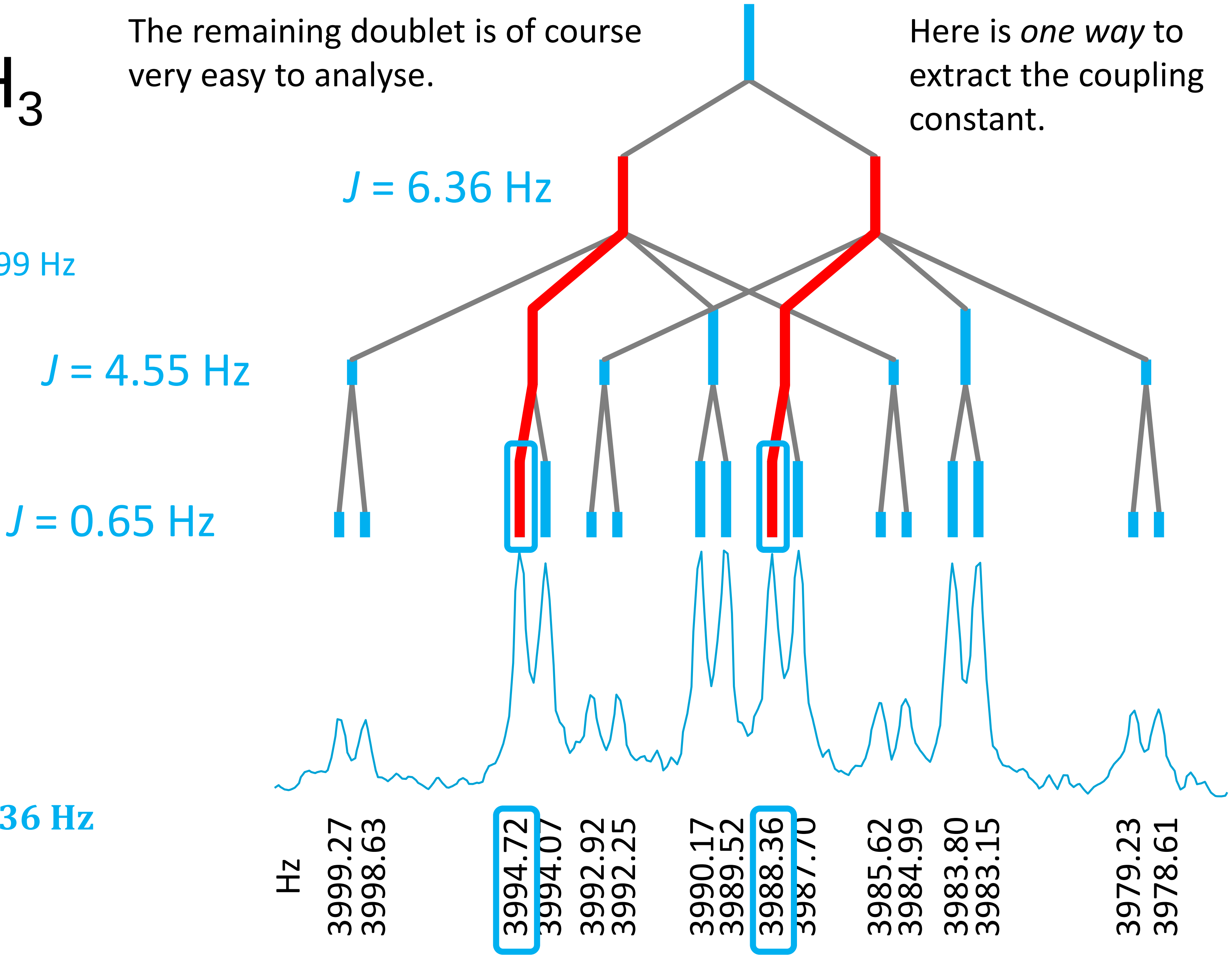
$$J = (3999.27\ \text{Hz} - 3985.62\ \text{Hz})/3 = \mathbf{4.55\ Hz}$$

Carbon multiplet detailed analysis

The remaining doublet is of course very easy to analyse.

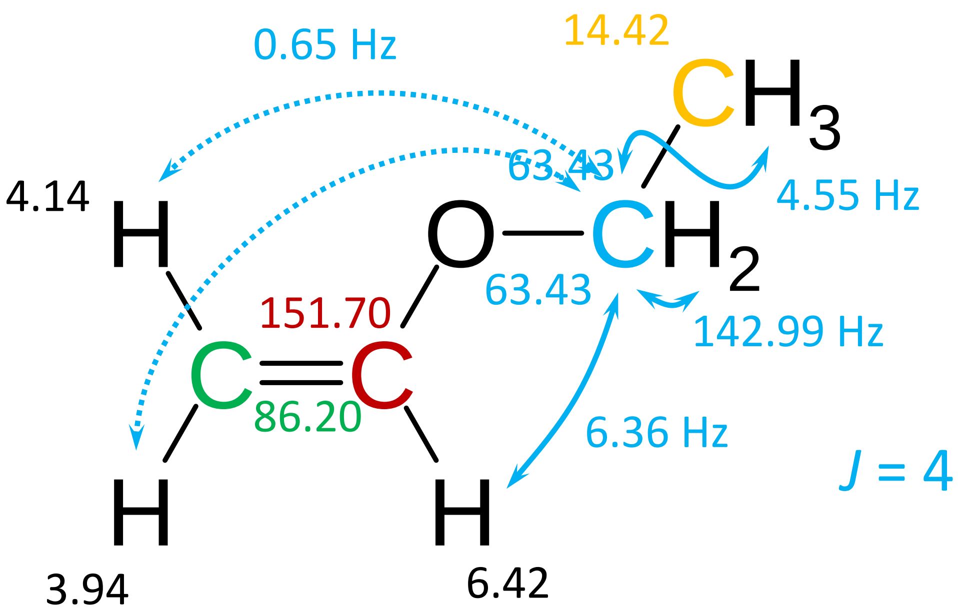
Here is *one way* to extract the coupling constant.

