Nuclear Magnetic Resonance Spectroscopy (NMR)

• Spectrum represents the different interactions of **stereochemically different** protons (\(^1\)H) with the applied magnetic field.

• We will focus on \(^1\)H NMR (proton, H\(^+\))

• **4 general rules for \(^1\)H NMR spectra**

  1. Only stereochemically different \(^1\)Hs give different signals.

     ![Diagram](image)

     CH\(_3\)CH\(_2\)-Cl
     Different H
     Different NMR signal

     CH\(_3\)CH\(_2\)CH\(_2\)CH\(_3\)
     Same H, symmetric
     Different H
     Different NMR signal

  2. Area covered under the signal is proportional to the number of \(^1\)Hs causing the signal and is usually represented by integrals.

     ![Diagram](image)

     1
     2
     3

     6  5  4  3  2  1  0

     PPM

  3. The **Chemical Shift** (where on spectrum each peak appears) depends on the “chemical environment” of each proton. (see above picture)

     a. \(^1\)Hs close to electronegative atoms (O, N, X (halogen)) or aromatics shift to the left (deshielded, downfield shifted)

     b. The larger the number of \(^1\)Hs on the same carbon the more to the right (shielded, upfield shifted) the NMR signal is.
4. The multiplicity of the NMR peak depends on the number of $^1$Hs on neighboring carbons, NOT the same carbon. $^1$Hs attached to **adjacent carbons** split each other into:

$$\text{(n+1) peaks}$$

\[ n = \text{number of } ^1\text{Hs on adjacent carbons} \]

\[ \text{not the same C} \]

![NMR spectrum diagram](image)

a. Exchangeable, acidic $^1$H (-OH, NH$_2$) DO NOT split $^1$Hs on adjacent carbons and show on the spectrum as broad singlets.

a.

![Exchangeable, acidic H diagram](image)

b. Identical Hs symmetric q (quartet) [3+1]

b.

![Identical Hs symmetric diagram](image)
b. Only **non identical** \(^1\)Hs split each other.

The shape/relative intensity of the peaks follows the algorithm of **Pascal’s Triangle**:

Pascal's Triangle

\[
\begin{array}{cccccc}
1 & 1 & 1 & 1 & 1 & 1 \\
1 & 2 & 3 & 4 & 5 & 6 \\
1 & 3 & 6 & 10 & 10 & 5 \\
1 & 4 & 10 & 10 & 5 & 1 \\
\end{array}
\]

- Calculating the degree of unsaturation for a compound (number of RDBs, Rings and Double Bonds) when the molecular formula is known.

\[
\text{#RDBs} = \frac{2n + 2 - \text{#Hs} - \text{#Halides} + \text{# N atoms}}{2}
\]

\(n = \text{# Cs}\) (Oxidens do not participate in this equation and can be ignored when RDBs are calculated)

i.e. \(\text{C}_9\text{H}_9\text{OCl}\) : \(\text{RDBs} = (2\times9 + 2 - 9 - 1)/2 = 5\)