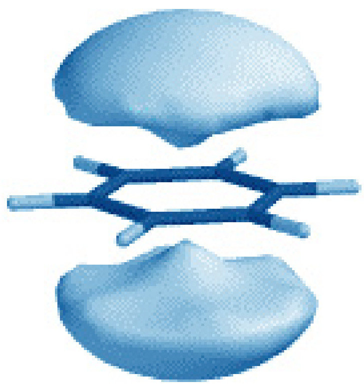
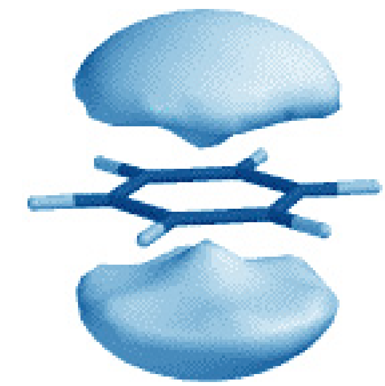


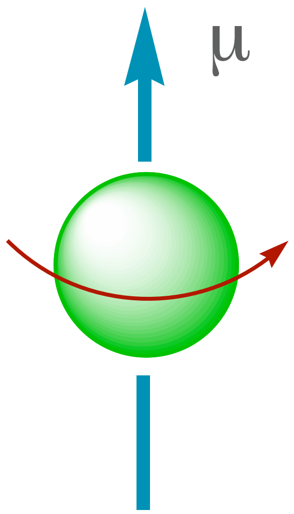
# Chem 342



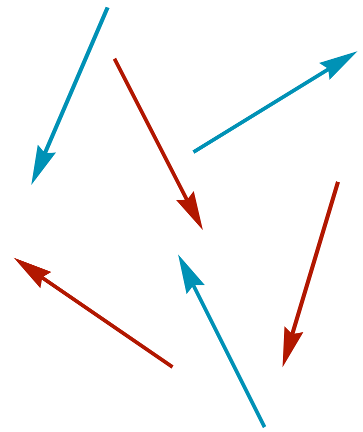
Organic Chemistry II
Spring 2004

cook.chem.ndsu.nodak.edu/chem342

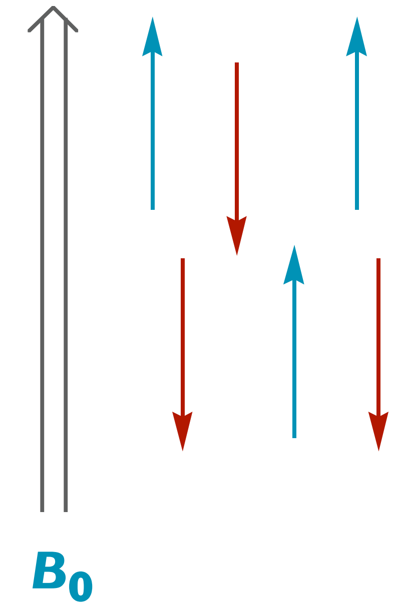
You can download a syllabus from the Handouts page

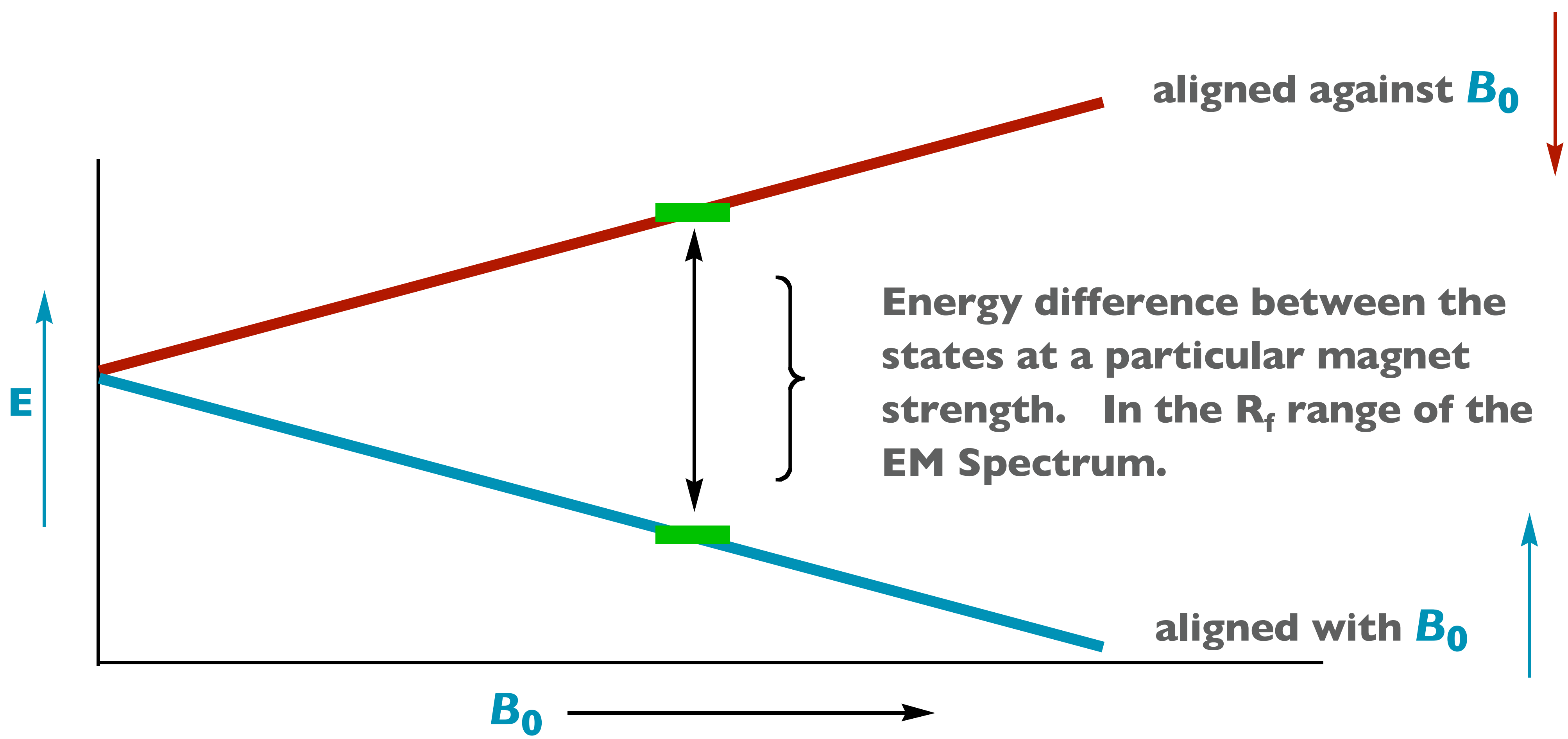



A spinning charged particle generates a magnetic field.
A nucleus with a spin angular momentum will generate a magnetic moment (m).



