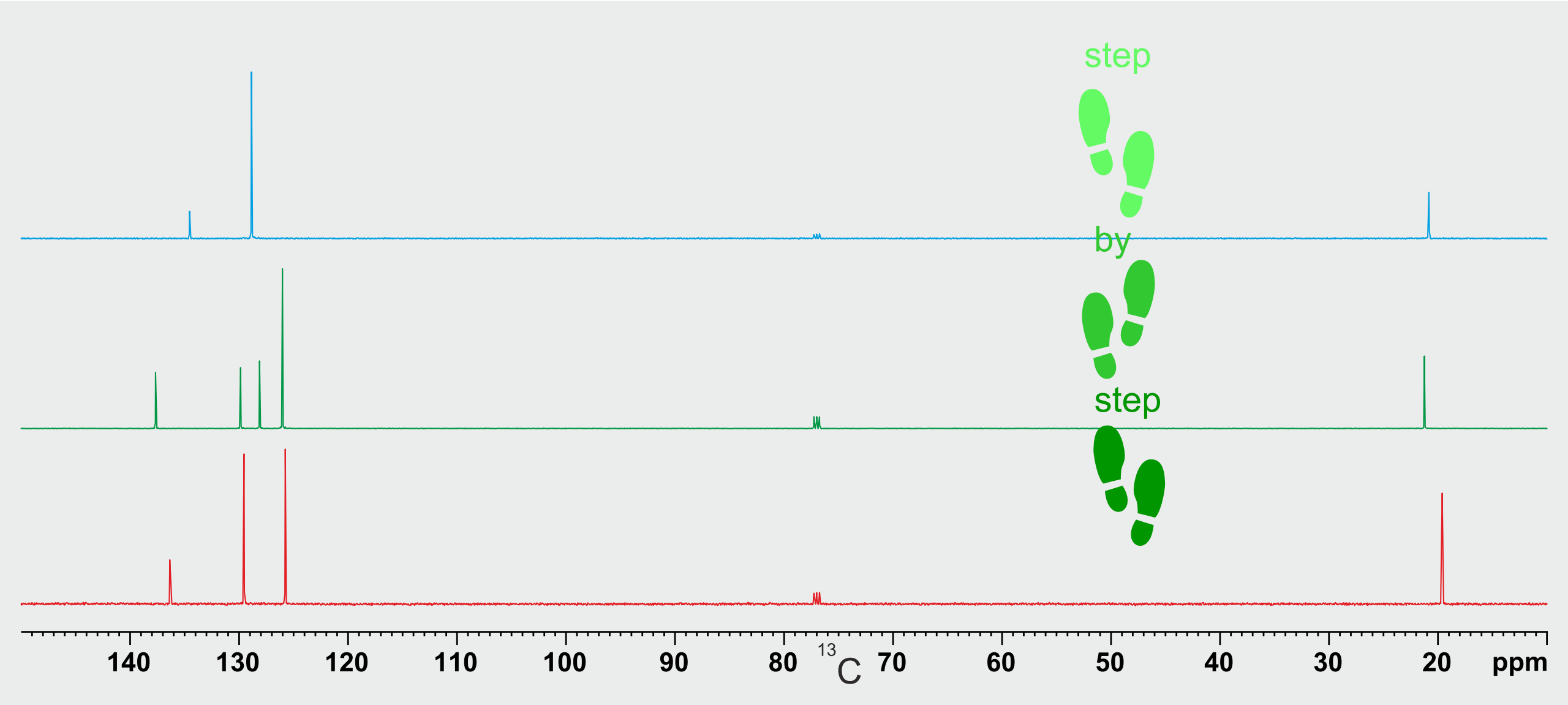
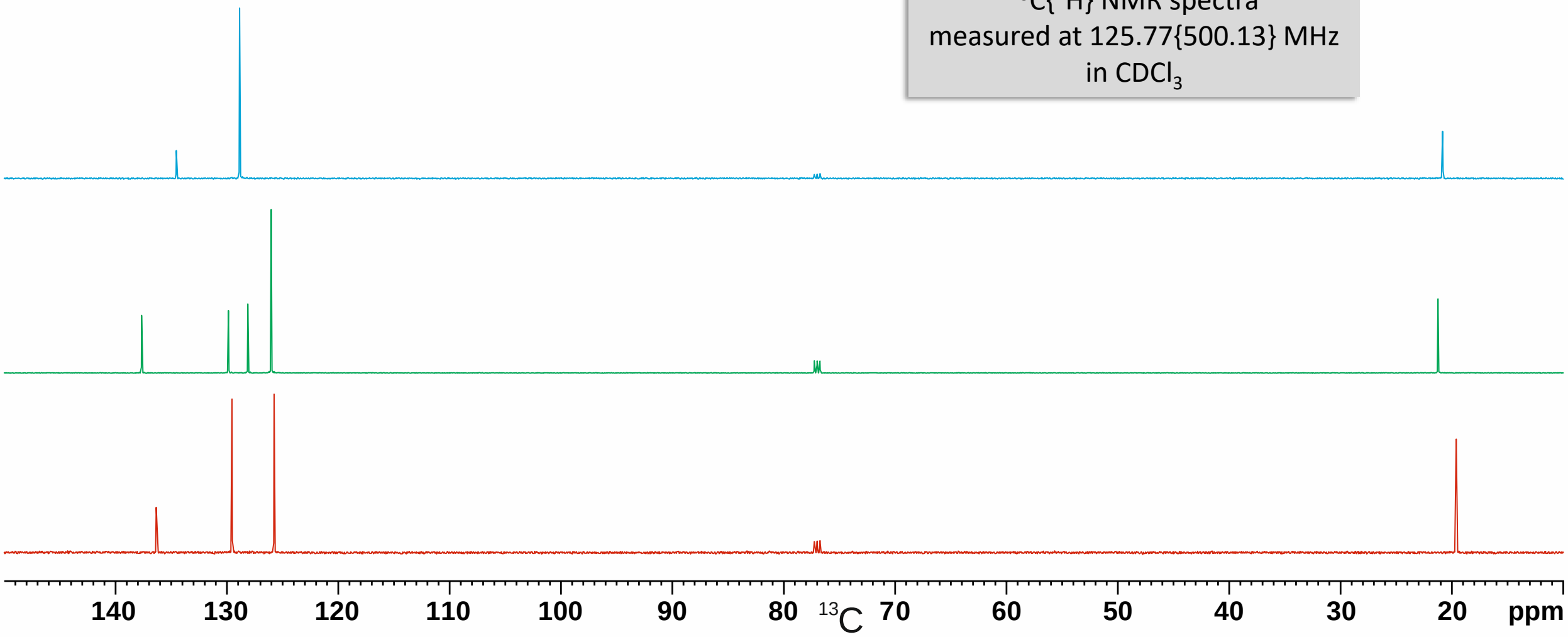
Exercise plus Solution – Quick PDF overview

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.

