Information in ^{1}H spectra

• Number of signals	***symmetry***
• Intensity	***number of equivalent nuclei***
• Chemical shift	***functional group***
• Fine structure and J-constants	***neighboring protons***

Information in13C spectra with decoupling

- Number of signals
- Chemical shift
- intensity does not correspond to number of equivalent nuclei

Information in APT/DEPT 13C spectra

- Multiplicity of carbons

Solving NMR spectra

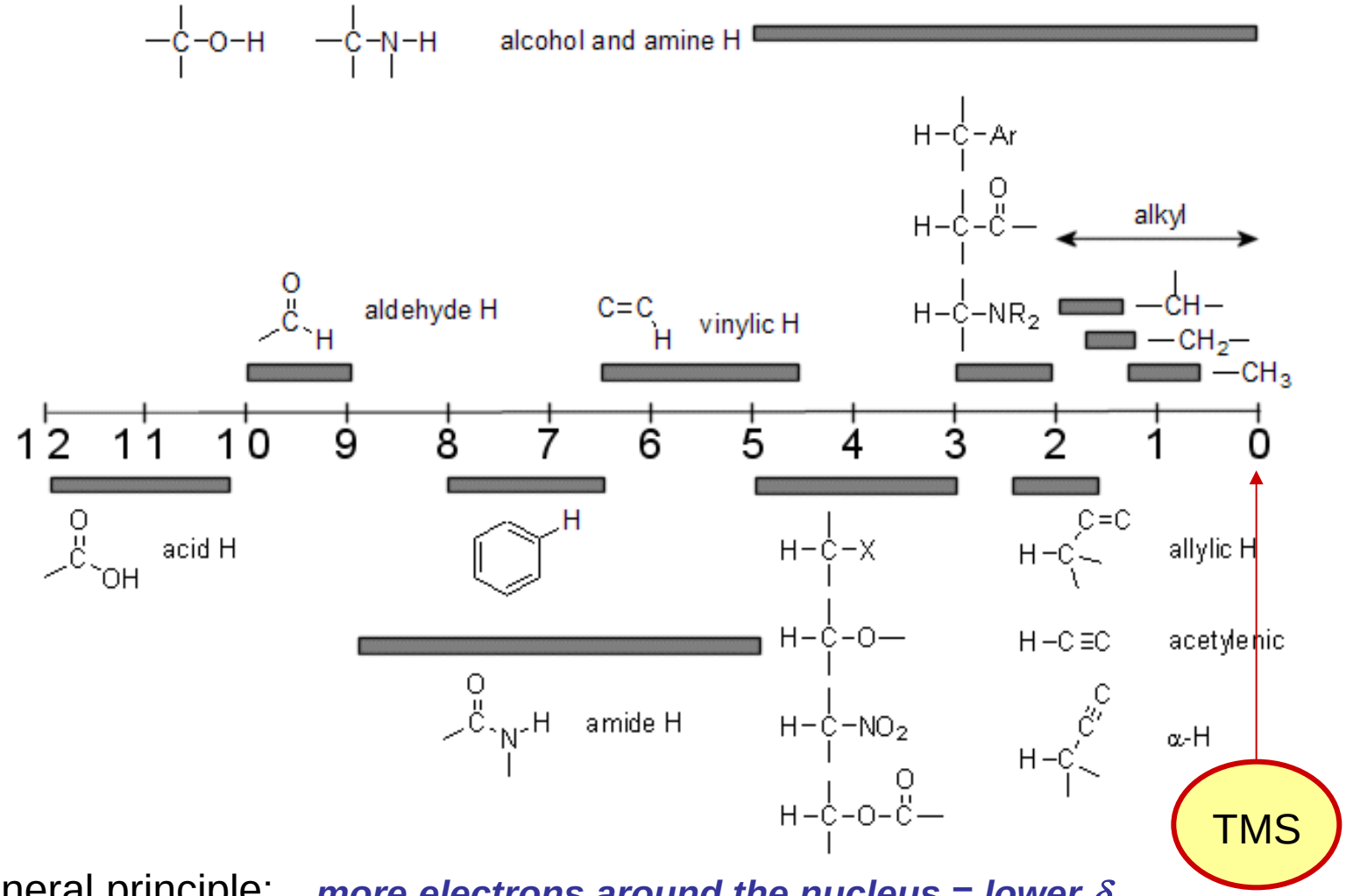
Information we get

- molecular formula (obtained e.g. by mass spectrometry)
- Set of spectra (1H, 13C, might have also APT or DEPT)

How to solve the structure

- identify signals, their number, position and intensity
- divide hydrogens into groups according to signal intensities
- analyze fine structure of multiplets, identify which groups of hydrogens will be next to each other
- complete the identification of functional groups, taking into account chemical shifts and other information (^{13}C spectrum, APT/DEPT)
- take into account the symmetry of the molecule (derived from the number of signals) and combine functional groups into a molecule
- for the proposed solution, to re-derive what spectrum it would provide, and thus verify whether the solution is correct

