# Nuclear Magnetic Resonance Spectroscopy (NMR)

- Spectrum represents the different interactions of **<u>stereochemically different</u>** protons ($^1H$) with the applied magnetic field.

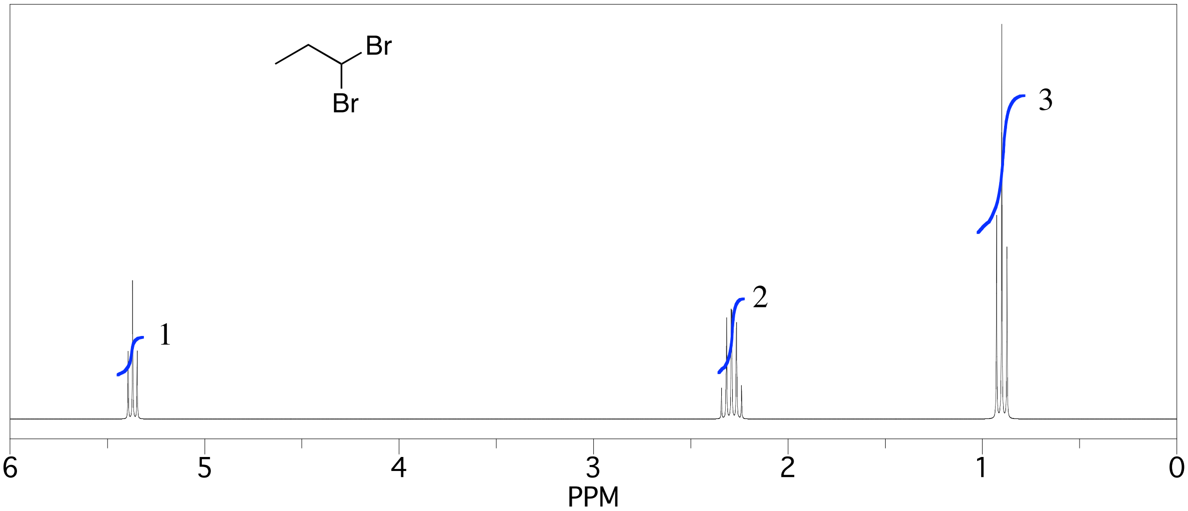
- We will focus on $^1H$ NMR (proton, $H^+$)

- **4 general rules for $^1H$ NMR spectra**

1. Only stereochemically different $^1H$s give different signals.

$$\underbrace{CH_3CH_2}_{\substack{\text{Different H}\\ \text{Different NMR signal}}}\text{-Cl} \qquad \overbrace{CH_3\underbrace{CH_2CH_2}_{\text{Same H, symmetric}}\underbrace{CH_3}_{\substack{\text{Different H}\\ \text{Different NMR signal}}}}^{\text{Same H, symmetric}}$$

2. Area covered under the signal is proportional to the number of $^1H$s causing the signal and is usually represented by integrals.