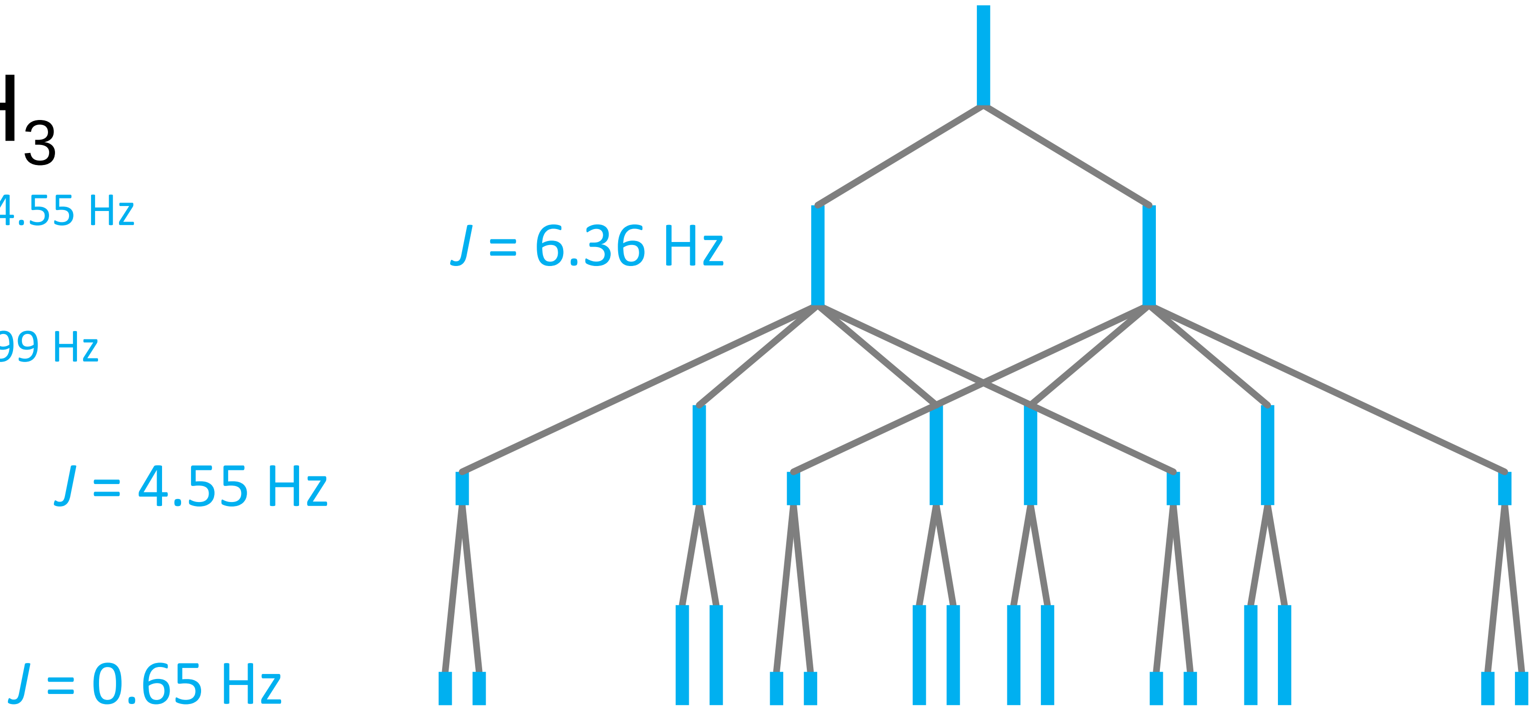




$$J = (3994.72\ \text{Hz} - 3988.36\ \text{Hz}) = \mathbf{6.36\ Hz}$$

Carbon multiplet detailed analysis





The assignment of the three coupling constants is not too difficult.

There is only one option for the quartet.

The source of the doublet with the coupling constant of **6.36 Hz** is one of three protons. Two of them are four bonds away from the carbon atom. **6.36 Hz** are extremely unlikely for such a 4-bond coupling constant.

The value of **0.65 Hz** *must be* a 4-bond coupling constant to one of the remaining two protons. Which of the two protons causes the splitting cannot be determined here.

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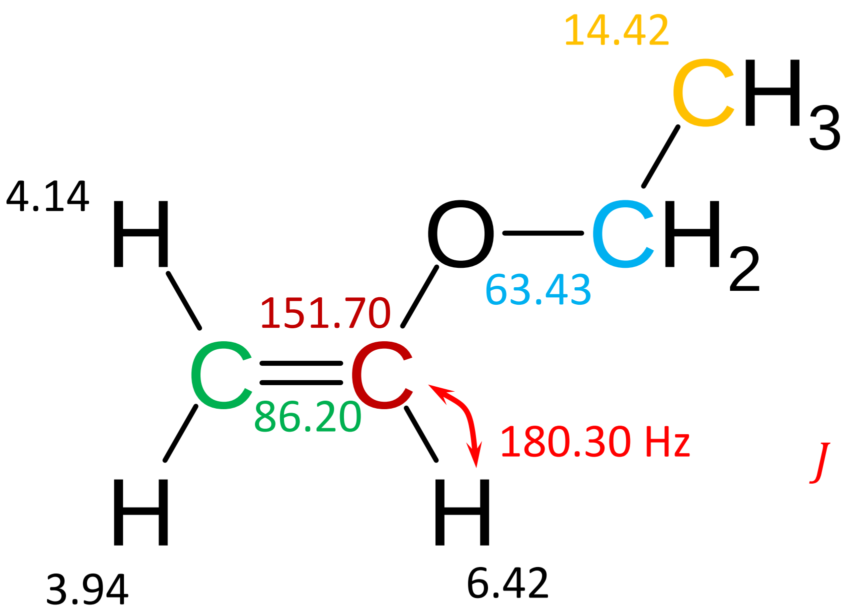

The basic structure of the multiplet of the carbon atom at 151.70 ppm is a doublet, caused by the proton at 6.42 ppm.

The coupling constant is determined from the difference of the mean value of the two partial multiplets with currently unknown fine structure.

$$J = \frac{(9639.42\ \text{Hz} + 9623.07\ \text{Hz})}{2} - \frac{(9459.10\ \text{Hz} - 9442.79\ \text{Hz})}{2} = \mathbf{180.30\ Hz}$$

To extract the other coupling constants, one of the two partial multiples is sufficient..

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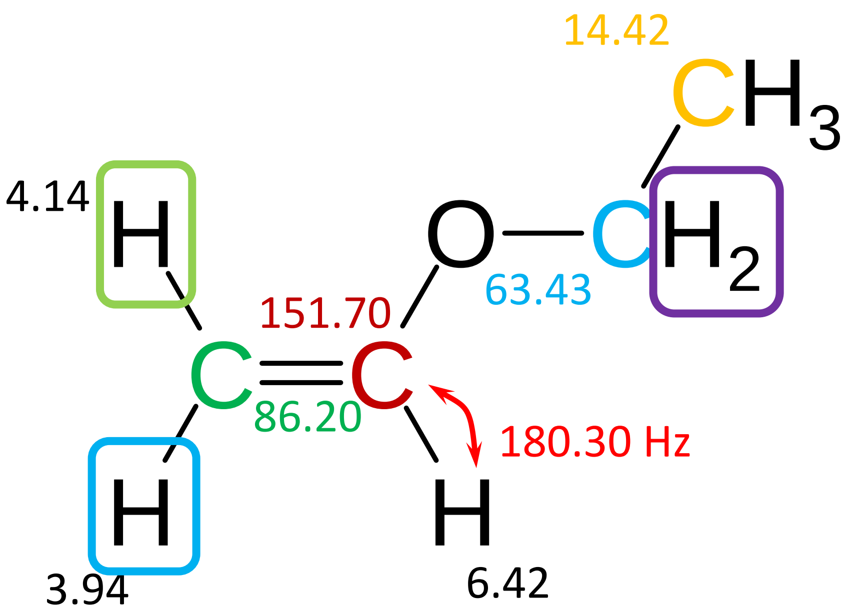


