**$^{13}$C NMR**

Any nucleus with an odd atomic number or odd mass will have a nuclear magnetic resonance.

A proton is the most common example in organic chemistry so by default when someone talks about NMR it usually means a $^1$H NMR.

Carbon-12, the most abundant source of carbon, has an even atomic number and even mass so therefore this nuclei is NMR inactive.

The isotope C-13, though, has an odd mass and is therefore NMR active.

Another very useful nucleus to determine organic structures.
Carbon-13

The natural abundance of C-13 isotope is ~1%

Therefore only 1% probability that a given carbon atom is NMR active
- therefore the signal-to-noise ratio for carbon NMR is less
Put another way – if studying 1-chloroethane only 1 in 100 molecules will be active at C1

In addition the gyromagnetic ratio, γ, for carbon is ~1/4 that of hydrogen
(remember that each nucleus has its own unique gyromagnetic ratio)
-this also causes a lower signal-to-noise for carbon relative to hydrogen NMR
$^{13}$C NMR Spectra
Unique Features of $^{13}\text{C}$ NMR Relative to $^{1}\text{H}$ NMR

1) The scale is much larger for $^{13}\text{C}$ than $^{1}\text{H}$ NMR
Notice spectrum is 0-200 ppm instead of 0-11 ppm,
due to carbon being more shielded than hydrogen
[8 electrons around carbon rather than 2 electrons around hydrogen]

2) Relative placement of functional groups though is the same in the above spectrum
Which functional group was more deshielded in $^{1}\text{H}$ NMR is still more deshielded in $^{13}\text{C}$ NMR
-aldehyde carbon 194 ppm, sp$^2$ carbons 158 and 133 ppm, sp$^3$ carbons below 40 ppm

3) Each carbon has its own unique chemical shift
big advantage with $^{13}\text{C}$ NMR, can instantly tell number of
distinct symmetrically different carbons
[the spectrum shown is a proton-decoupled $^{13}\text{C}$ NMR, most common example]

4) Do not observe $^{13}\text{C}$-$^{13}\text{C}$ splitting
Due to low probability of finding two adjacent carbons both $^{13}\text{C}$ isotope with only 1%
probability for each
Splitting

Notice that carbon-carbon splitting is not detected in NMR

Can still detect $^{13}\text{C}$-$^1\text{H}$ splitting from hydrogens attached to carbon of interest
    This is called off-resonance decoupled
    Have same N+1 rule

Normally, though, a $^{13}\text{C}$ NMR is proton spin decoupled
    In this mode a sharp singlet is observed for each carbon
    -far easier to interpret spectra
Remember to look for symmetry
Only distinguish symmetrically different carbons
Peak Areas

Unlike $^1$H NMR we cannot integrate peaks in $^{13}$C NMR to detect relative abundance.

In a typical $^{13}$C NMR, the peak areas are dependent upon how many hydrogens are attached to carbon, not the relative number of carbons causing the signal.

$\text{CH}_3$ groups are the biggest followed by $\text{CH}_2$, $\text{CH}$ and quaternary carbons are the smallest.
Position of Functional Groups in $^{13}$C NMR

The relative placement is similar to $^1$H NMR, but the scale is much larger.

Observe all carbons
(Obviously do not “see” carbons that have no hydrogens attached in $^1$H NMR)
Examples
Examples
MRI Imaging

MRI (magnetic resonance imaging) is in theory identical to our discussions
MRI = NMR

Consumers are hesitant with anything that has “nuclear”
in its descriptor so the name was changed

One main difference is that instead of spinning the sample to make the magnetic field
homogeneous throughout the sample in a NMR experiment
(thus the chemical shift will be identical for all hydrogens
with the same amount of shielding),
in MRI the field is inhomogeneous throughout the sample

This inhomogeneity allows one to measure either placement of protons in a body
(where is the water)
or also changes in movement of the protons
(i.e. how mobile is water inside a tumor relative to a normal tissue)
Use all the spectroscopic tools we have learned to determine the exact structure.