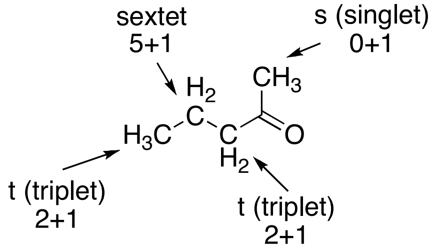


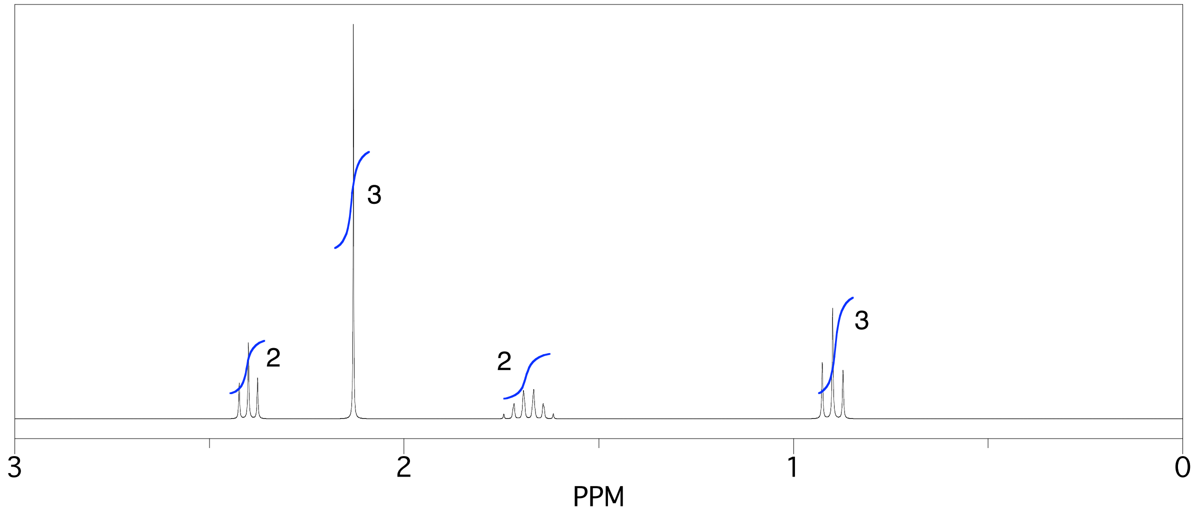
3. The **Chemical Shift** (where on spectrum each peak appears) depends on the "chemical environment" of each proton. (see above picture)
    a. $^1H$s close to electronegative atoms (O, N, X (halogen)) or aromatics shift to the left (deshielded, downfield shifted)
    b. The larger the number of $^1H$s 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:

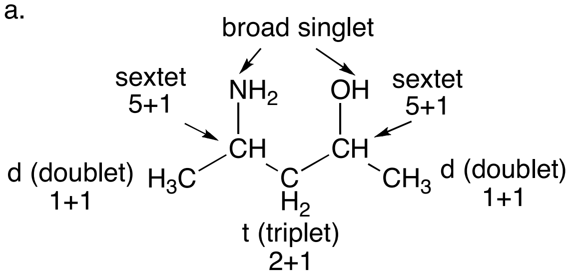
(n+1) peaks

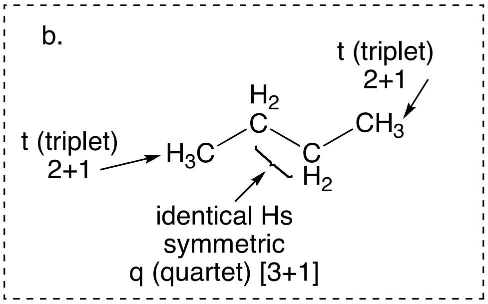
n = number of 1Hs on adjacent carbons
(not the same C)

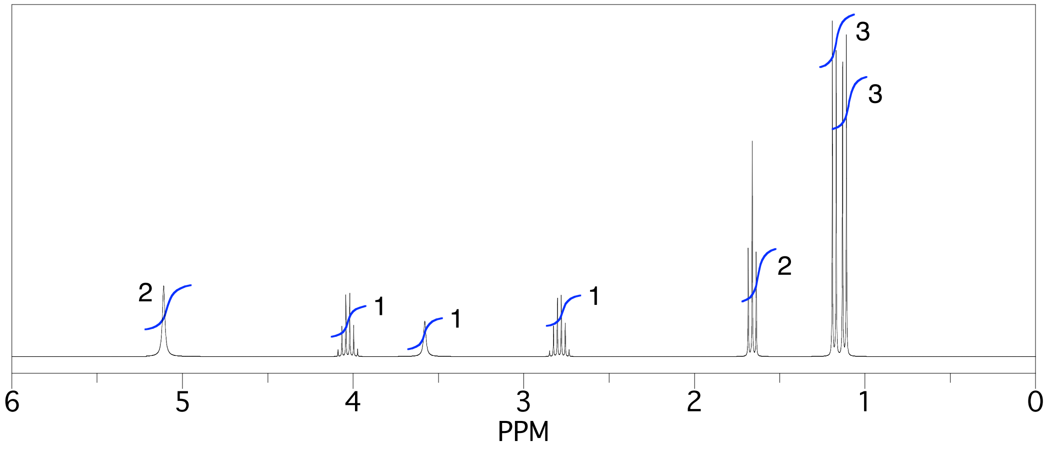




a. Exchangeable, acidic $^1$H (-OH, $NH_2$) DO NOT split $^1$Hs on adjacent carbons and show on the spectrum as broad singlets.