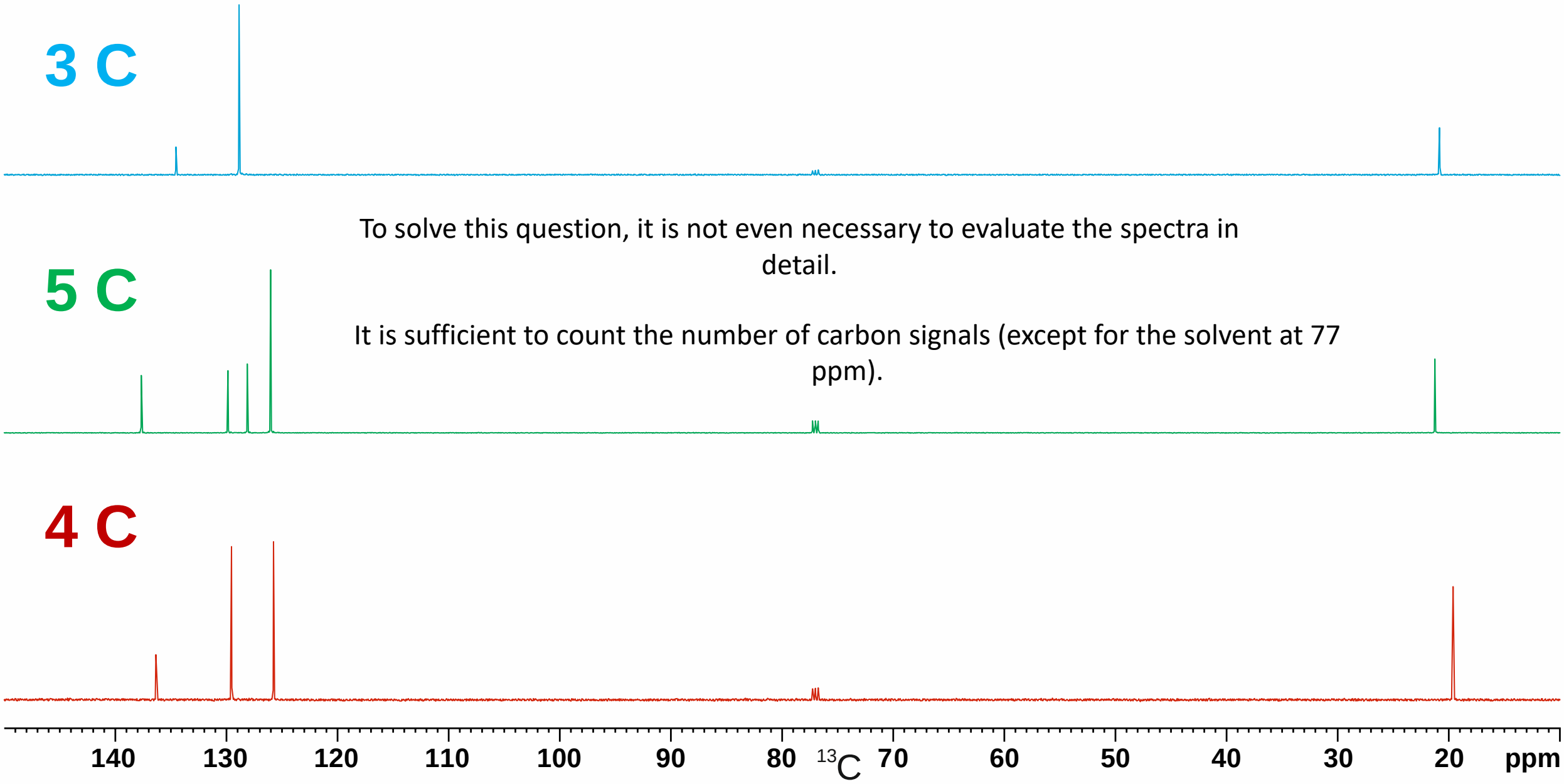


Which ^{13}C NMR spectrum belongs to which of the three isomeric xylenes?

$^{13}C\{^{1}H\}$ NMR spectra
measured at 125.77{500.13} MHz
in $CDCl_3$



KISS (Keep it simple and straightforward)



To solve this question, it is not even necessary to evaluate the spectra in detail.

It is sufficient to count the number of carbon signals (except for the solvent at 77 ppm).