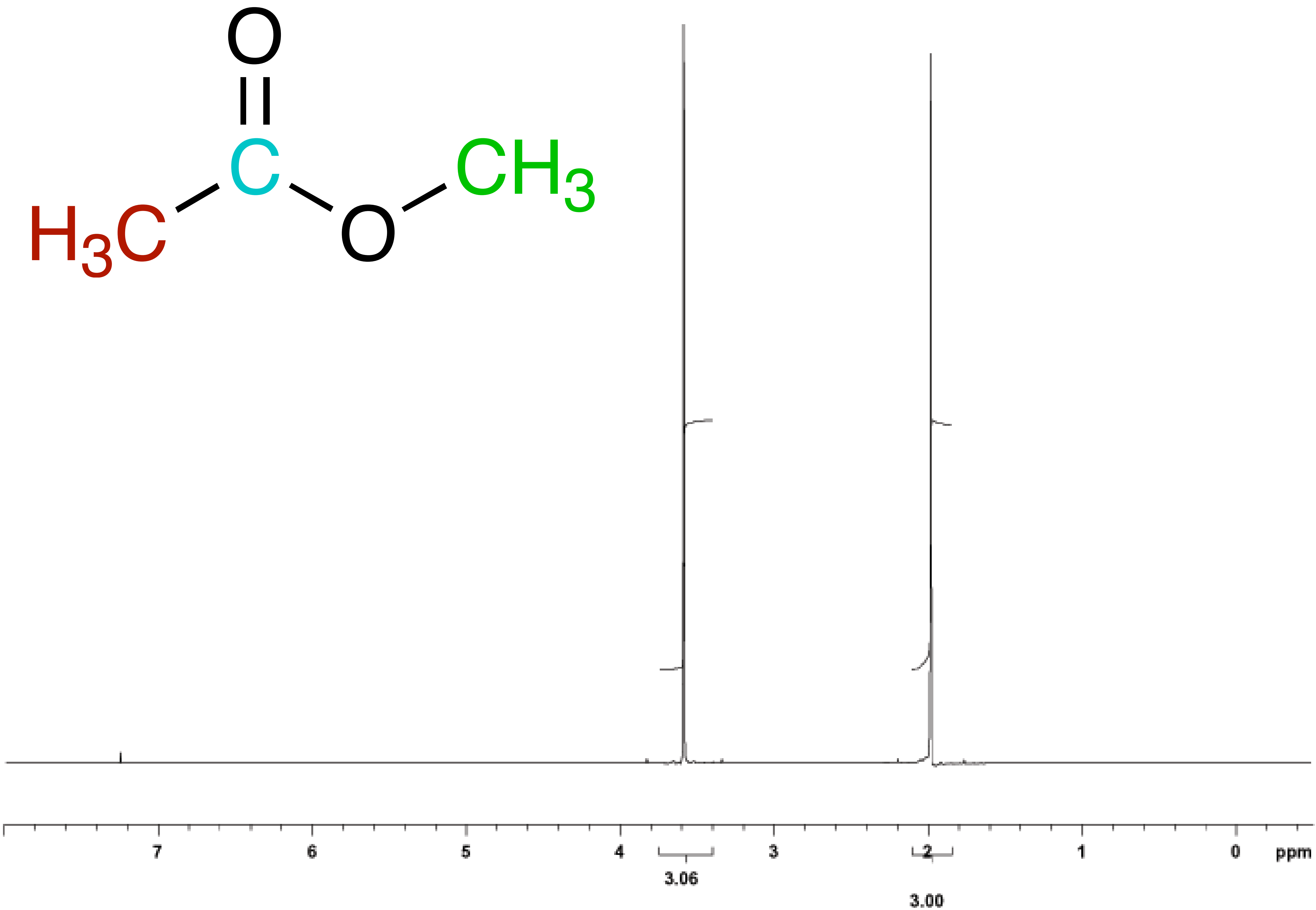
When placed in a magnetic field (*Bo*), they will adopt two different states - one aligned with the field and one aligned against the field.