This partial multiplet should be an

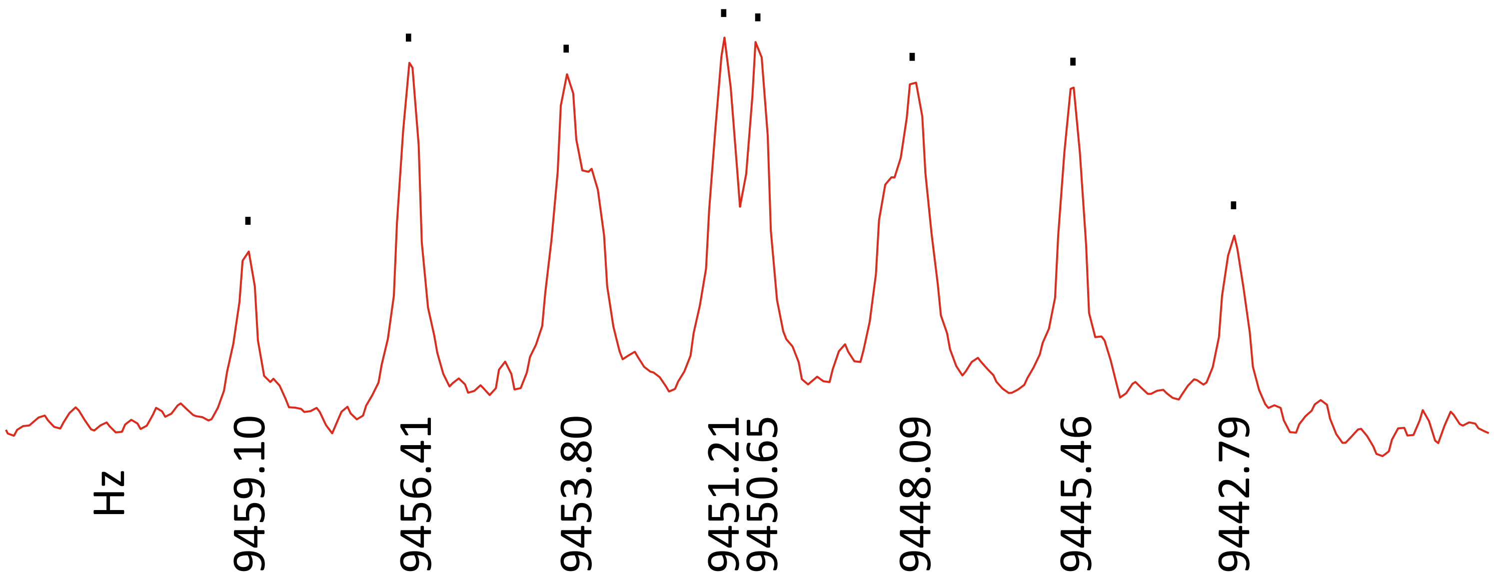
doublet

of doublets

of triplets

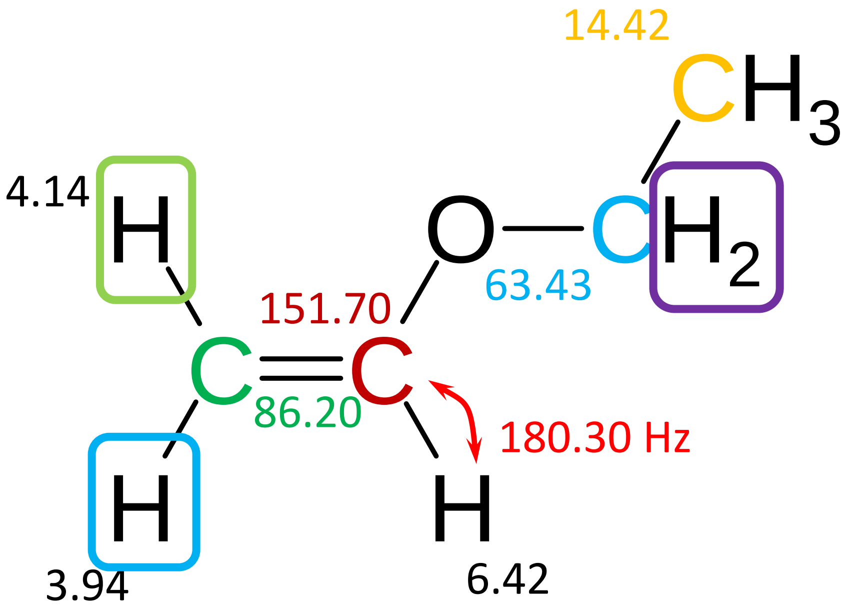
with alltogether 12 lines.

Eight of these lines are visible (ten, if you include two shoulders).



Translation in progress beyond this slide.

Analyse der Kohlenstoffmultipletts

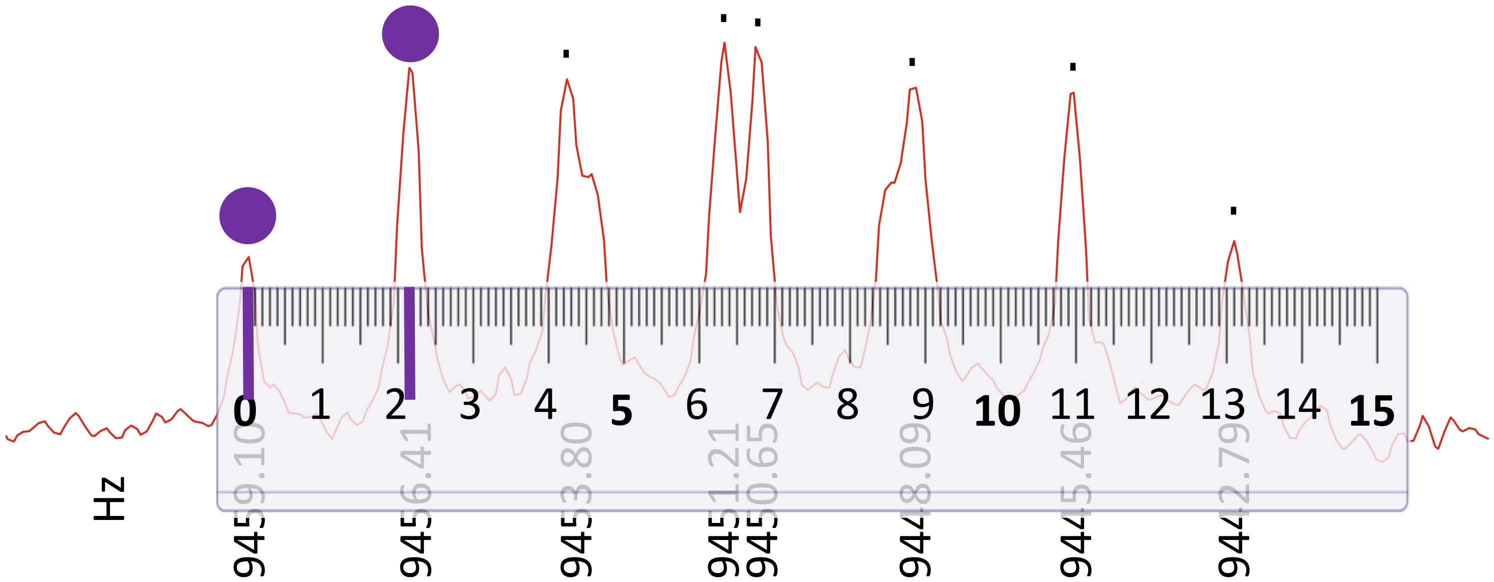


Am leichtesten sollte man eine Triplettstruktur erkennen können, vorausgesetzt, mindestens zwei der drei Linien des Tripletts zeigen keine Überlagerung mit anderen Linien.

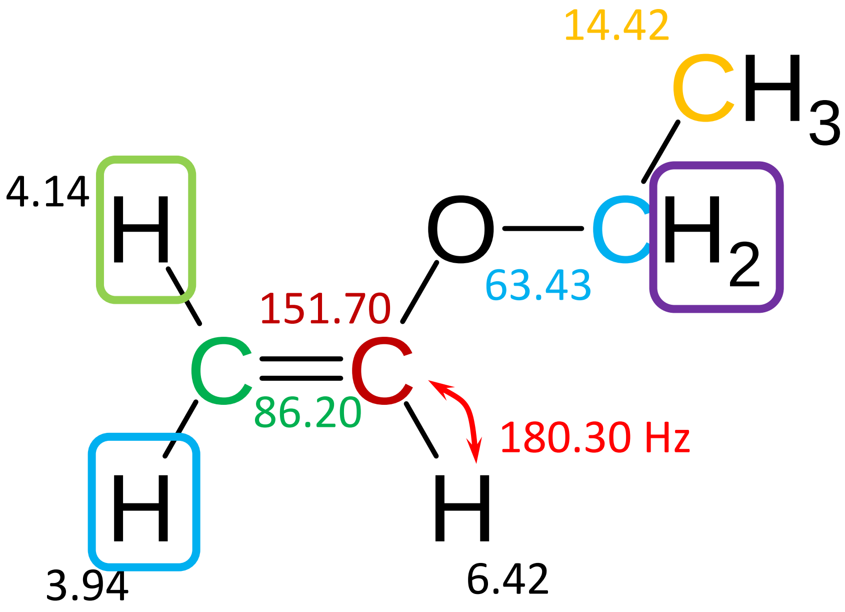
Zwei der Linien des Multipletts scheinen im Intensitätsverhältnis **1** : **2** vorzuliegen.

Markieren wir versuchsweise diese beiden Linien und markieren gleichzeitig die Differenz auf einem Lineal.

Finden wir durch Verschieben des Lineals die dritte Linie des Tripletts? Versuchen wir es einfach.