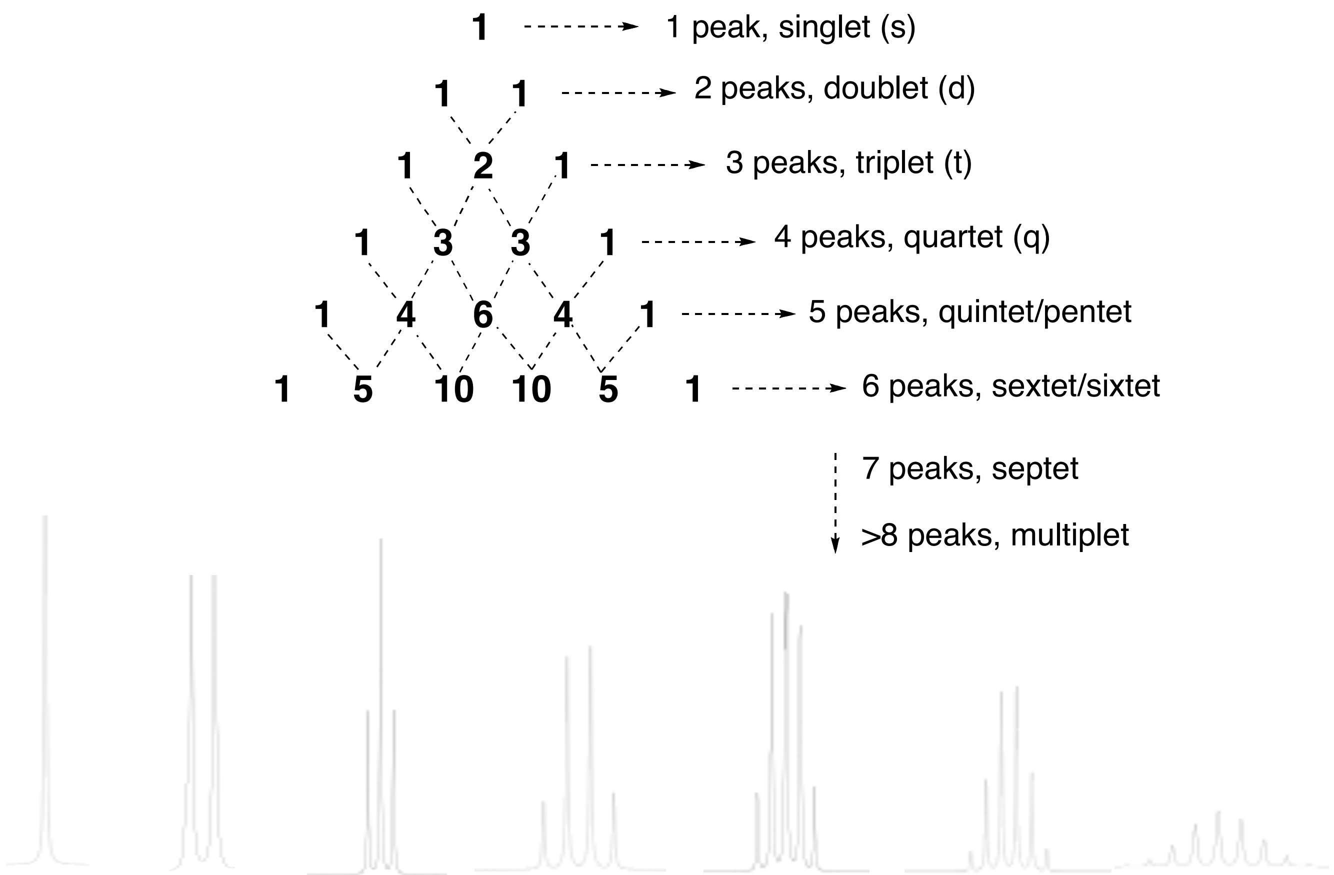




b. Only **non identical** $^1$Hs split each other.

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

Pascal's Triangle



1 peak, singlet (s) | 2 peaks, doublet (d) | 3 peaks, triplet (t) | 4 peaks, quartet (q) | 5 peaks, quintet/pentet | 6 peaks, sextet/sixtet | 7 peaks, septet

- 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 = # Cs
(Oxygens do not participate in this
equation and can be ignored when
RDBs are calculated)

i.e. $C_9H_9OCl$ : RDBs = (2x9 + 2 – 9 – 1)/2 = 5