How we come to know a chemical structure

\[ m_s \rightarrow \# \text{ of carbons} \]

\[ I_2 \rightarrow \text{Type of Bonds} \rightarrow \text{functional Group} \]

The last piece of the puzzle - **NMR (Nuclear Magnetic Resonance)**

- Give the carbon chain/connectivity

**Theory**

Hydrogen nuclei have a magnetic moment \( \textit{H} \)

When placed in a magnetic field have 2 'spin states' \( \uparrow \) \( \downarrow \)

\[ E = \gamma B_0 \text{ magnetic field (that H feels)} \]

\( \Delta E = \hbar (2\pi) \) between spin states

The energy difference between spin states sets us up for Spectroscopy (\( \Delta E \))

When \( \Delta E = \text{Energy of light} - \text{light will be absorbed} \)

\[ \Delta E \quad \text{"Flip the spin"} \quad \nu \]

No magnetic field

If all protons have the same \( \Delta E \) then they all give just one signal

But the \( \Delta E \) will change depending on electron density about the proton.

\[ C \quad \downarrow \quad H \]

Proton feels sum of both fields + smaller due to electrons in the bond = \( \Delta E \) is smaller = easier to "flip the spin"
Protons with high e- density we call 'shielded' \( \rightarrow \) smaller AE Gap, easy to flip

Compare CH₄ and CH₃-F

- CH₄ has less e- density around H
- CH₃-F has more e- rich
- more shielded
- AE is smaller, need less energy to flip

NMR Spectra

CH₃F - AE larger

'deshielded' protons

less e- density

Chemical Shift (δ) units ppm

standard for 0 ppm \( \rightarrow \) TMS Tetramethylsilane

\[
\begin{align*}
\text{CH}_3 & \quad \uparrow 1 \quad \text{CH}_2 \quad \text{very e- rich proton/} \\
\text{CH}_3 & \quad \text{vs} 2 \quad \text{CH}_2 \quad \text{poor}
\end{align*}
\]
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**Equivalent Protons**

- All equivalent protons have the same chemical shift (S).
- Non-equivalent protons do not have the same chemical shift (S).

**2 Signals**

- B: upfield, C- rich
- A: downfield, C-poor

**3 NMR signals**

- Aldehyde
- Aromatic
- Vinyl Hydrogen

**Chemical Shifts (S) of Some Common Protons**

- Aldehyde
- Aromatic
- Vinyl Hydrogen
- Halogen, Oxygen
- α Hydrogen: CHy Alkanes

**TMS**
- **Anisotropy**: Double bonds cause protons to go way down field 5-8 ppm.

- **Protons on Nitrogen + Oxygen**
  - NH\_2 \rightarrow 0.5-4 ppm
  - OH \rightarrow 1.5-4 ppm
  - R-\(\dot{\text{O}}\)-H Tend to be broad

Have 3 aspects/qualities about the NMR signal N-H 1-4 ppm to be broad:

1. **Chemical Shift**: Location in ppm → Tells Type of Proton
2. **Integration**: Size of Peak/Area → From the # of Protons - 1st is H Large Peak
3. **Splitting Pattern**: How the carbons are connected.

**Splitting of the Signal**

- **Tri-bromo ethanol**
  - Br-\(-\text{C}-\text{C}H_A\)
  - H\_8 \rightarrow 1 proton
  - H\_8 \rightarrow \(\frac{1}{2}\) proton

- **Br-\(-\text{C}-\text{C}H_A\)**
  - H\_8 \rightarrow 2 protons