Analyse der Kohlenstoffmultipletts



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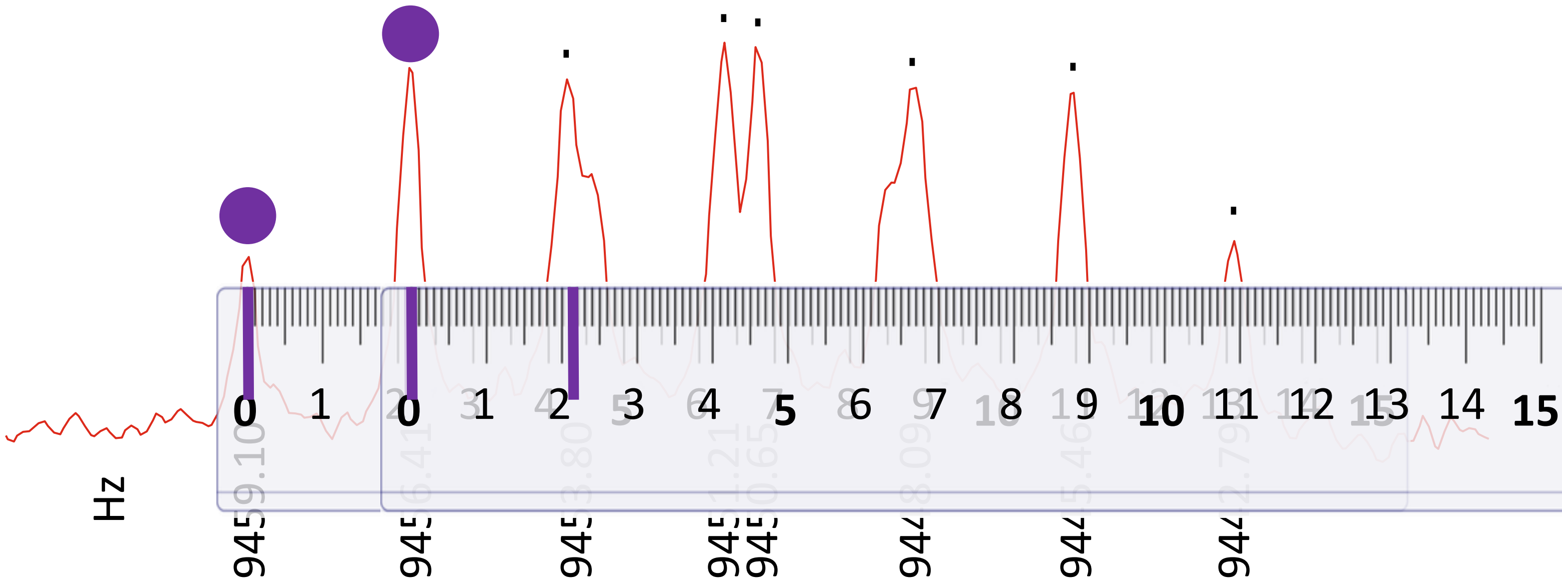
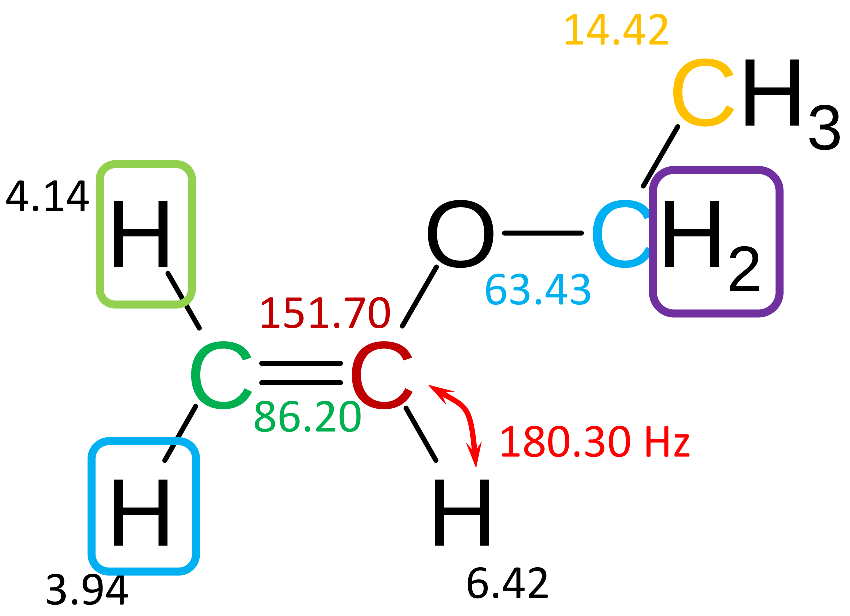


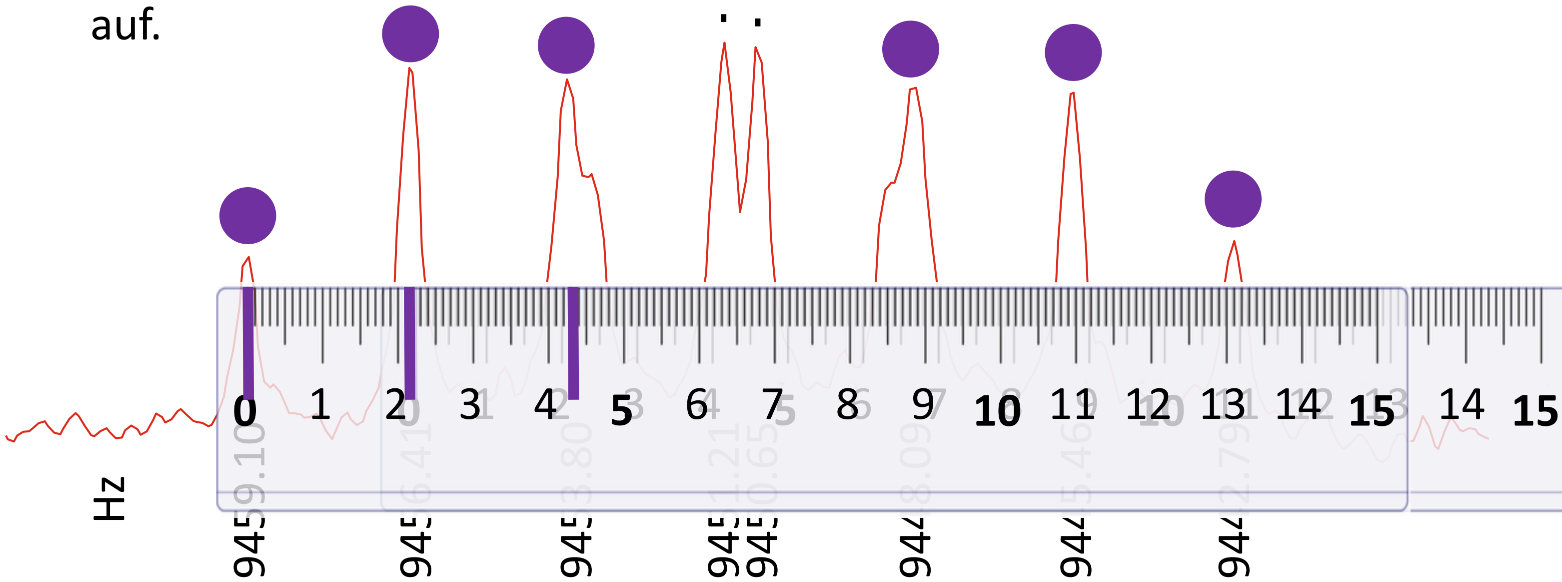
Analyse der Kohlenstoffmultipletts



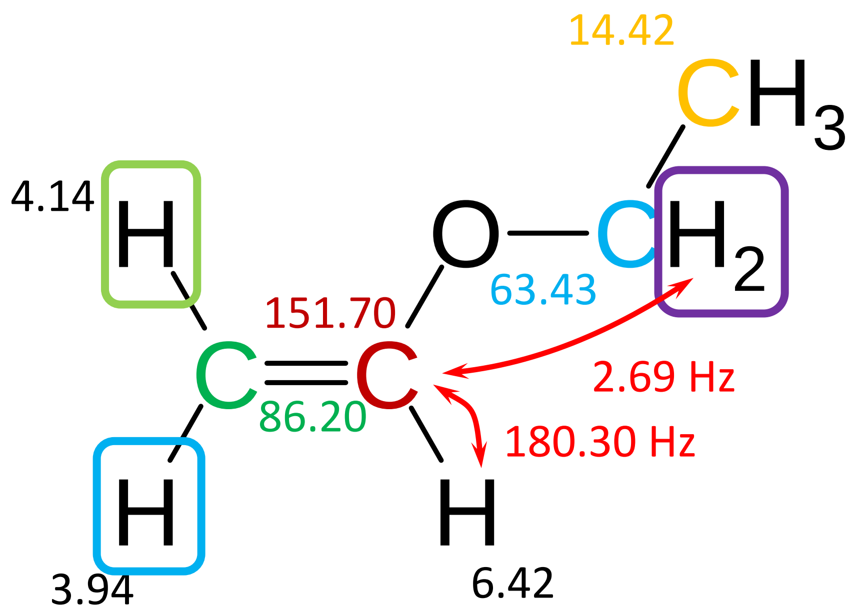
Die dritte Linie unseres Tripletts könnte sich in diesem Bereich überlagerter Linien verbergen.

Setzen wir eine Markierung und markieren anschließend das komplette Triplett auf dem Lineal.

Die gleiche Struktur finden wir auf der rechten Seite des Multipletts noch einmal. Wir können jetzt aus beiden Tripletts die Linie rekonstruieren, aus der durch Koplung mit den Methylenprotonen die Triplettstruktur entsteht. Das Lineal mit den drei Markierungen heben wir für eine spätere Verwendung auf.