o-Xylene

3 C

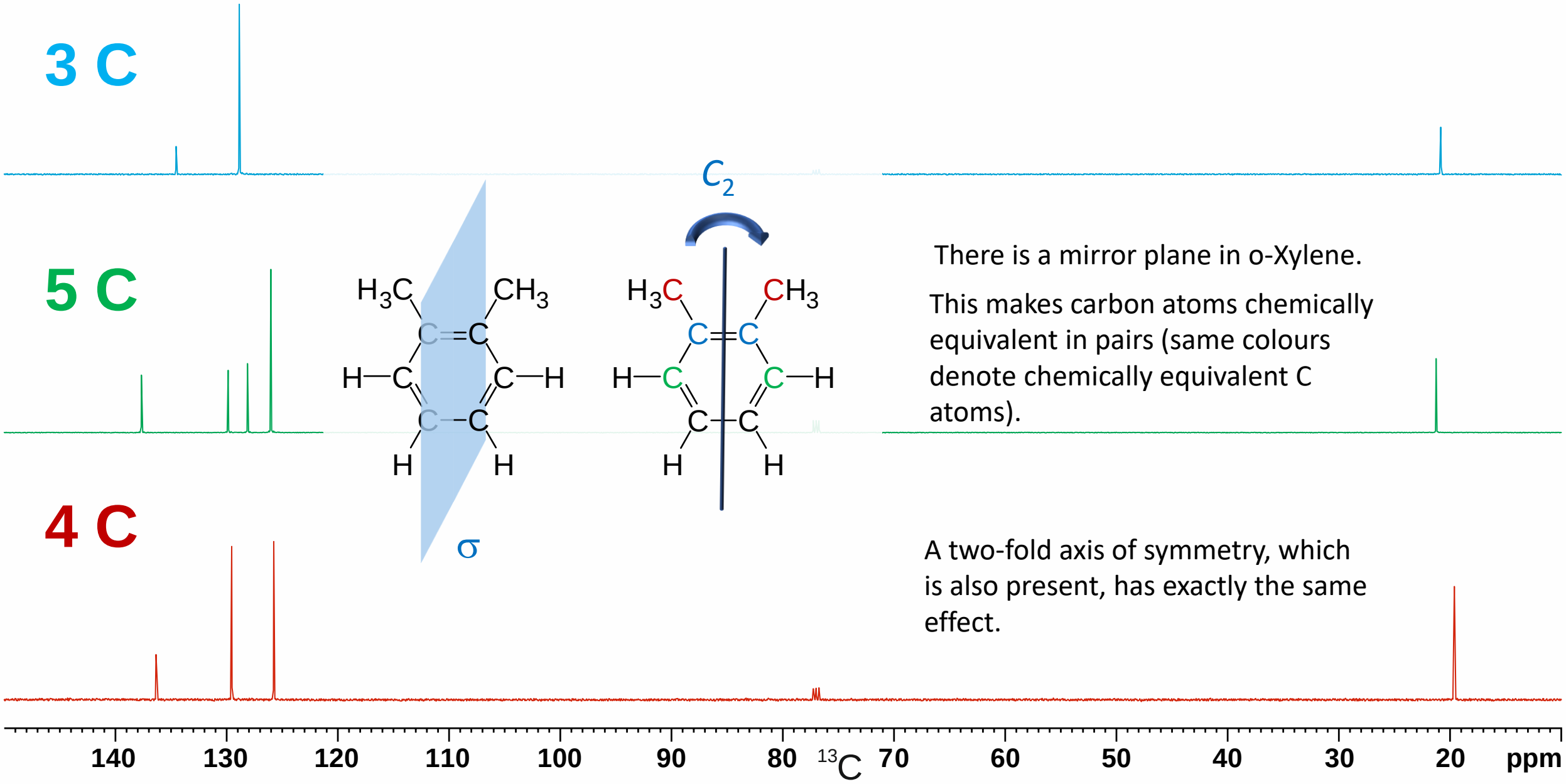
5 C

4 C

There is a mirror plane in o-Xylene.

This makes carbon atoms chemically equivalent in pairs (same colours denote chemically equivalent C atoms).

A two-fold axis of symmetry, which is also present, has exactly the same effect.

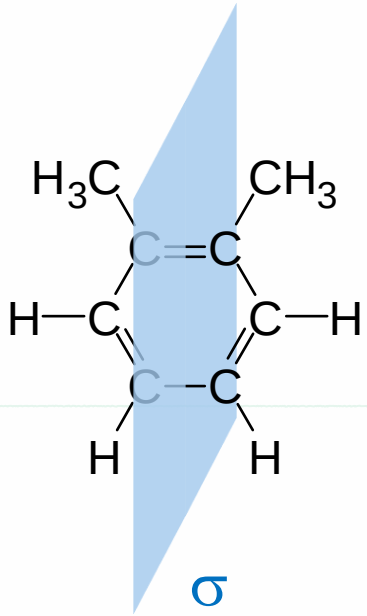


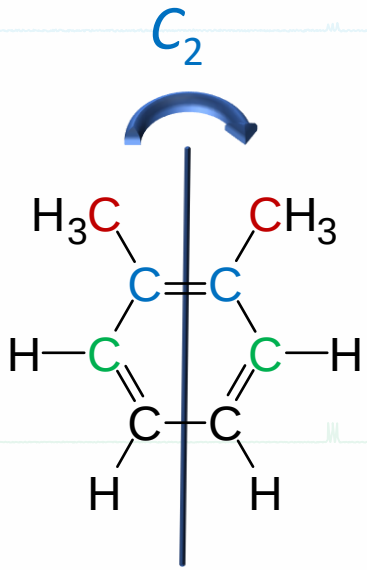
o-Xylene

3 C

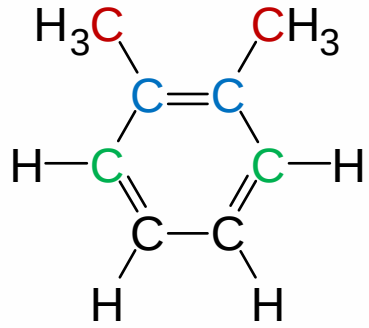
5 C

4 C





o-Xylene has 4 distinguishable carbon atoms.



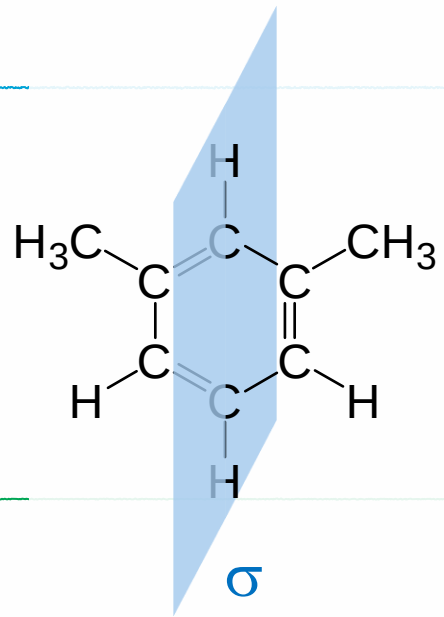
140 130 120 110 100 90 80 ^{13}C 70 60 50 40 30 20 ppm