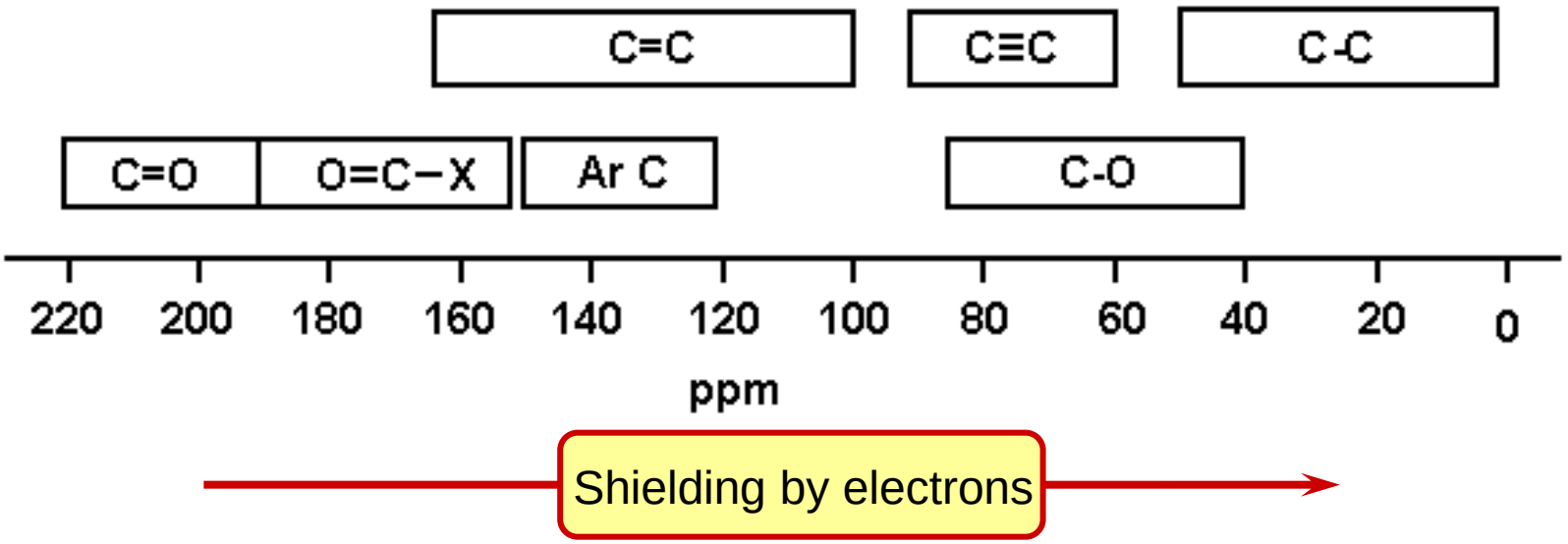
^{1}H chemical shifts



General principle: ***more electrons around the nucleus = lower δ***

http://www.chemistry.ccsu.edu/glagovich/teaching/316/index.html

Chemical shifts ^{13}C

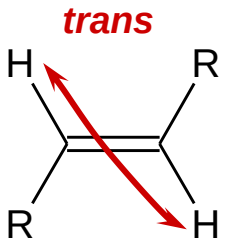


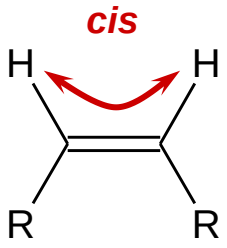
General principle: ***more electrons around the nucleus = lower δ***