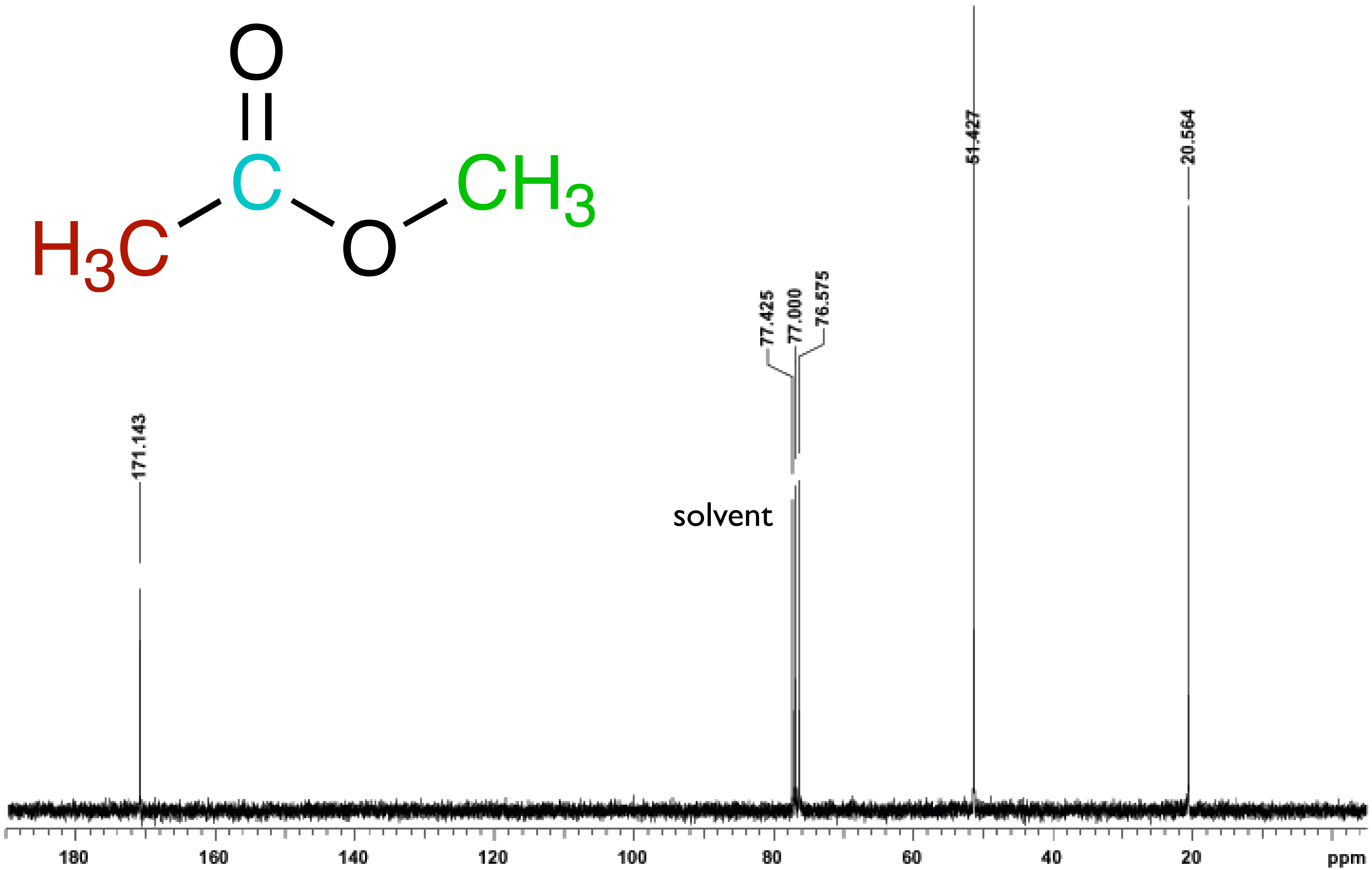




**Energy difference between the states at a particular magnet strength. In the $R_f$ range of the EM Spectrum.**

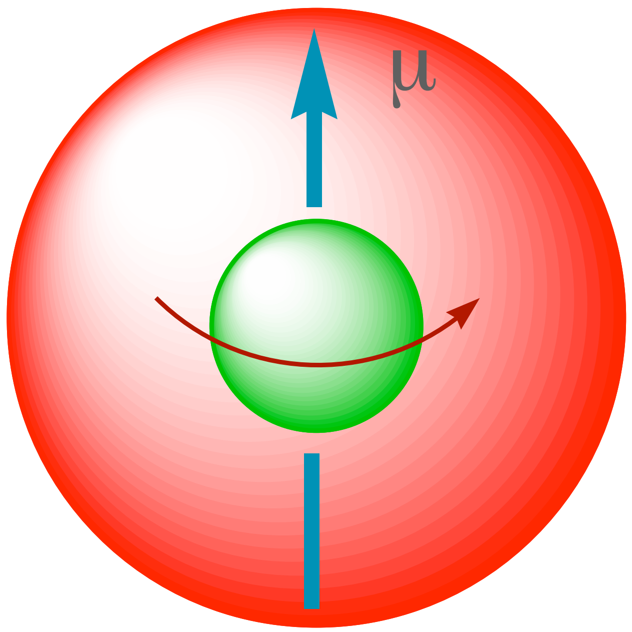
# Methyl Acetate - Proton NMR

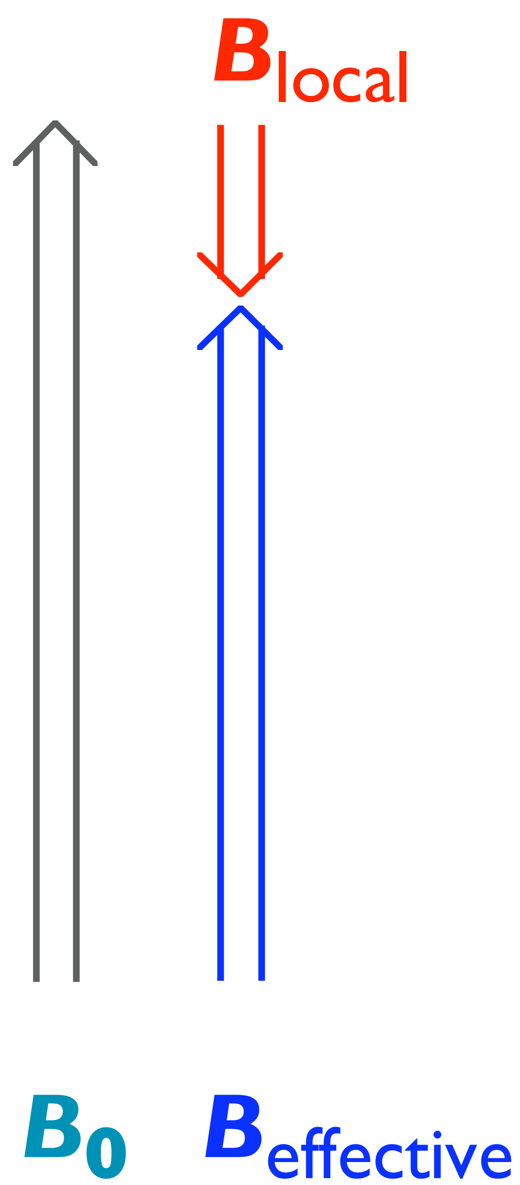


# Methyl Acetate - Carbon NMR



# Electronic Shielding - Local Environments

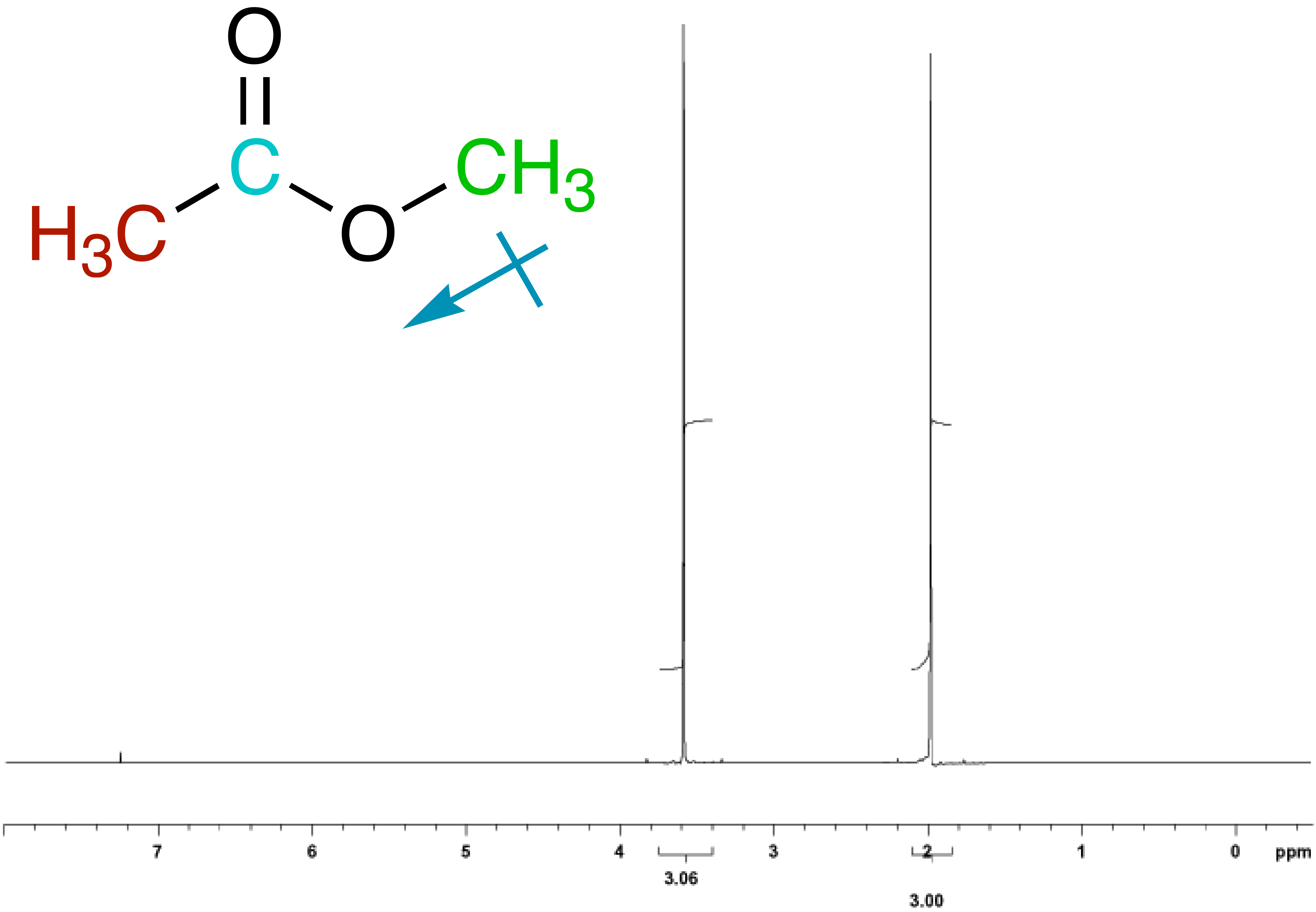


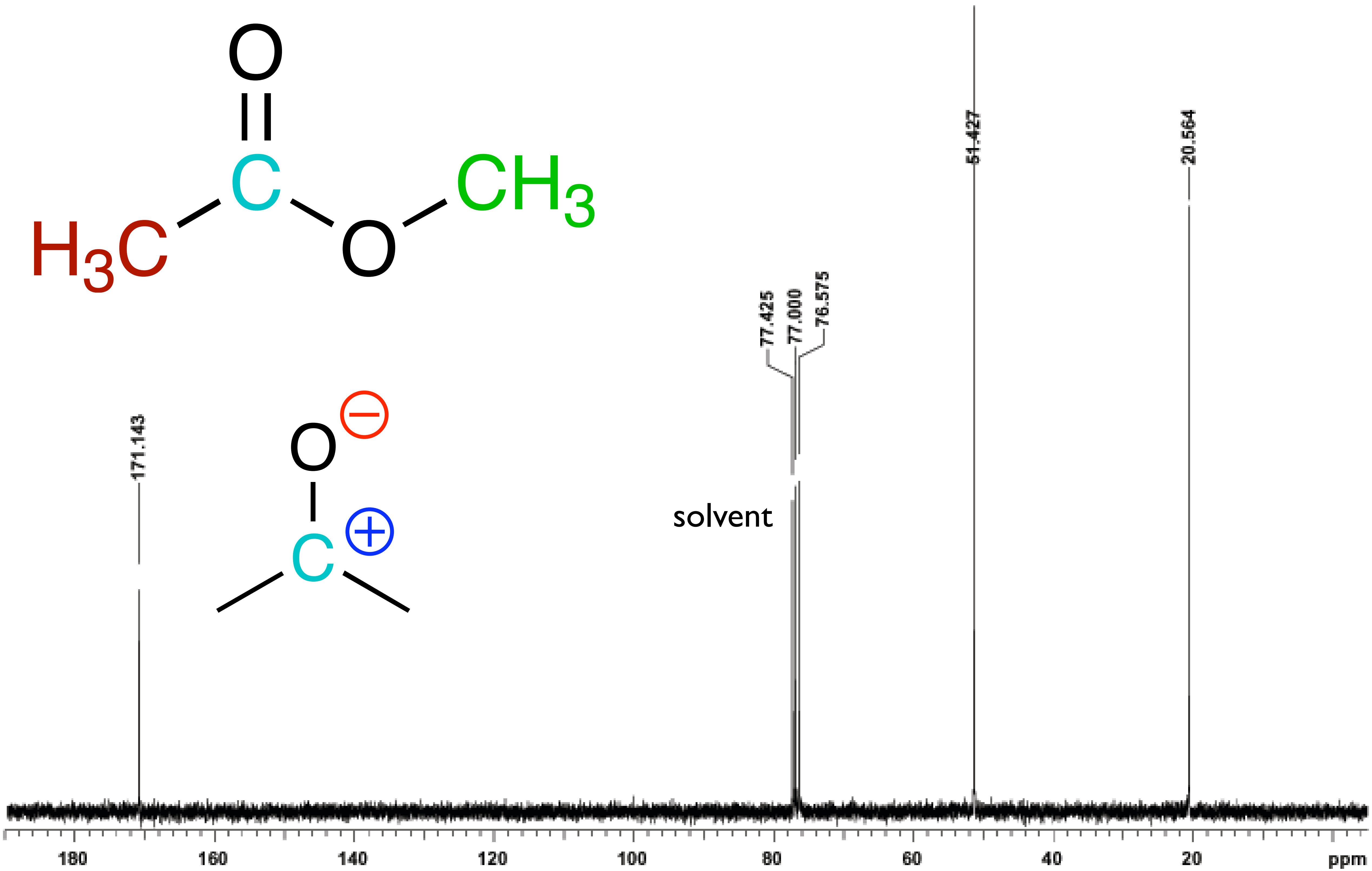