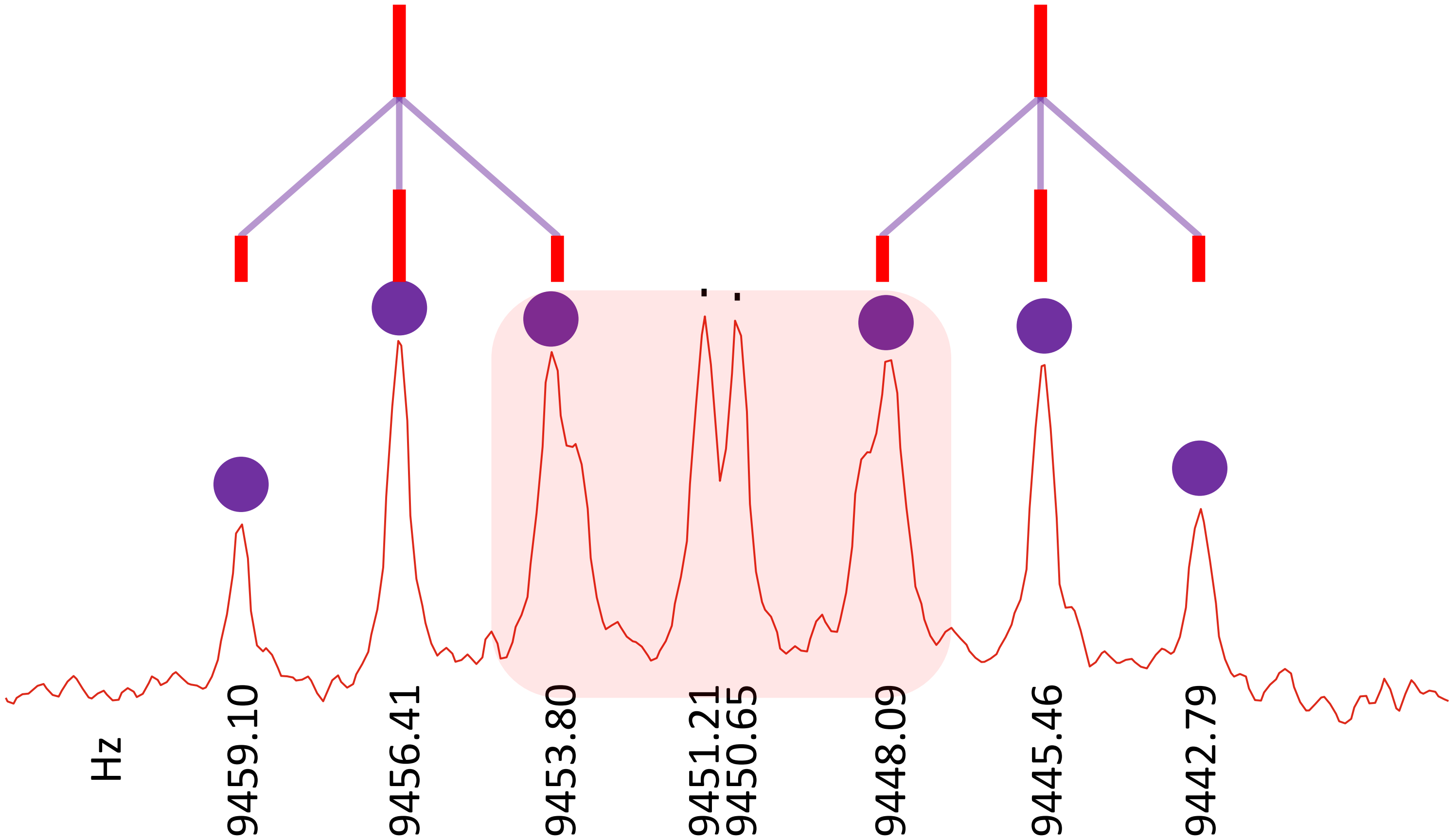
Analyse der Kohlenstoffmultipletts



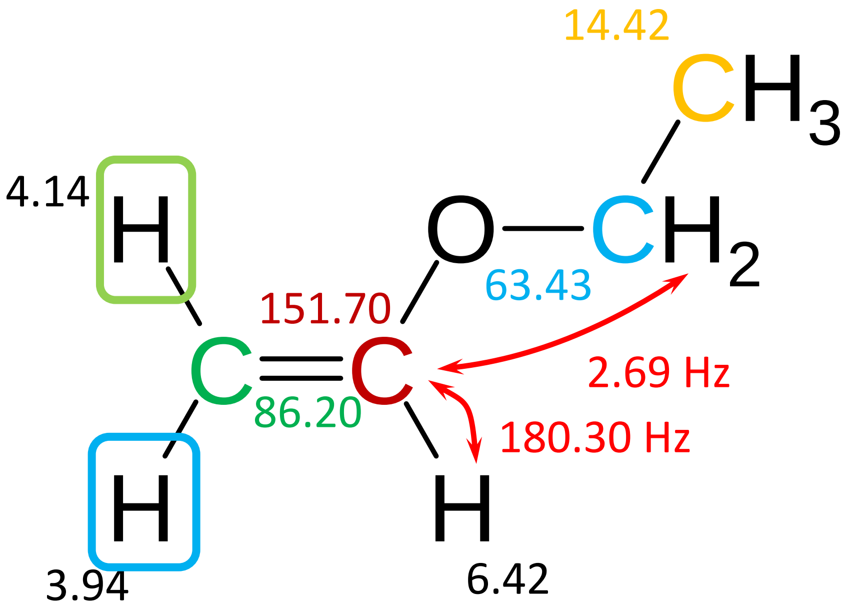
J = 9459.10 Hz – 9456.41 Hz = **2.69 Hz**

Um das theoretisch vorausgesagte Dublett von Dubletts von Tripletts zu erhalten, müssten sich in dem Multiplett noch zwei weitere Tripletts verstecken.

Hierfür kommt nur der markierte Bereich des Multipletts in Frage.
Die Linien außerhalb des Bereiches werden mit sehr hoher Sicherheit durch die bereits gefundenen Tripletts vollständig erklärt.