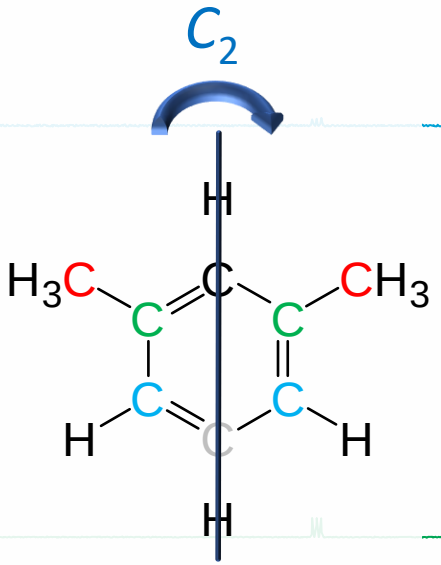
m-Xylene

3 C

5 C

4 C

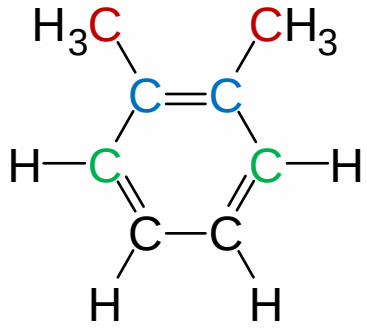




There is a mirror plane in m-Xylene as well.

This makes carbon atoms chemically equivalent in pairs (same colours denote chemically equivalent C atoms).

And like o-Xylene, m-Xylene too has a two-fold axis of symmetry, which make the same carbon atoms identical like the mirror plane.



140 130 120 110 100 90 80 ^{13}C 70 60 50 40 30 20 ppm

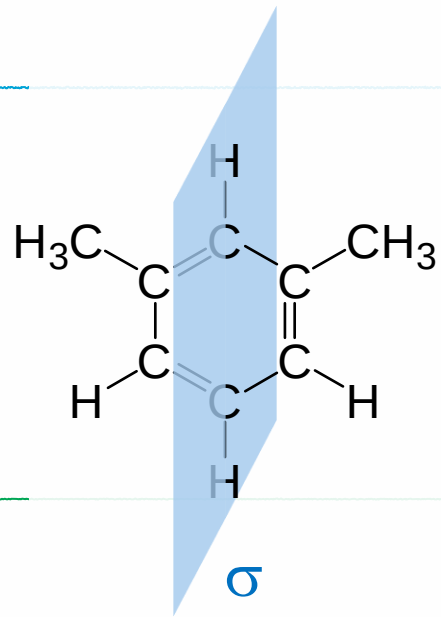
m-Xylene

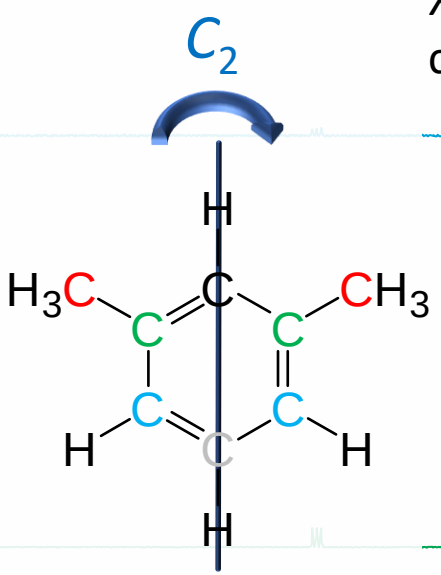
3 C

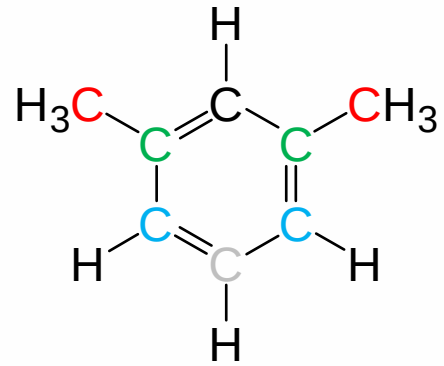
5 C

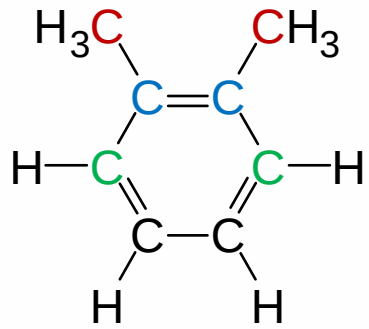
4 C

Because of the 30° rotated position of the symmetry elements compared to o-Xylene, m-Xylene has 5 distinguishable carbon atoms.









140 130 120 110 100 90 80 ^{13}C 70 60 50 40 30 20 ppm

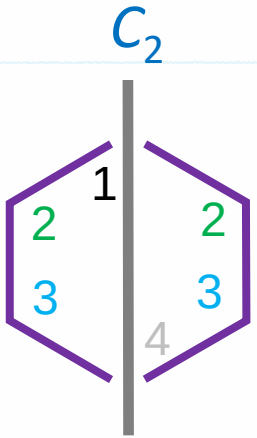
m-Xylene

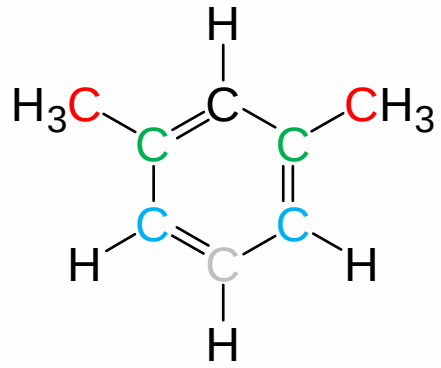
3 C

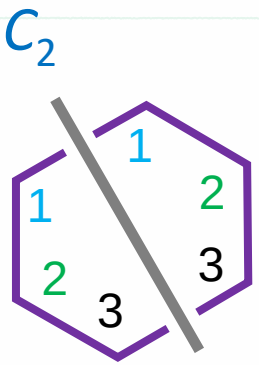
5 C

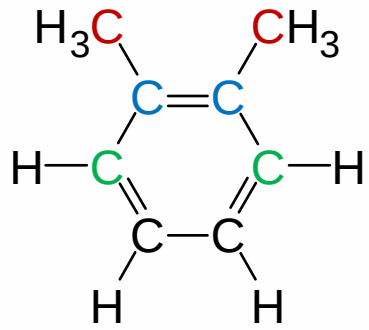
4 C

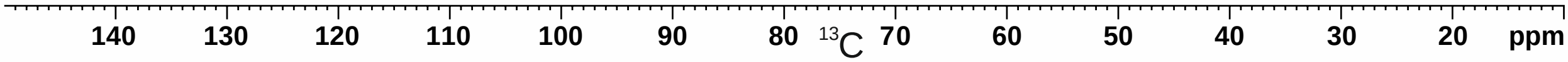
To understand the effect of the symmetry elements rotated by 30 degrees, this hexagon with a two-fold rotation axes might be helpful.