$$B_{effective} = B_0 - B_{local}$$

Actual magnetic field felt by the nucleus

# Methyl Acetate - Proton NMR

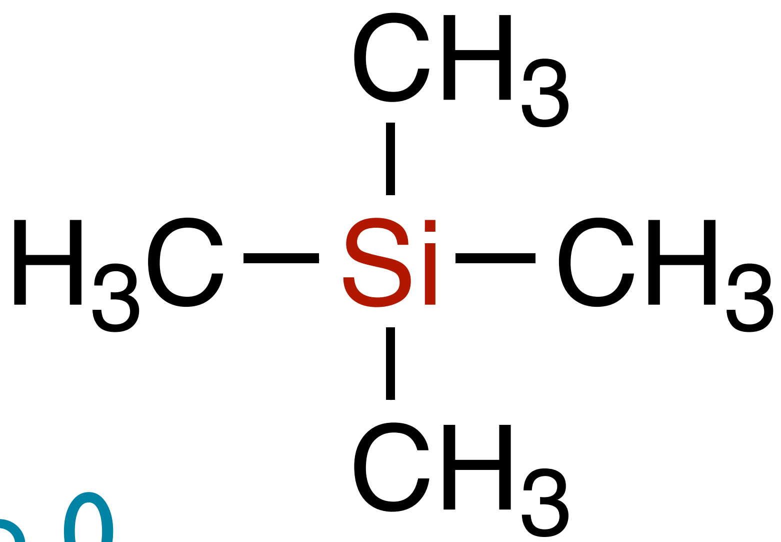


# Methyl Acetate - Carbon NMR



# Chemical Shift

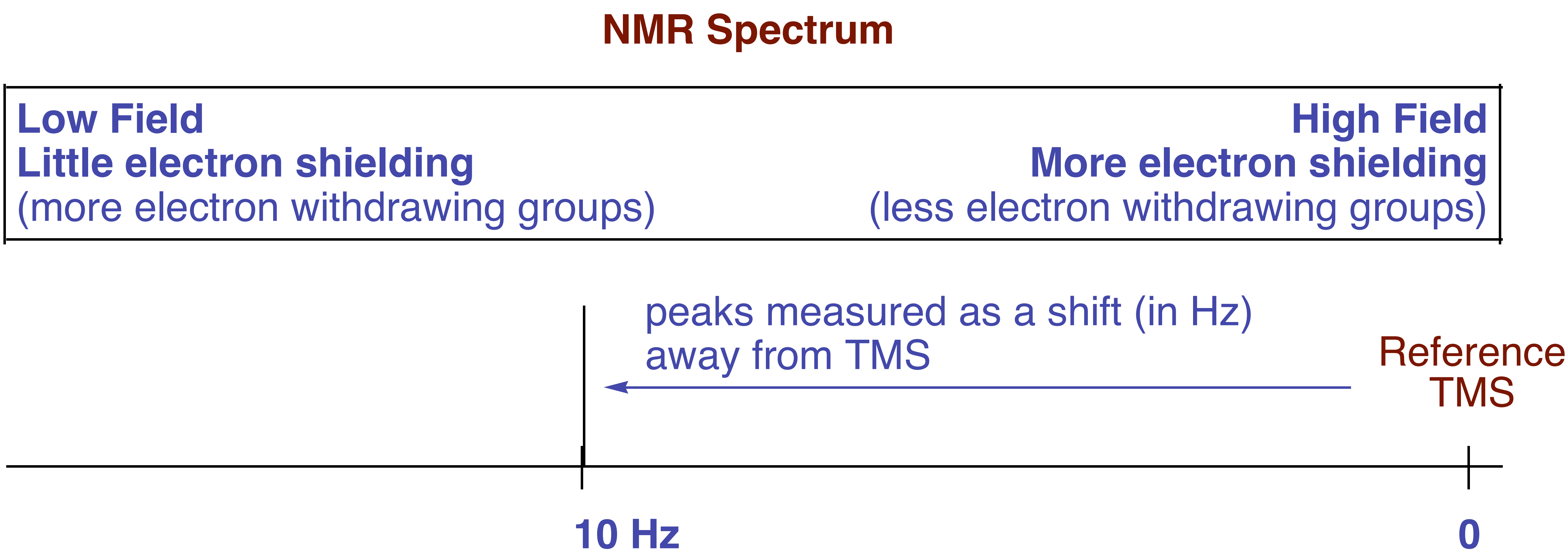
- The difference in resonance frequency of a nuclei relative to a standard
  - Most Shielded
  - Relatively Inert
  - Volatile
- Resonance of standard is set to 0




