Nuclear Magnetic Resonance (NMR) Spectroscopy

- Most important technique for organic chemists.
- Uses same technology as MRI.
- Noninvasive diagnostic tool.

NMR: $^1H$, $^{13}C$, and other "spin-active" nuclei.

tumor
How does it work?

- Detects very low energy transitions of atomic nuclei with nuclear spin

  > Atoms with odd number of protons or neutrons (or both)

  ex: $^1\text{H}$, $^{12}\text{C}$, $^{13}\text{C}$

Spin gives nuclei a magnetic dipole moment. Spin-active nuclei behave as dipoles.

In presence of external magnetic field, nuclei align like bar magnets.
In the absence of an applied magnetic field,

In the presence of an applied magnetic field, $B_0$

- Aligned against the field: higher energy $\beta$ hydrogens
- Aligned with the field: lower energy $\alpha$ hydrogens

$B_0$ Applied magnetic field

Figure 15.18
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In the absence of a magnetic field, both spin states have equal energy
In a strong magnetic field, the energy level difference corresponds to the energy of radio waves.

\[ \Delta E = h\nu \]
Figure 15.19
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RF transmitter

RF Receiver

Note modern NMRs use superconducting magnets to attain very strong magnetic fields
Nuclei that matter in organic chemistry: $^{13}\text{C}$, $^1\text{H}$

$^{13}\text{C}$ NMR

Recall: Most C is $^{12}\text{C}$ (invisible by NMR)
Only $^{13}\text{C}$ is spin-active (~1%)

What does it tell you?
Tells you how many types of C are in your molecule (and what types)

Different types of C appear at different frequencies
because the e-s around nuclei "shield" them from external magnetic field.
4 C's, but only 1 type

1 peak in 13C NMR
Solving the Structure of an Unknown... (or 2)...

Molecular Formula: \( C_3H_8O \) → \( \frac{\text{HCF}}{C_3H_8} \) \( \frac{\text{Sat. Alkane}}{C_3H_{(2n+2)}} \)

\( n = 3 \)

\( \varnothing \) degrees of unsaturation.

No \( \pi \) bonds, No rings.

\( \text{H}_3\text{C} - \text{CH}_2 - \text{CH}_2 - \text{OH} \)

3 \( ^{13}\text{C} \) signals

\( \text{H}_3\text{C} - \text{CH}_2 \text{O} - \text{CH}_2 \text{CH}_3 \)

2 signals in \( ^{13}\text{C} \) NMR
Both unknowns are alcohols.

Ruled out ether structure.

$\text{H}_3\text{C} - \text{O} - \text{CH}_3$
The diagram represents the 13C NMR of an unknown sample labeled #1. The graph shows three signals, with peaks at different ppm values. Arrows indicate 'Upfield' and 'Downfield' directions. The chemical structures H3C-OH are annotated near the peak locations.
$^{13}$C NMR of unknown #2

$\text{H}_3\text{C} - \text{OH}$

2 signals
Where a peak appears (0–200 ppm) = **CHEMICAL SHIFT**

- hybridization of C
- electronegativity of attached atom(s)
Midterm 1:

Average: 183 / 250

A: 220 - 250
B: 183 - 219
C: 121 - 182