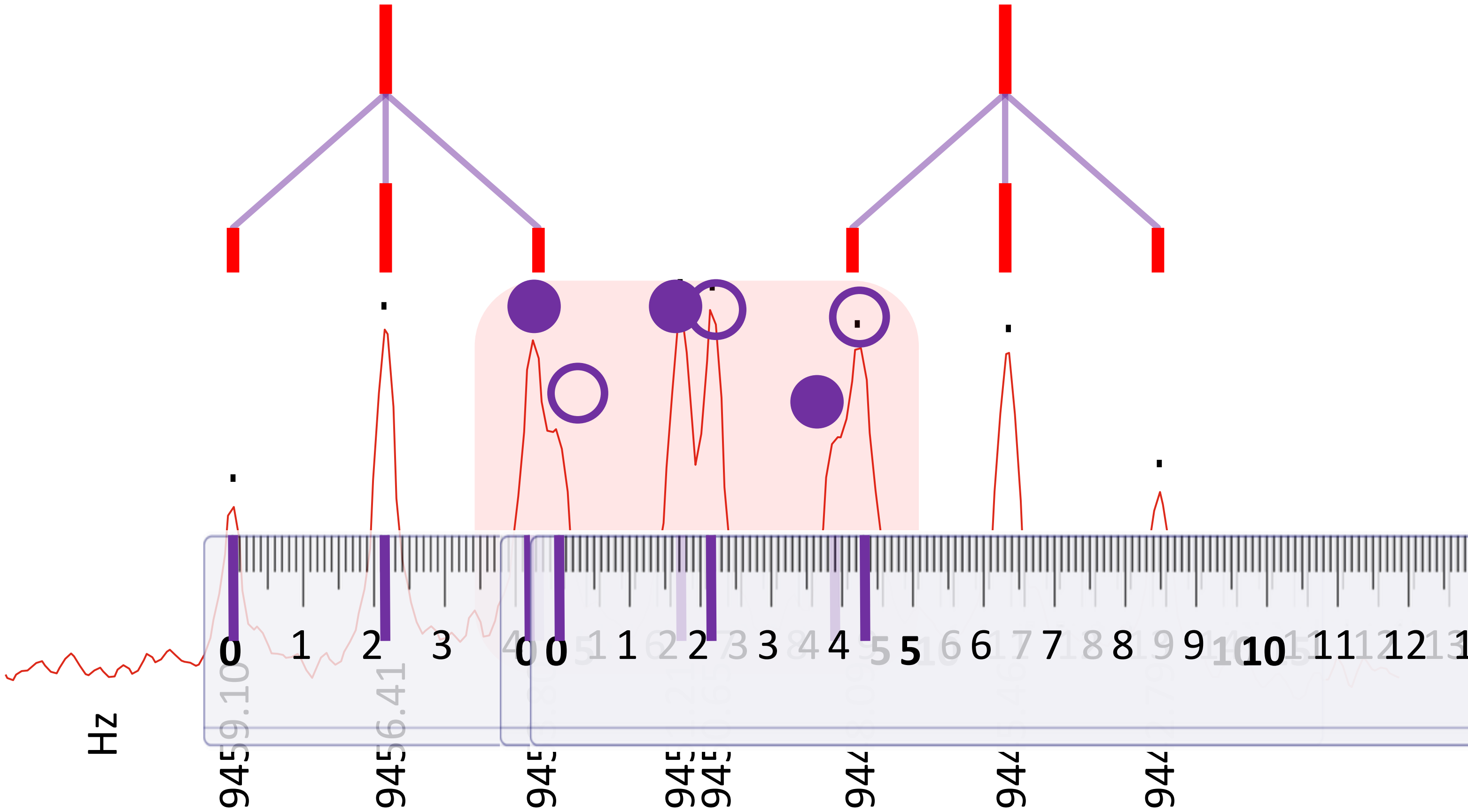
Analyse der Kohlenstoffmultipletts



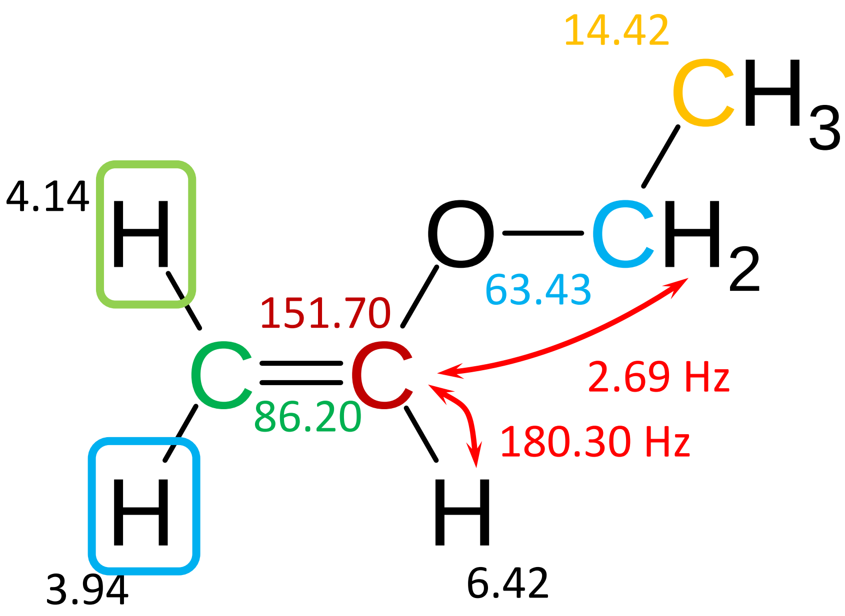
Probieren wir es wieder mit dem Lineal, auf dem bereits die drei Linien des Tripletts markiert sind.

Hier scheint sich ein Triplett zu befinden.

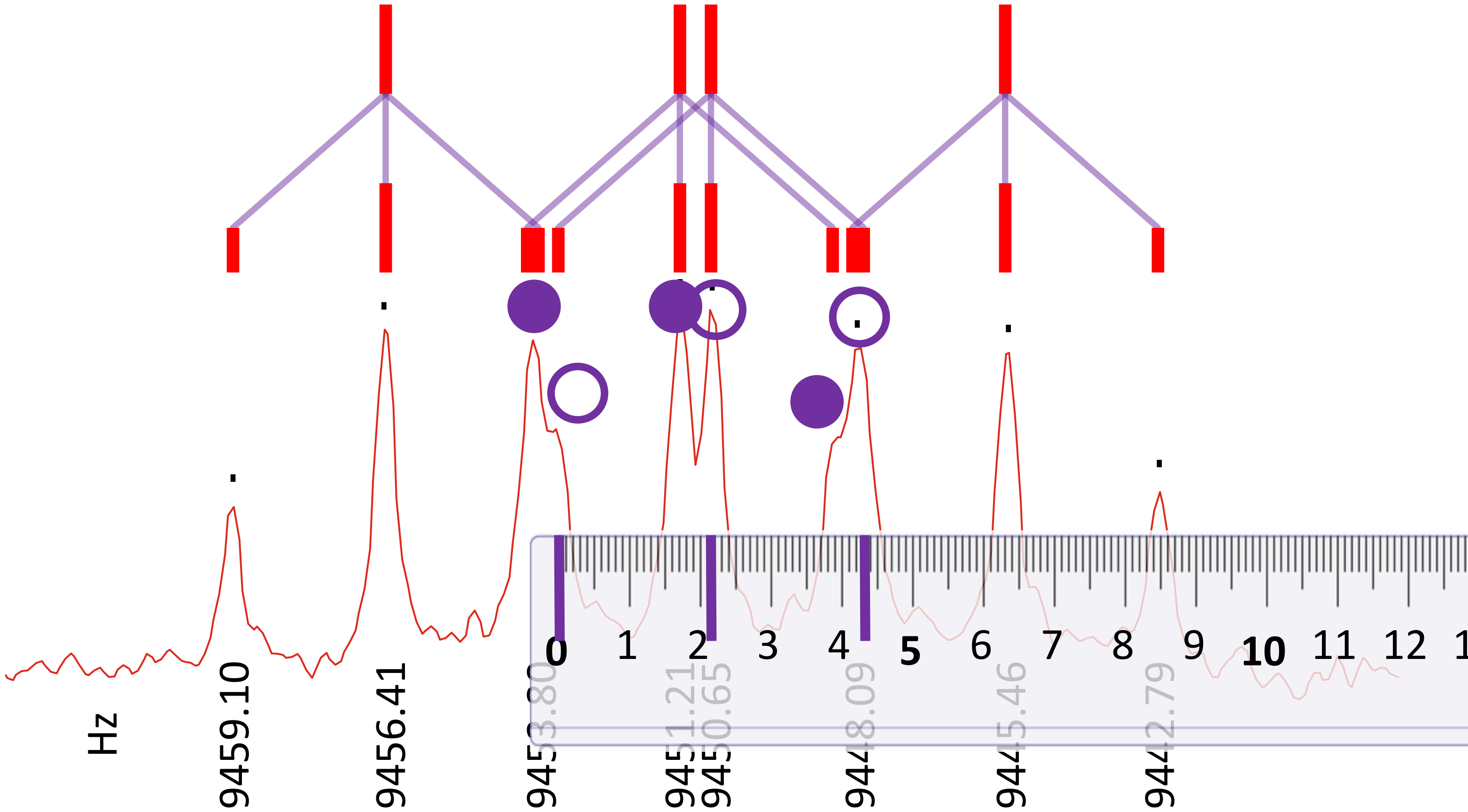
Und hier ein weiteres Triplett.