**TMS**

**TetraMethylSilane**

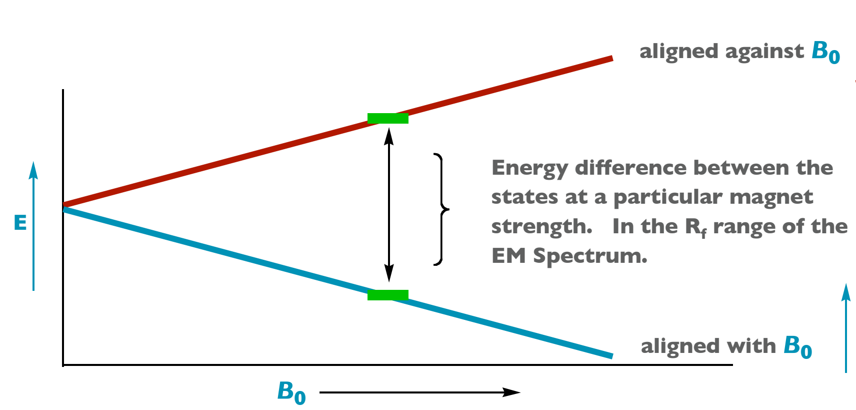
## X-Axis - frequency axis



# Different Spectrometer Frequencies

- Each specific instrument has it's own magnetic field strength - resonace occurs at different frequencies.

100 MHz NMR
300 MHz NMR



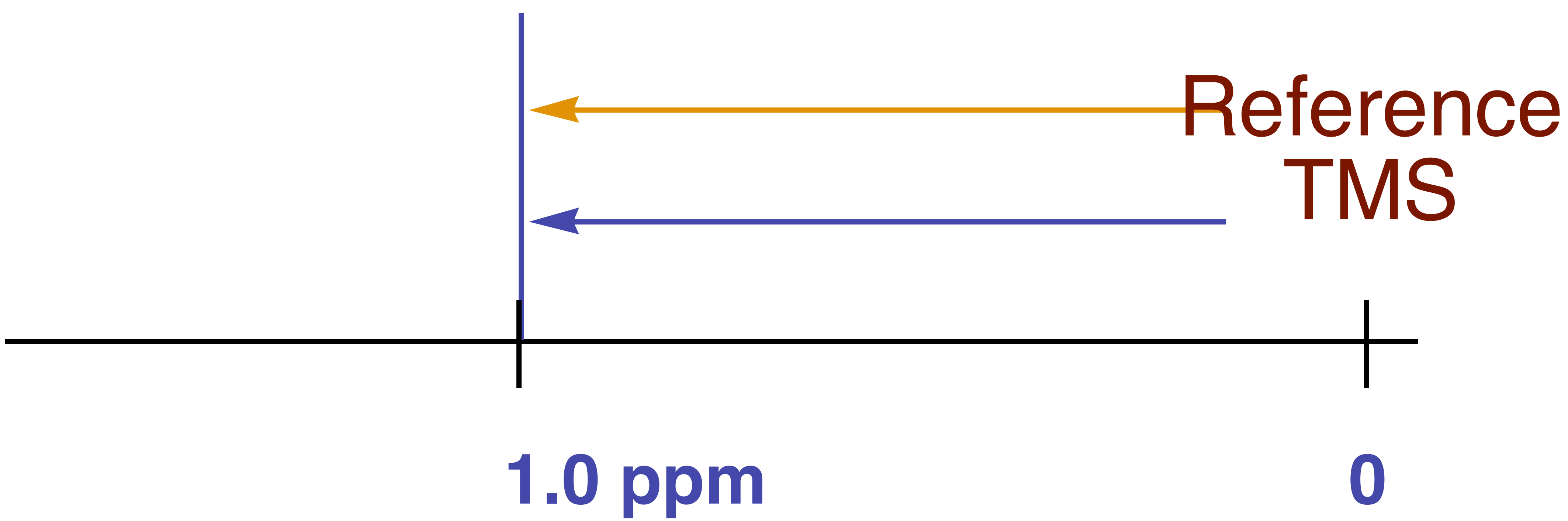

# Standard Scale

- $\delta = \text{ppm} = \dfrac{\text{Chemical Shift from TMS (Hz)}}{\text{Spectrometer Frequency (MHz)}}$

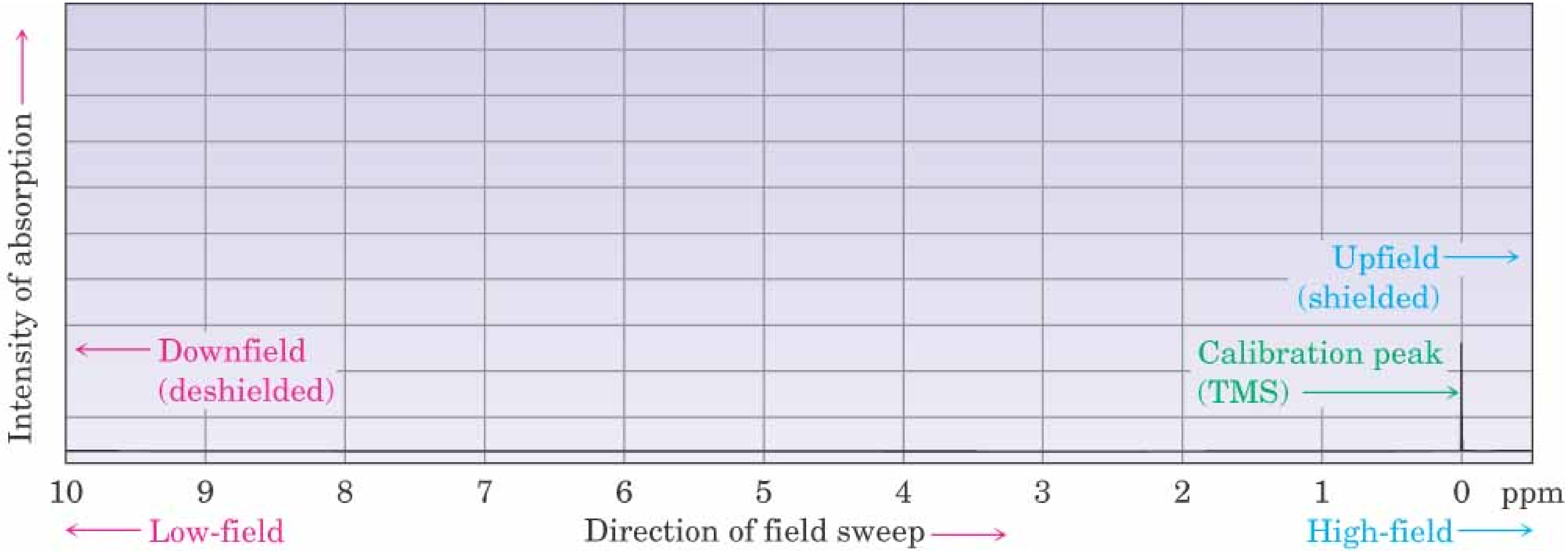
$$\frac{100\ \text{Hz}}{100\ \text{MHz}} = 1.0\ \text{ppm}$$