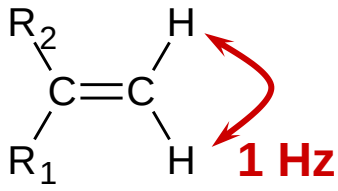
Values of J couplings

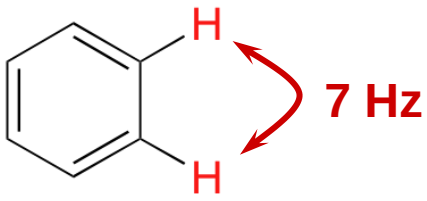
Hydrogen – Hydrogen

without conformational preference

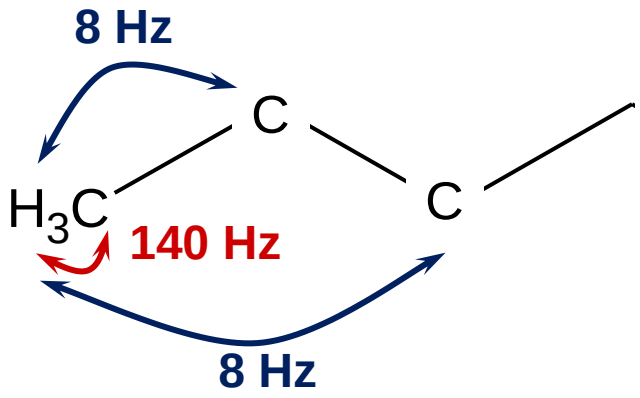




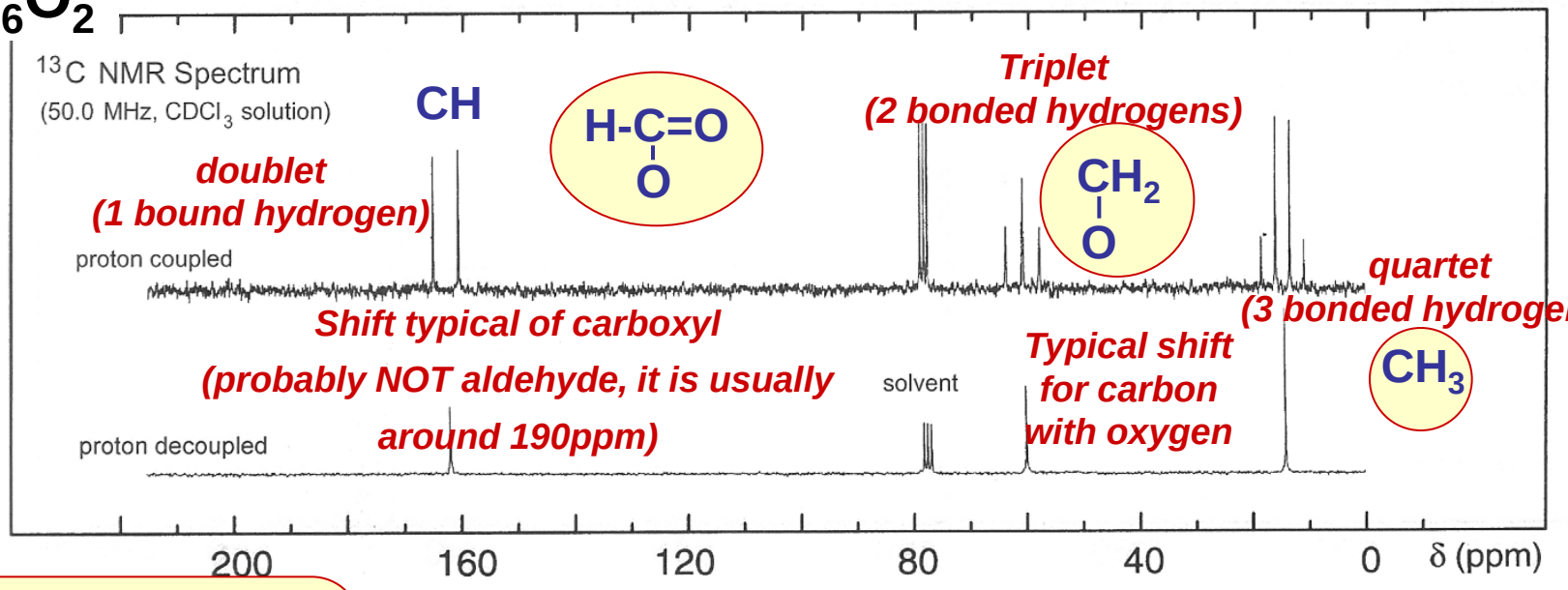


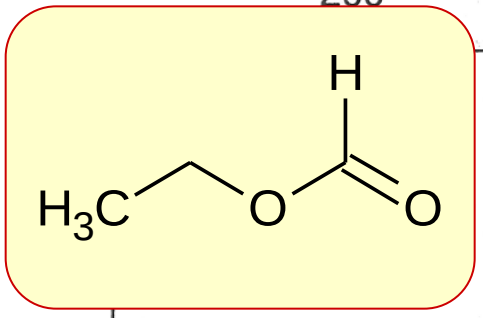


Hydrogen – carbon



$C_3H_6O_2$


^{13}C NMR Spectrum
(50.0 MHz, $CDCl_3$ solution)
CH
H-C=O
O
Triplet
(2 bonded hydrogens)
CH_2
O
doublet
(1 bound hydrogen)
proton coupled
quartet
(3 bonded hydrogens)
CH_3
Shift typical of carboxyl
(probably NOT aldehyde, it is usually
around 190ppm)
solvent
Typical shift
for carbon
with oxygen
proton decoupled
200
160
120
80
40
0
δ (ppm)


H
H_3C
O
O

quartet of doublets
(coupling with 3 hydrogens + 1 more)
Triplet
(coupling with 2 hydrogens)
small J
over 4 bindings
CH_2
O
CH_3
TMS
probably CH
1
probably J coupling
2
J coupling
= Neighboring groups
3
Typical shift of
Methyl
Shift typical of hydrogen next to oxygen
10
9
8
7
6
5
4
3
2
1
0
δ (ppm)