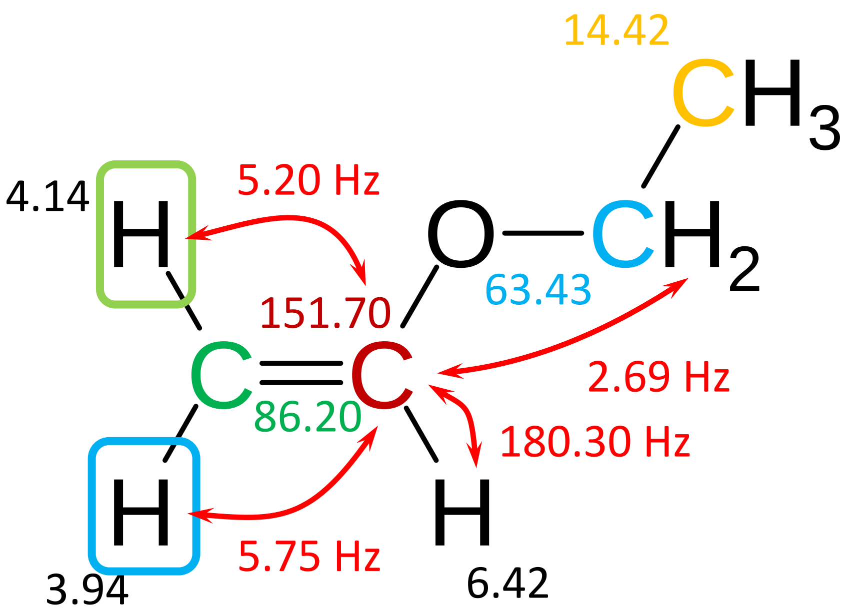
Analyse der Kohlenstoffmultipletts

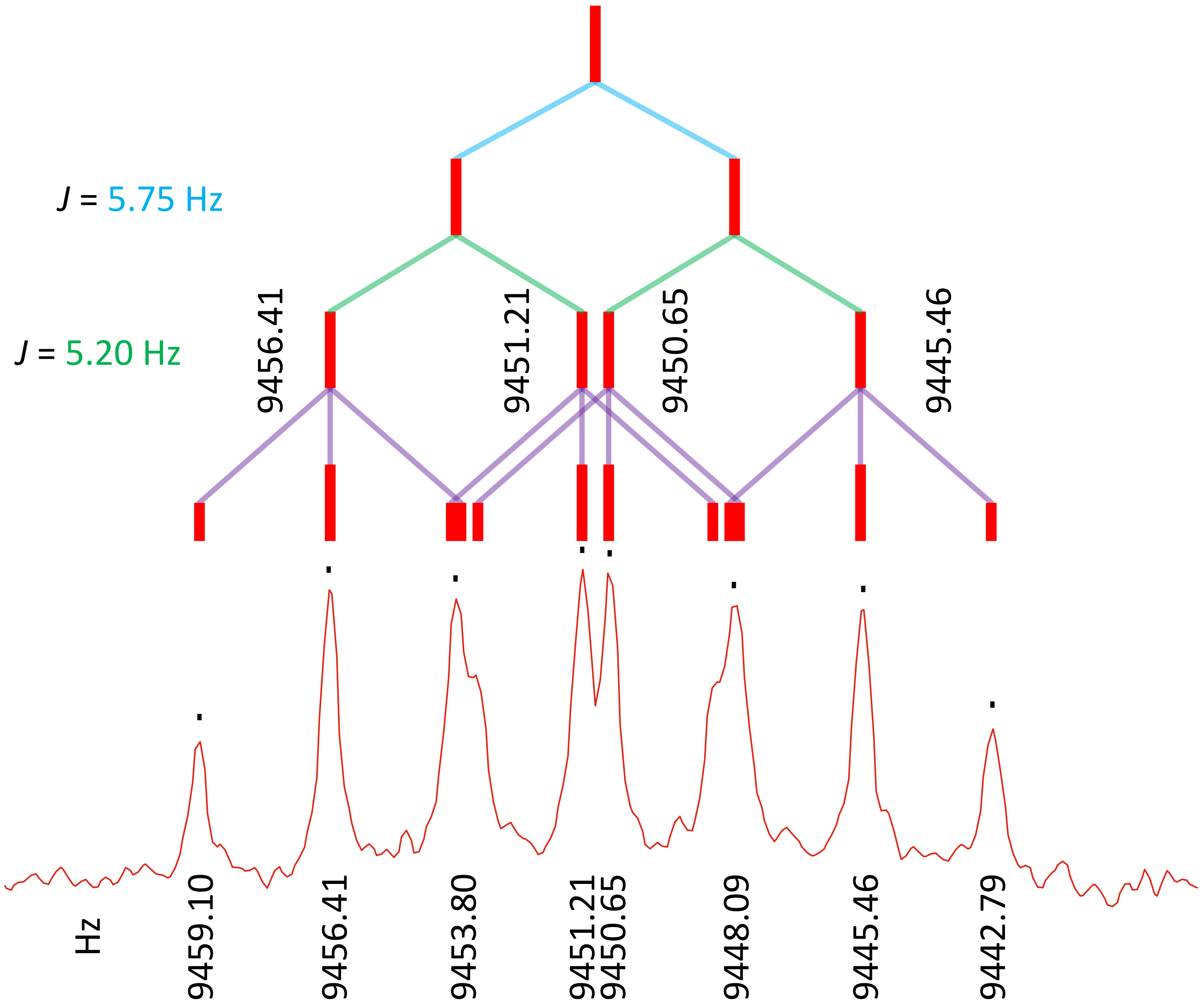


Nur für die mittlere Linie der beiden Tripletts beobachtet man keine Überlagerung. Eine Kopplungskonstante kann hier nicht gemessen werden, die ist allerdngs auch bereits bekannt.