$$\frac{300\ \text{Hz}}{300\ \text{MHz}} = 1.0\ \text{ppm}$$

100 MHz NMR
300 MHz NMR

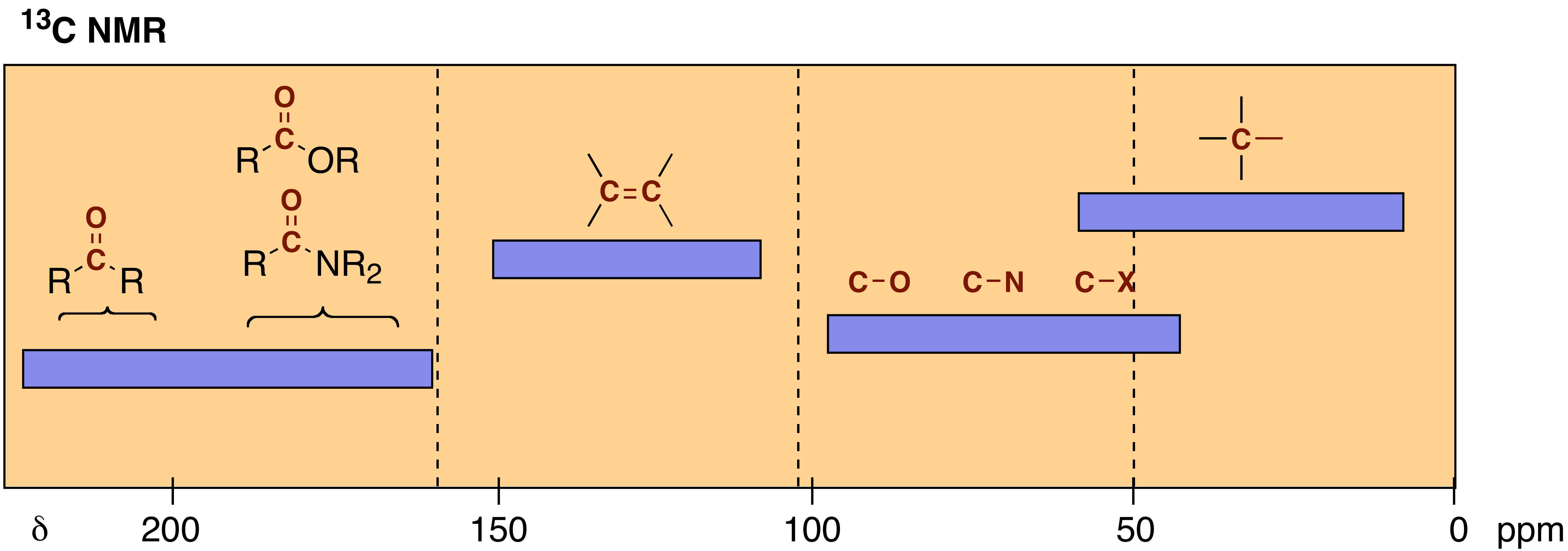


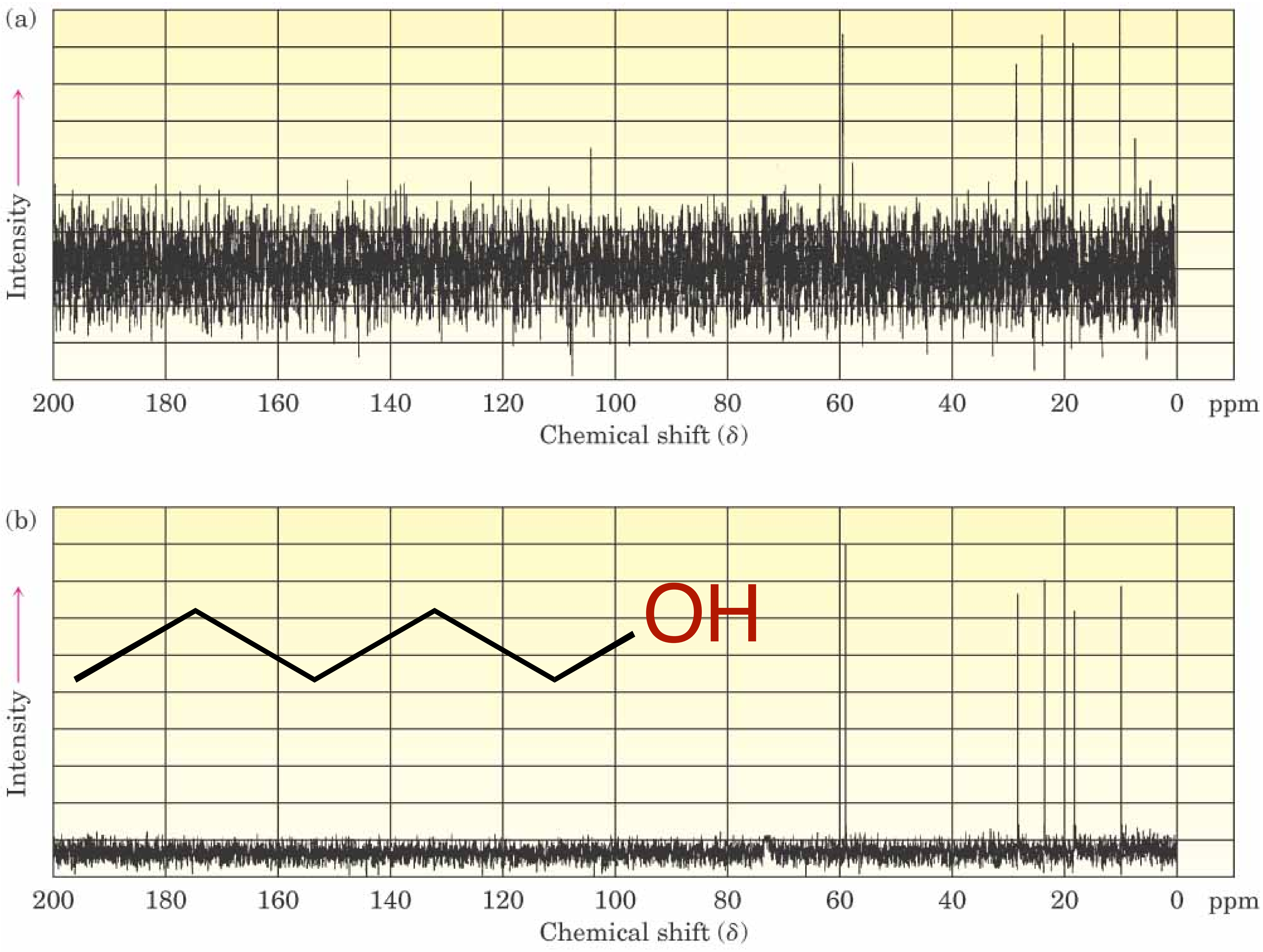
# NMR Scale



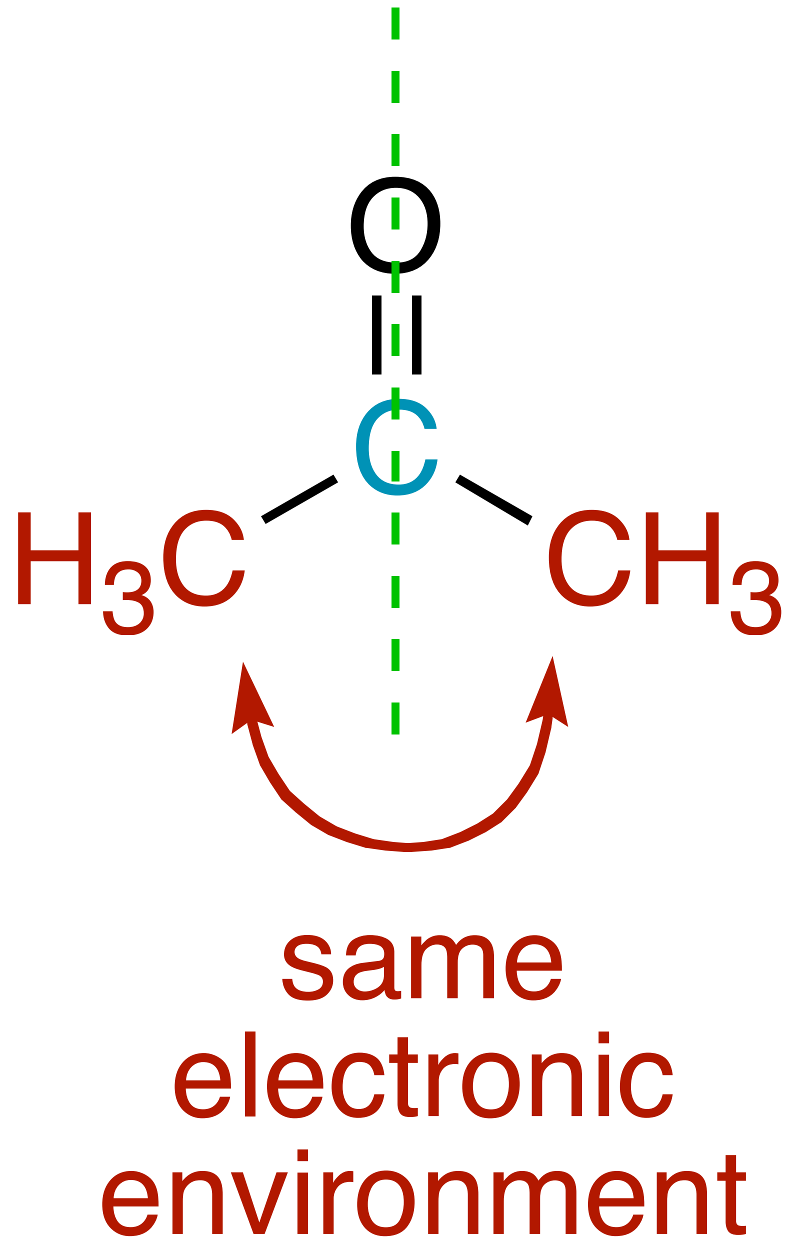
Intensity of absorption
Upfield
(shielded)
Downfield
(deshielded)
Calibration peak
(TMS)
10
9
8
7
6
5
4
3
2
1
0
ppm
Low-field
Direction of field sweep