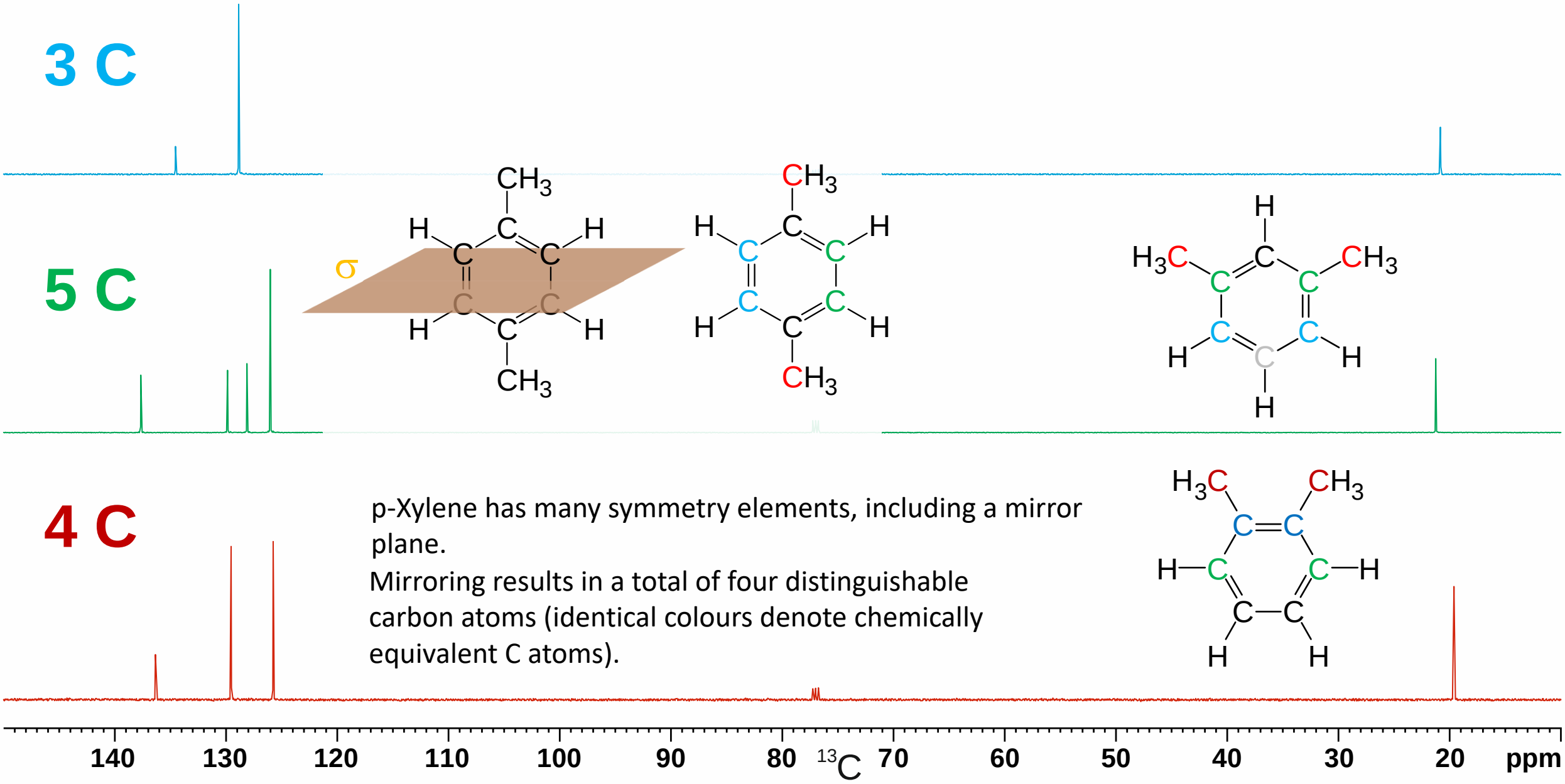
p-Xylene

3 C

5 C

4 C

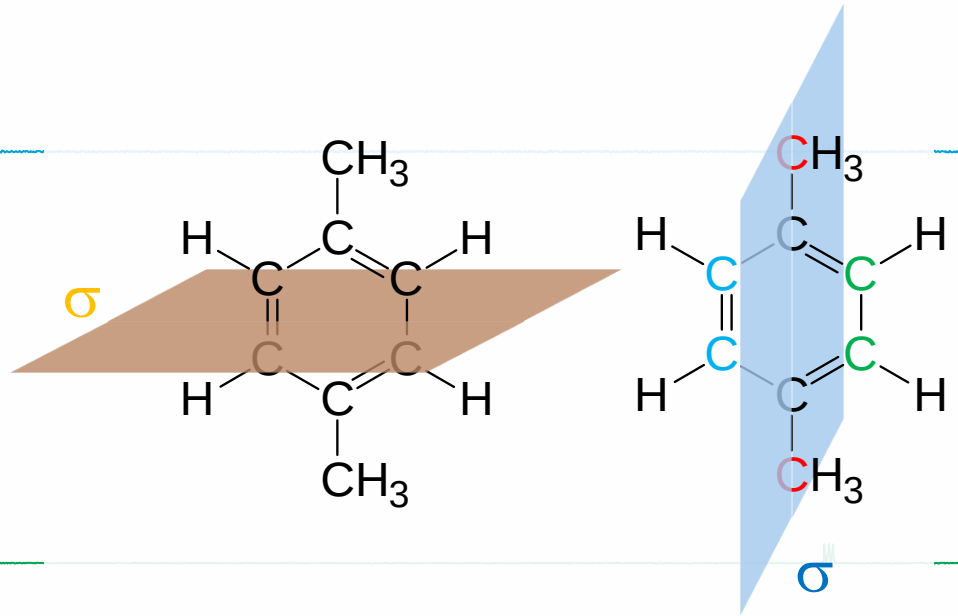
p-Xylene has many symmetry elements, including a mirror plane.
Mirroring results in a total of four distinguishable carbon atoms (identical colours denote chemically equivalent C atoms).

