Chapter 13 - Nuclear Magnetic Resonance Spectroscopy

$^1$H NMR Spectroscopy

More complicated splitting occurs when there are non-equivalent hydrogens coupling the same nucleus with different coupling constants. The patterns can be predicted by building a splitting tree diagram with one nuclear coupling at each level.

The pattern is NOT a triplet if the coupling constants are not identical.

The more couplings that are present, the more complicated the pattern peaks can be. Again, if all coupling constants are the same, the peak pattern can be predicted by the n+1 rule.
Strategies for determining unknowns.
Determine units of unsaturation
Identify functional groups
Identify pieces of the molecule
Put the pieces together in a reasonable way
Double check that your structure matches all the data

General Formula for Units of Unsaturation

\[
\text{UN} = \frac{(2n+2) - \#H - \#X + \#N}{2}
\]

- \(2n+2\) is the number of H’s if completely saturated
- \(\#H\) is the actual number of H’s in the molecule
- \(\#X\) is the actual number of halogens
- \(\#N\) is the actual number of nitrogens
- divide by 2 because each unit of unsaturation removes 2 H’s from the molecule

For example

\[
\text{C}_8\text{H}_8\text{CINO} \quad \text{UN} = \frac{(16+2) - 8 - 1 + 1}{2} = \frac{10}{2} = 5
\]