High-field

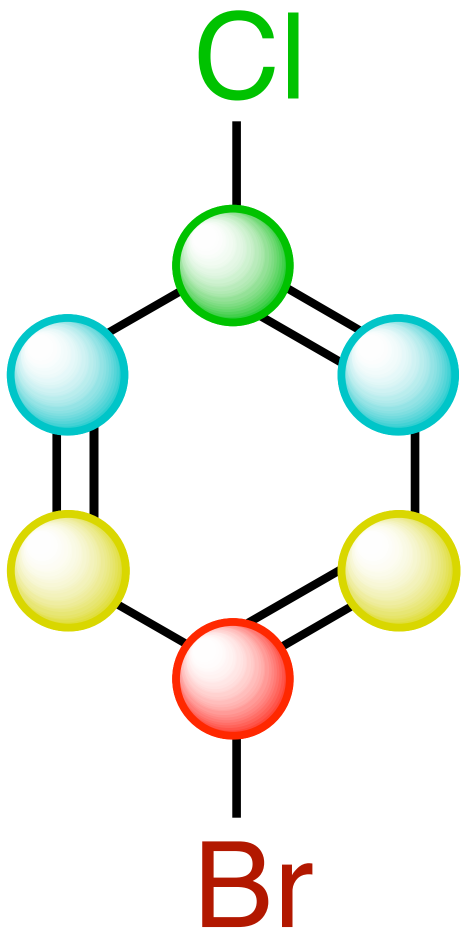
- Difficult - Carbon 13 only 1.1% of all carbon.
- Number of different carbons
- Functional Group Regions



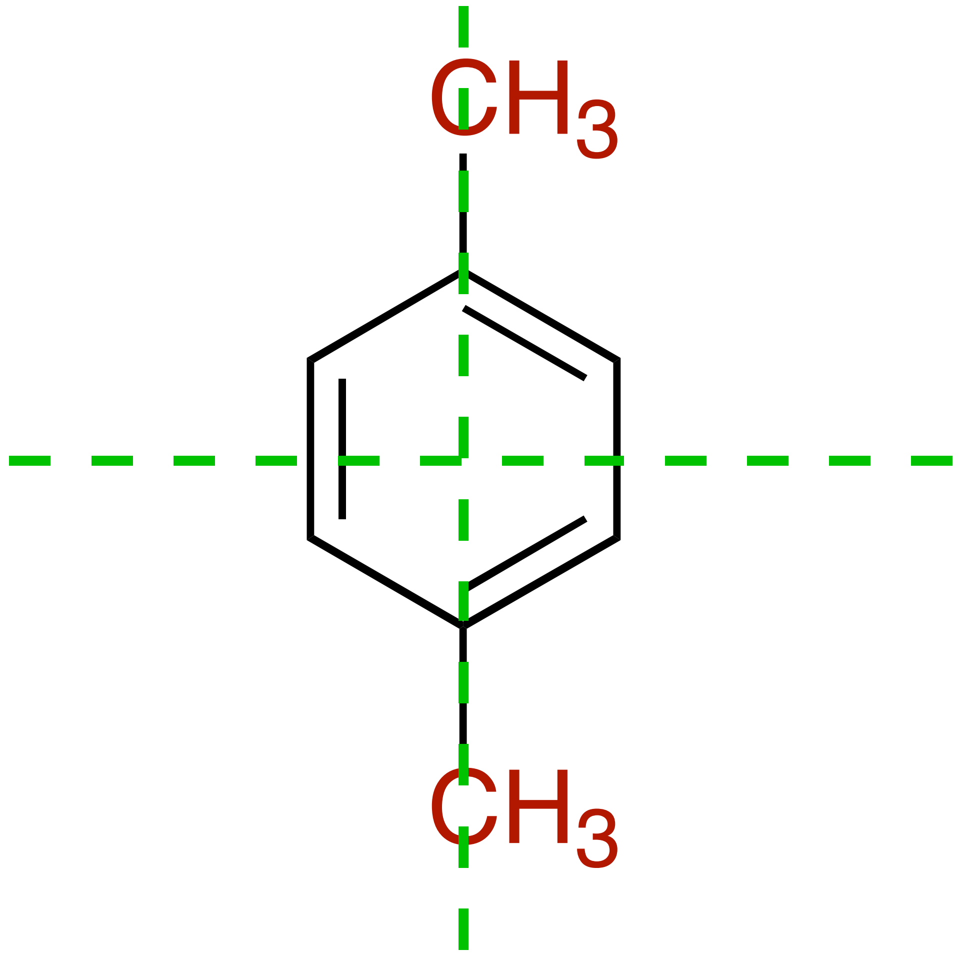

(a)
Intensity
200
180
160
140
120
100
80
60
40
20
0
ppm
Chemical shift (δ)
(b)
OH
Intensity
200
180
160
140
120
100
80
60
40
20
0
ppm
Chemical shift (δ)