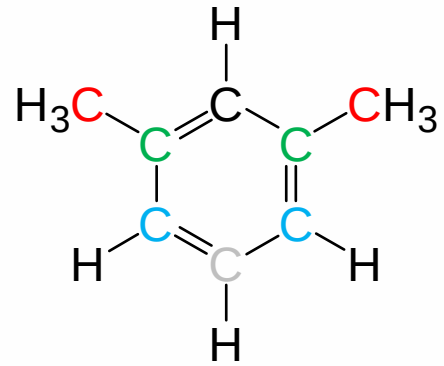


p-Xylene

3 C

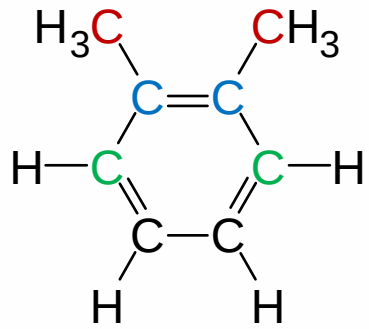
5 C

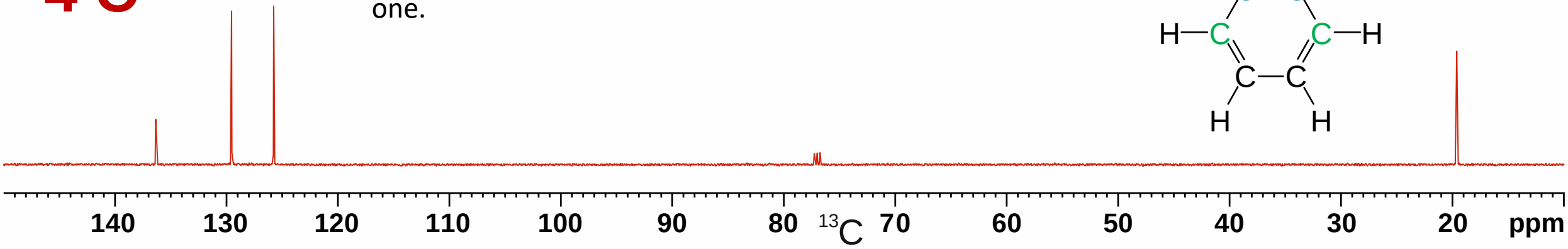




4 C

Another mirror plane is arranged perpendicular to the first one.

