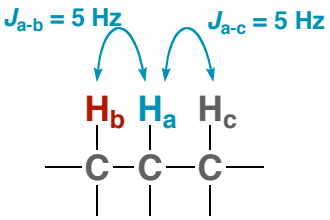
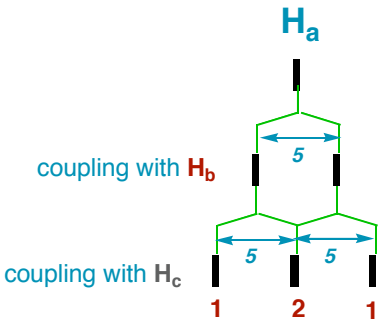
Chapter 13 - Nuclear Magnetic Resonance Spectroscopy

^{1}H NMR Spectroscopy

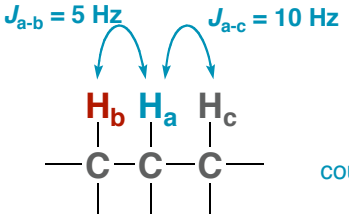
More complicated splitting occurs when there are non-equivalent hydrogens coupling the same nucleus with different coupling constants. The patterns can be predicted by building a splitting tree diagram with one nuclear coupling at each level.

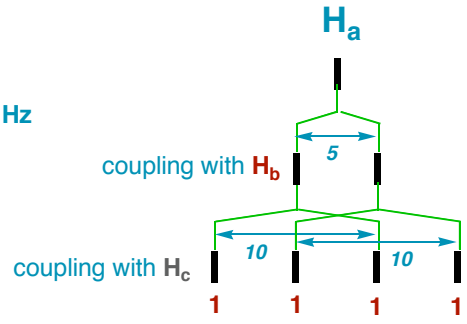




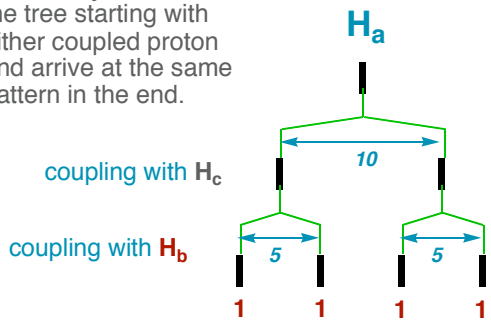
If the couplling constants are the same, it looks just like coupling with a CH_2 group.

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

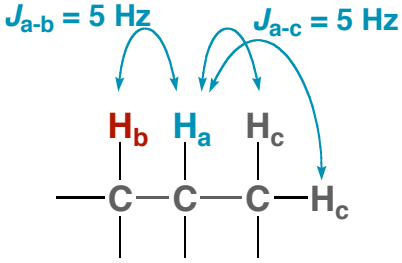


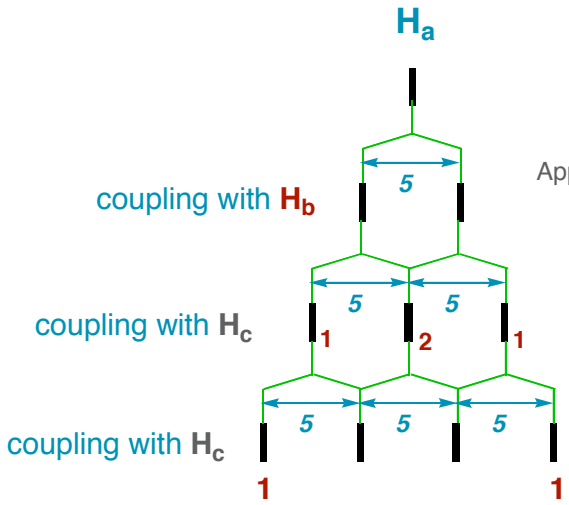


Note that you can draw the tree starting with either coupled proton and arrive at the same pattern in the end.

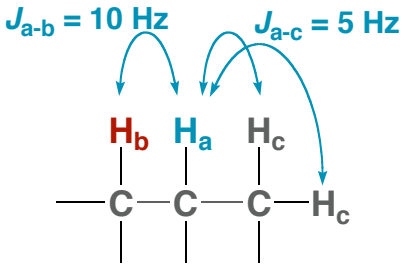


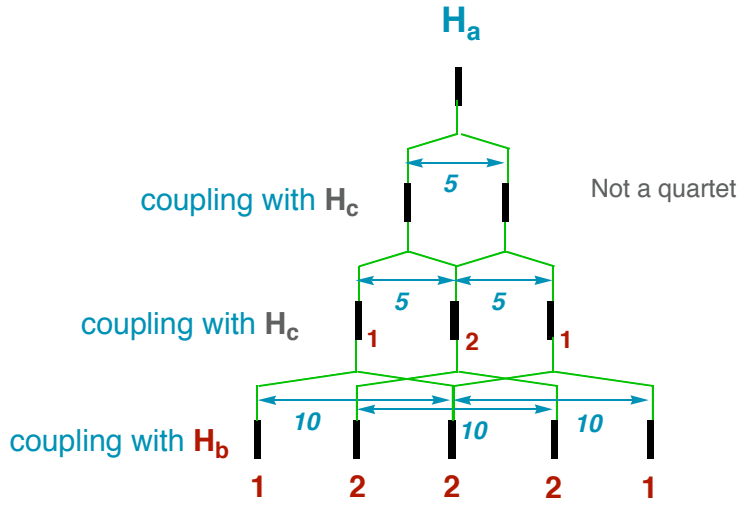
The more couplings that are present, the more complicated the pattern peaks can be. Again, if all coupling constants are the same, the peak pattern can be predicted by the n+1 rule.





Appears like a quartet





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

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

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 numnber of nitrogens
divide by 2 because each unit of unsaturation removes 2 H's from the molecule

For example

C_8H_8ClNO

$$UN = \frac{(16+2) - 8 - 1 + 1}{2} = \frac{10}{2} = 5$$