NMR continued.

- Splitting by $n$ neighbors gives $n+1$ lines.

- Circle absorbing H's
  - Underline splitting H's (neighbors)

- $\text{C}_3\text{H}_3\text{Br}$
  - IHD: 0
  - $\text{IHD} = \frac{2C + 2 - H - X + N}{2}$
  - Gives # of double bonds or rings

- Close to EFG (Br)
  - Highest frequency, most out of field

- Equivalent H's Do not split each other.

- Integra: the intro of integrals tells you how many H's are causing each peak.
Submit a Single-sided Copy to the Office
DO NOT STAPLE

Trends in δ values

<table>
<thead>
<tr>
<th></th>
<th>CH₃Cl</th>
<th>CH₂Cl₂</th>
<th>CHCl₃</th>
</tr>
</thead>
<tbody>
<tr>
<td>1H</td>
<td>1.06</td>
<td>1.25</td>
<td>1.56</td>
</tr>
<tr>
<td>13C</td>
<td>0.00</td>
<td>10-526</td>
<td>15-566</td>
</tr>
</tbody>
</table>

Compare 1H for CH₃Cl & CH₃Br

which is high free & why.

CH₃Cl is higher, Cl is more electronegative than Br
so...

CH₃F > CH₃Cl > CH₃Br > CH₃I

Higher Magnetic Field Magnets separate peaks better than lower field Magnets.
- Peaks will come at different frequencies - Confusing
  some use S to normalize

\[ S = \frac{\text{h}z \text{ from TMS}}{\text{spectroscopic frequency}} \]
Reference for NMR = TMS (tetramethylsilane) or (trimethylsilylacetone)

1) Has 12 equivalent H's
2) Si is electropositive compared to carbon
3) Volatile, Boils @ 23°C (easy to remove from sample)

Solvent for NMR, cannot have H's

CCl₄ is not a very good solvent

CDCl₃ is good but it has an H, so we use

CDCl₃ deuterio chloroform, D does not interact w/ H NMR

CDCl₃ will always contain a small quantity of CHCl₃ that can be seen in the spectrum

δ (ppm) = \( \frac{\Delta \nu (\text{MHz})}{\nu (\text{MHz})} \)

\( \text{H}_3 \text{C} \quad \text{H}_3 \text{C} \)

100 MHz instant, can @ 200 MHz from TMS

300 MHz 600 Hz

δ (CH₃) = \( \frac{200 \text{ Hz}}{100 \text{ MHz}} = \frac{600 \text{ Hz}}{300 \text{ MHz}} = 2.6 \)

CH₃-CH₂-OH → CH₃-CH₂-O⁻ + CH₃-CH₂-O⁻ → CH₃-CH₂-O⁻ + CH₃-CH₂-O⁻

- Protons on O, N can change environment through exchange
- Often will not show splitting w/ neighbors
- Often broad
\[ \text{CH}_3\text{-CH}_2\text{-OH} + \text{D}_2\text{O} \rightarrow \text{CH}_3\text{-CH}_2\text{-O}\text{-D} \text{ H is now gone.} \]

3 different H's

\[ \text{Cl} \quad \begin{array}{c} \text{O} \\ \text{H} \\ \text{H}_a \\ \text{H}_b \\ \text{H}_c \end{array} \]

1H 1H 1H first order spectrum

\[ \text{12} \quad 6 \quad 5 \quad 1 \]

distance between peaks in a doublet/multiplet = J

\[ J_{ab} = J_{ba} = 10 \text{ Hz in this case.} \]

H's on double bonds are more dampened than you would expect due to magnetic anisotropy

\[ J \text{ 1st order} \]

Peaks for apart

Leaving

\[ \text{Singlet when the same} \]

when peaks are leaving towards each other they are splitting each other
why splitting occurs.

\[ \begin{align*}
\text{H}_b & \text{ alone} \\
\text{H}_a & \text{ can be } +\frac{1}{2} \text{ or } -\frac{1}{2}
\end{align*} \]

\[
\begin{align*}
\text{Bo} & \\
\text{B}_0 + \frac{1}{2} & \text{ or } \text{B}_0 - \frac{1}{2}
\end{align*}
\]

\[
\begin{align*}
\text{H}_b & \text{ alone} \\
\text{H}_a & +\frac{1}{2} -\frac{1}{2} \\
\text{H}_b & +\frac{1}{2} -\frac{1}{2}
\end{align*}
\]

Splitting is determined by Pascal's Triangle

1

single

doublet

triplet

quartet

pentet

quintet

1 5 10 10 5 1 grief