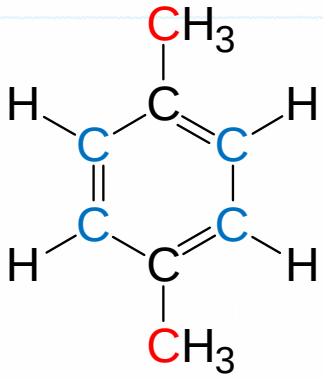


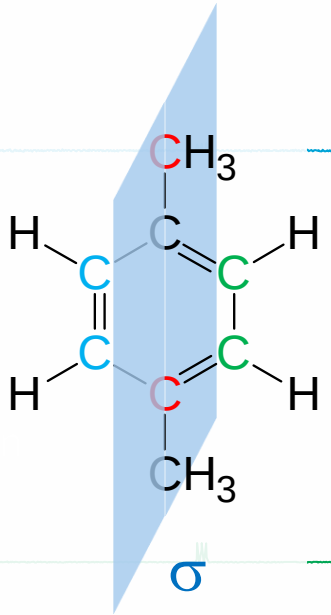


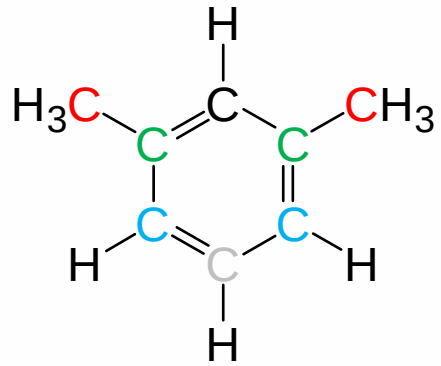
p-Xylene

3 C

5 C



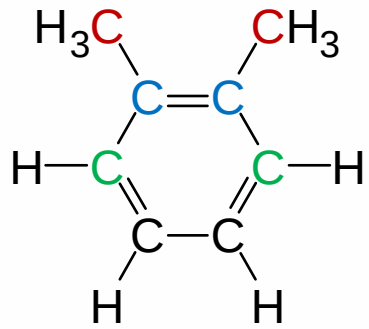


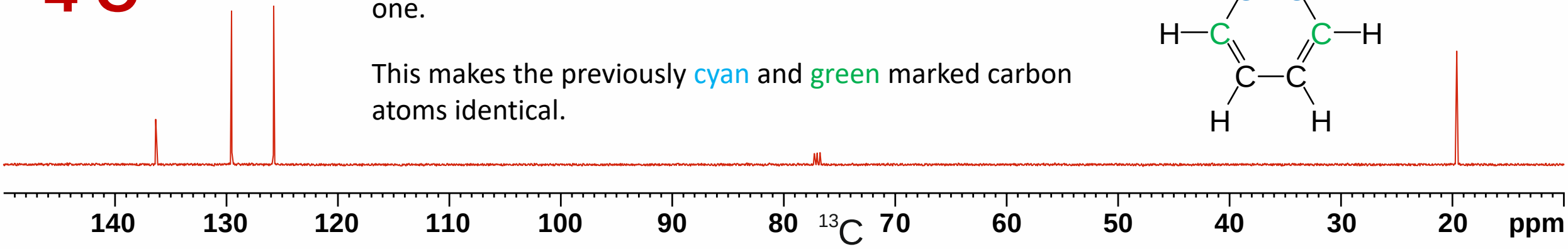


4 C

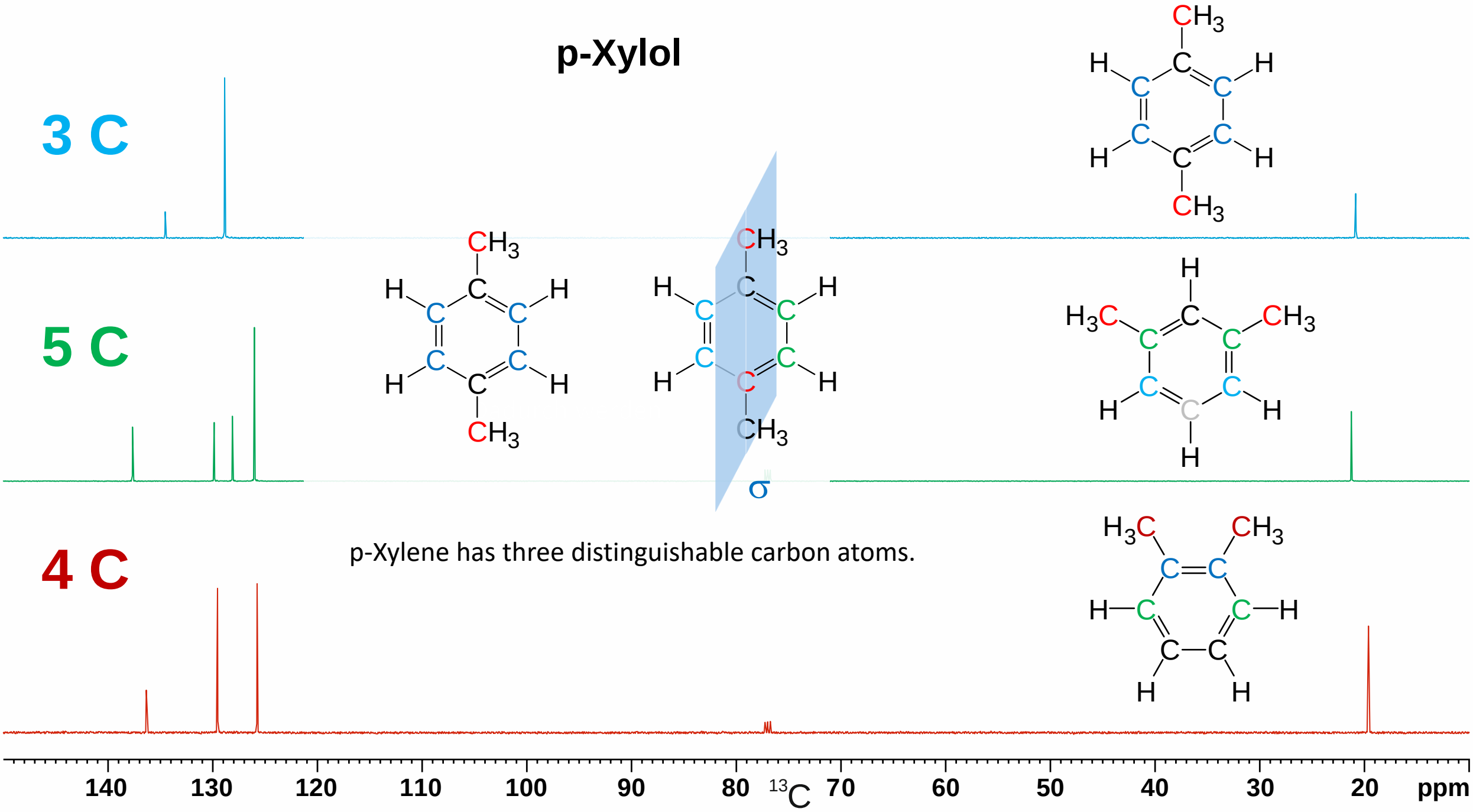
Another mirror plane is arranged perpendicular to the first one.

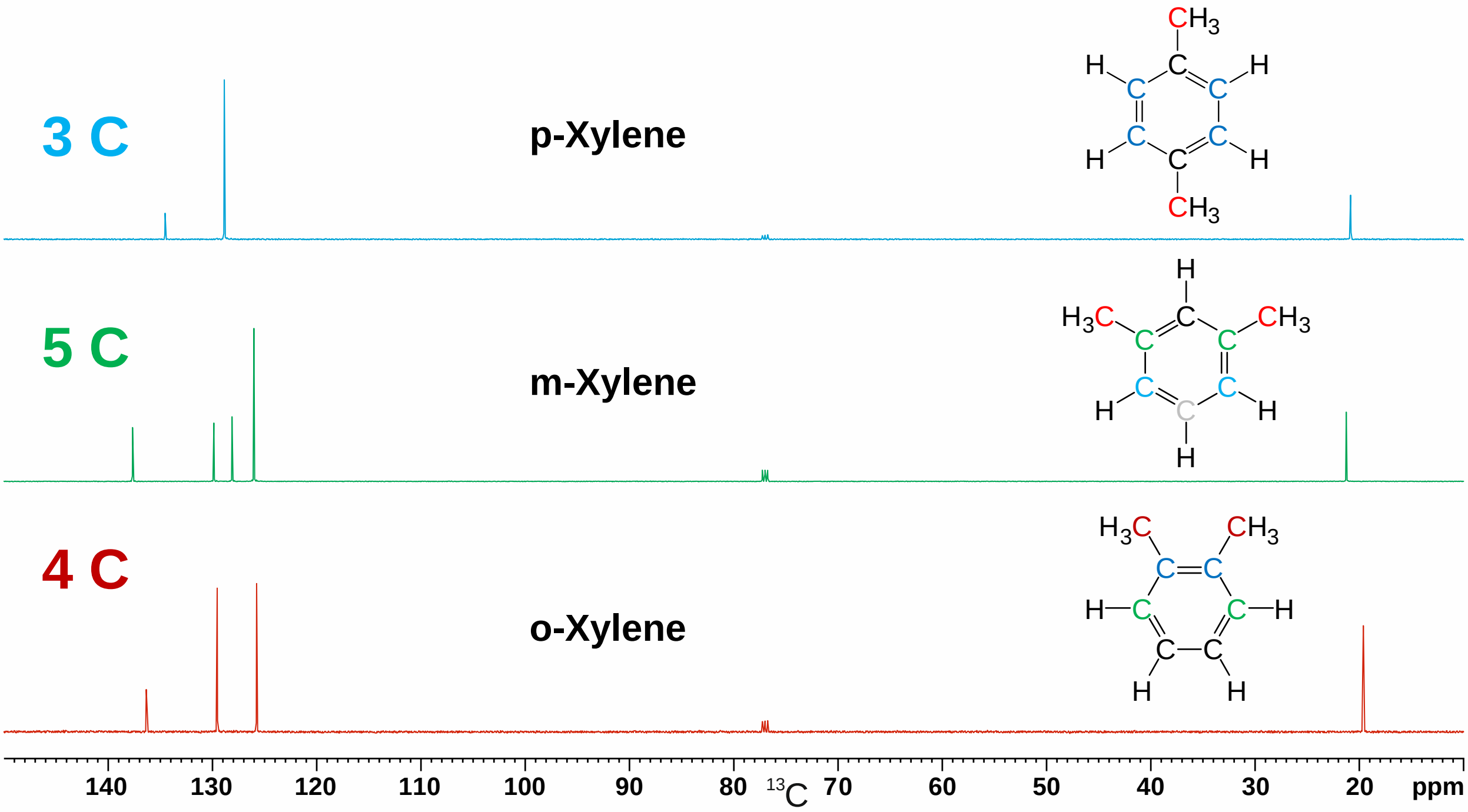
This makes the previously cyan and green marked carbon atoms identical.