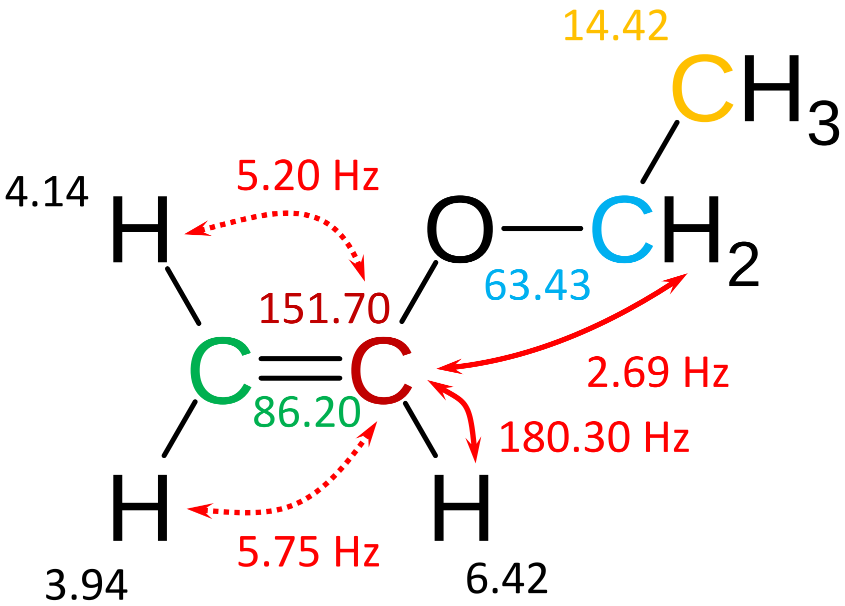
Analyse der Kohlenstoffmultipletts

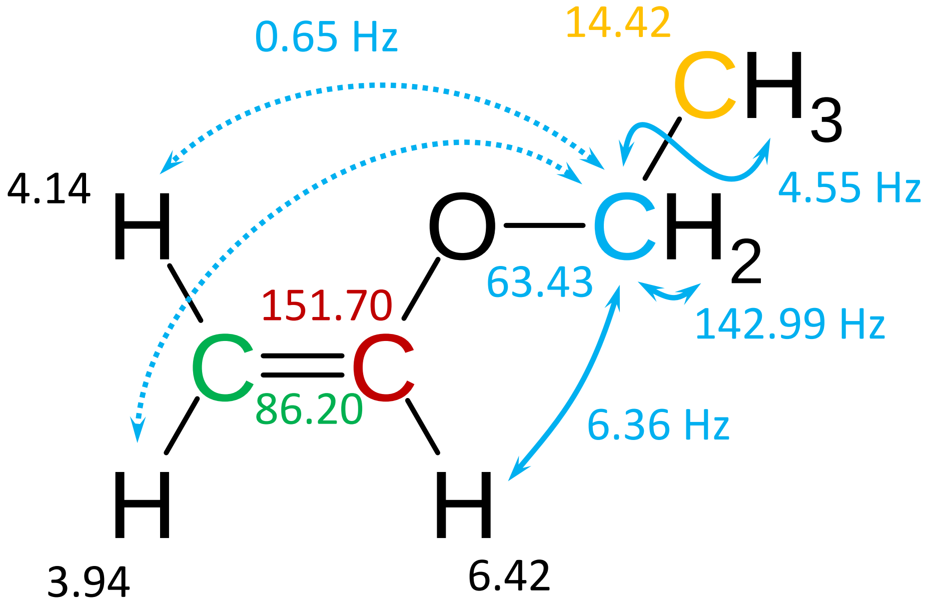


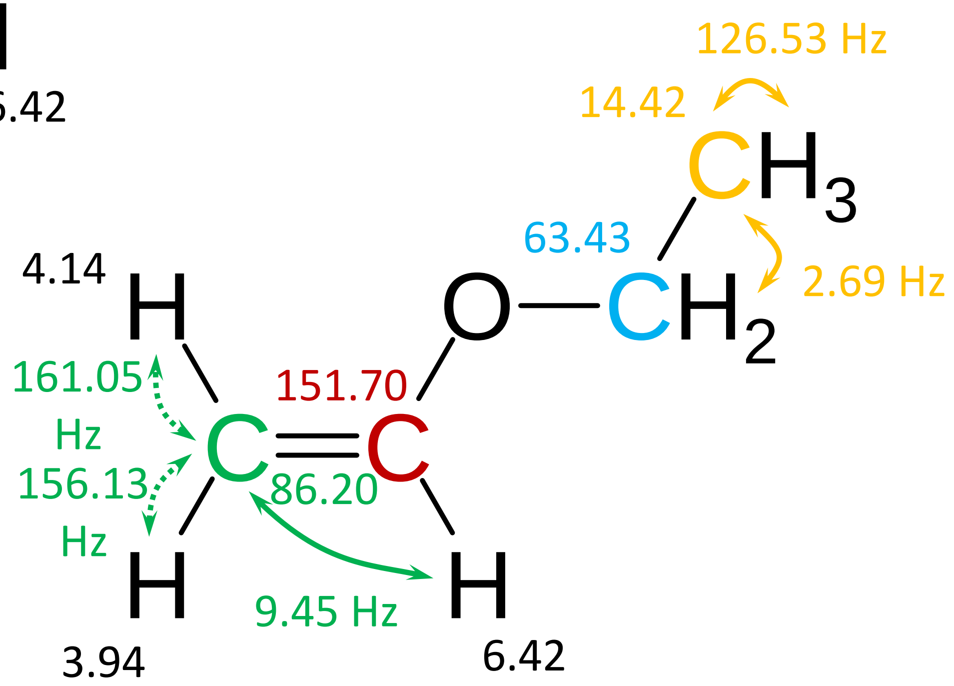


Die Analyse des verbleibenden Dubletts von Dubletts ist jetzt einfach.
Die nötigen chemischen Verschiebungen können ohne Rechnung direkt dem Multiplett entnommen werden.

Carbon chemical shifts and carbon proton coupling constants

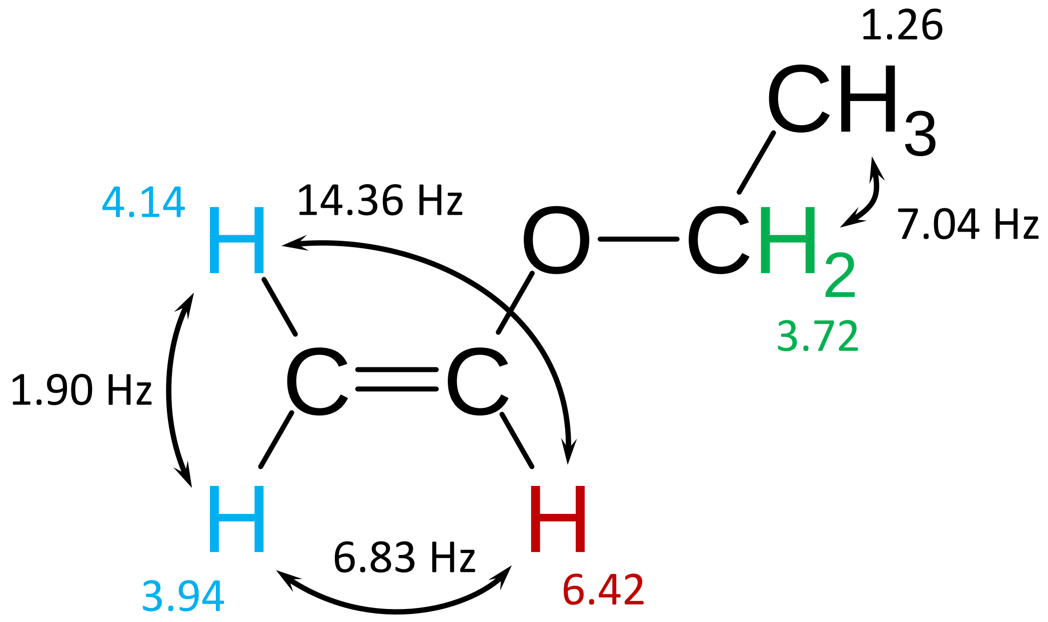






(Bei den gestrichelten Linien ist die Zuordnung nicht eindeutig.)

Proton chemical shifts and proton proton coupling constants



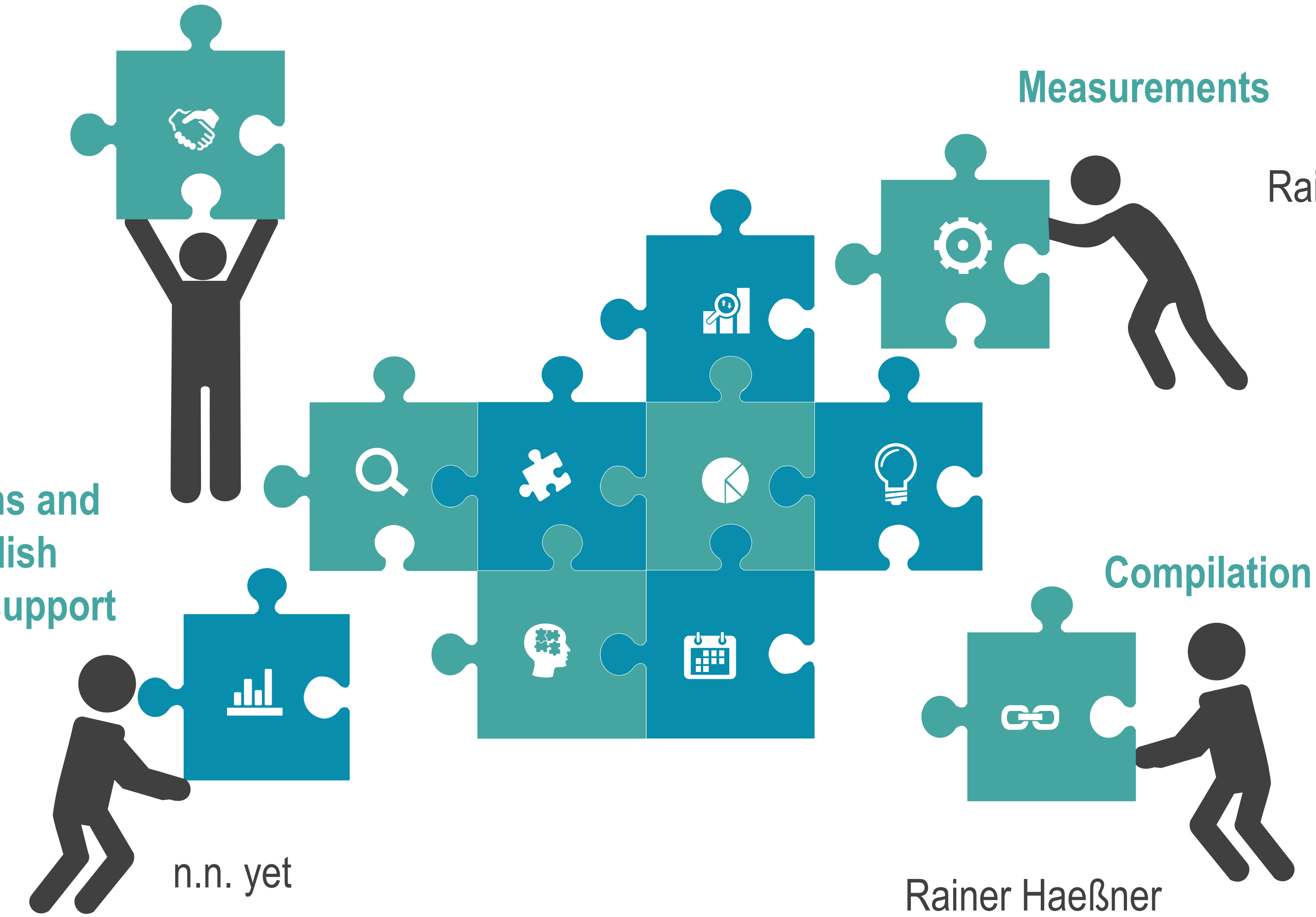
Contributions

Spectrometer time

TU Munich

Measurements

Rainer Haeßner



Discussions and native English language support

n.n. yet

Compilation

Rainer Haeßner

More exercises …