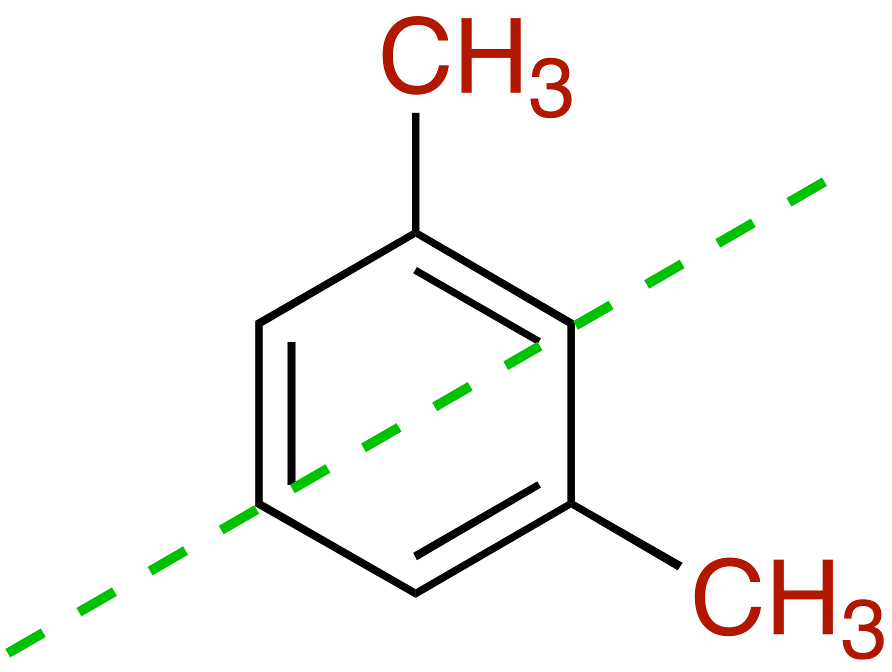
- Symmetry in molecules can make carbons "Chemically Equivalent"



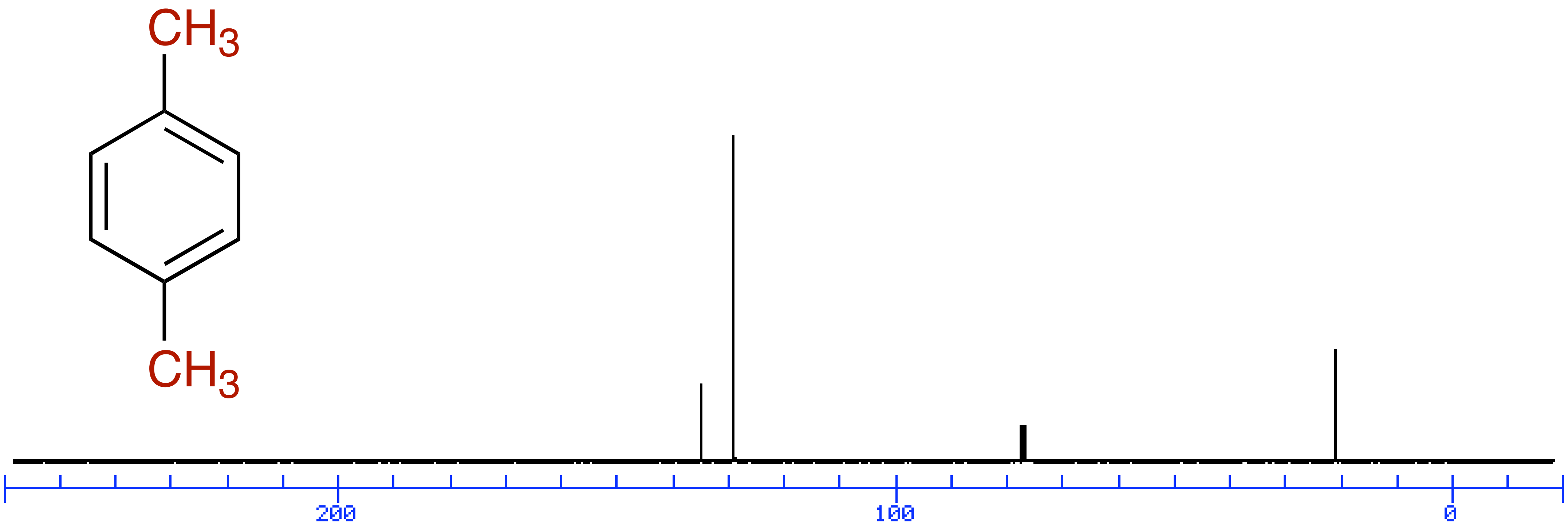



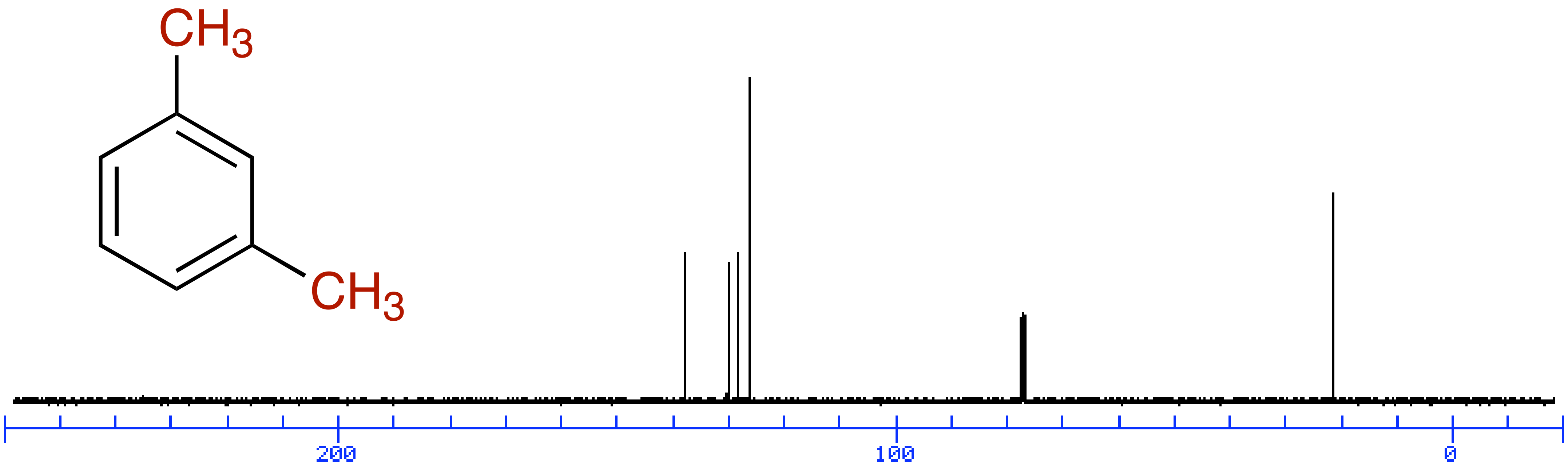
- Some molecules have more than one mirror plane



# Symmetry



# Symmetry