p-Xylol


3 C
5 C
4 C
σ
p-Xylene has three distinguishable carbon atoms.
140
130
120
110
100
90
80
^{13}C
70
60
50
40
30
20
ppm


3 C
p-Xylene
5 C
m-Xylene
4 C
o-Xylene
140
130
120
110
100
90
80
^{13}C
70
60
50
40
30
20
ppm

Contributions

Spectrometer time

TU Munich

Measurements

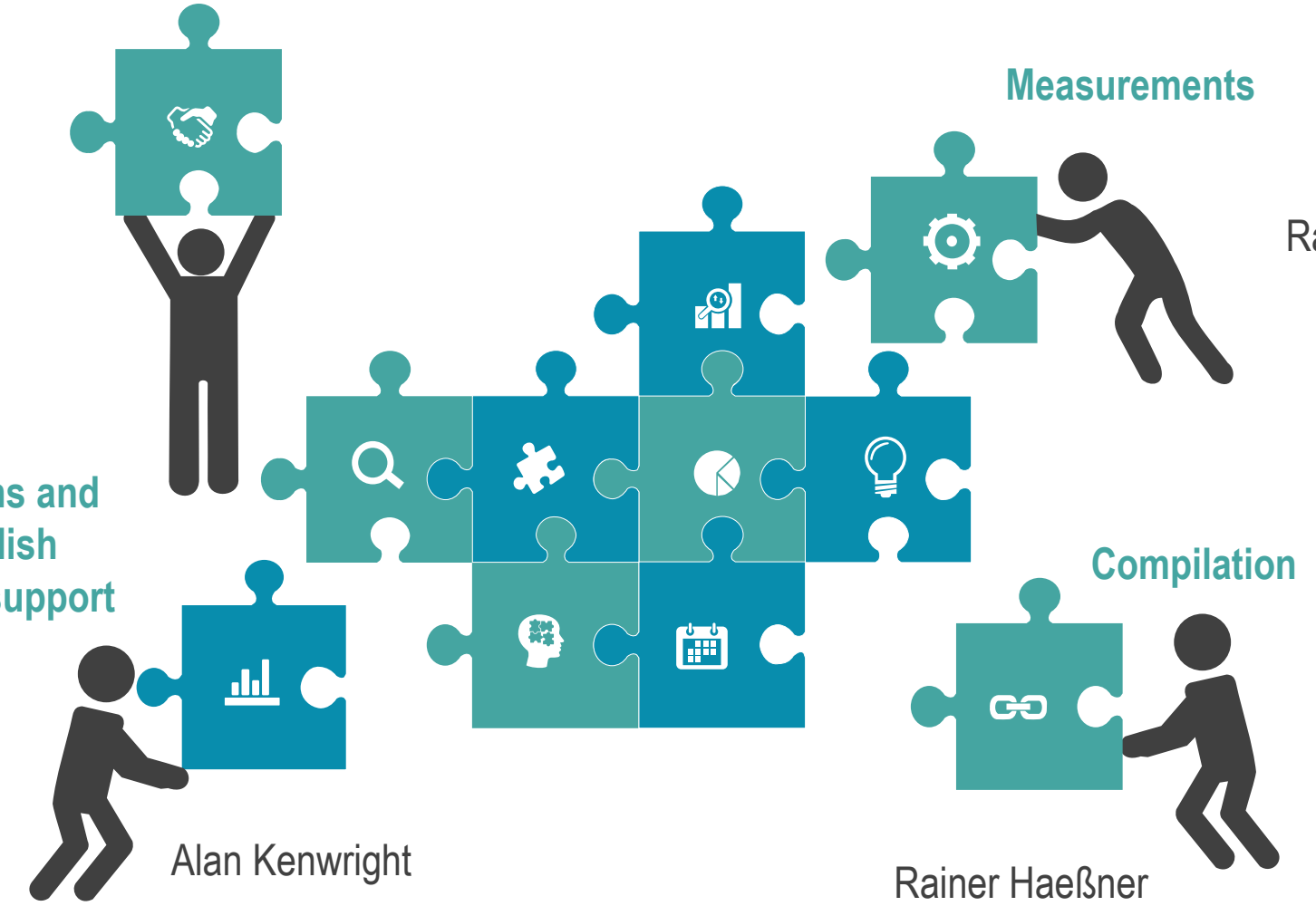
Rainer Haeßner

Discussions and native English language support

Alan Kenwright

Compilation

Rainer Haeßner



More exercises …