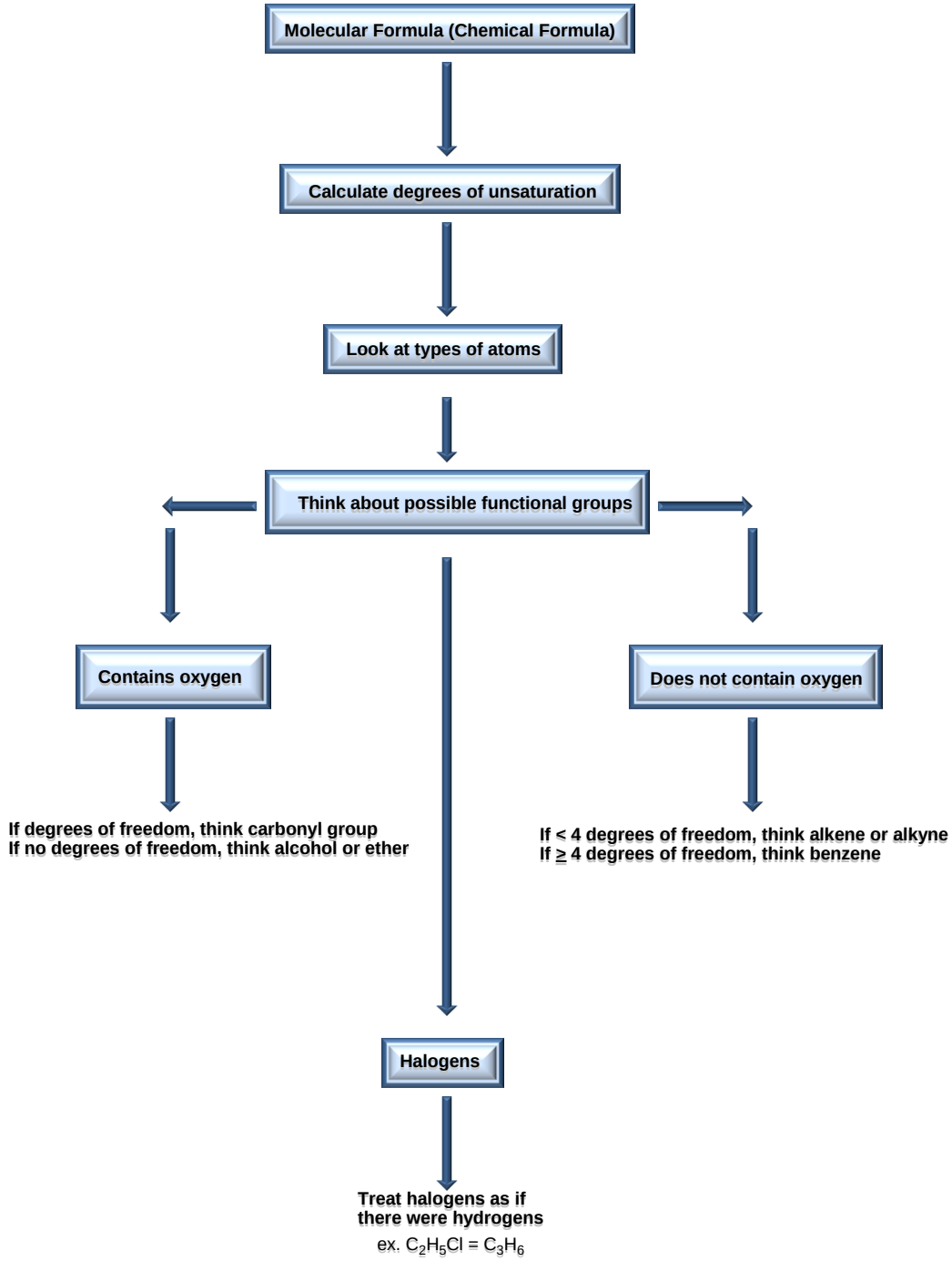
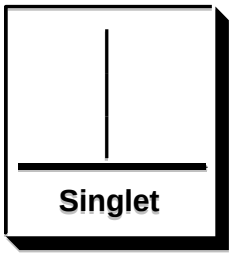
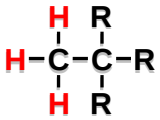
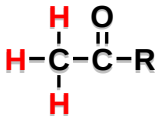
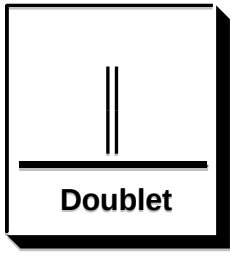

Molecular Formula (Chemical Formula)
Calculate degrees of unsaturation
Look at types of atoms
Think about possible functional groups
Contains oxygen
Does not contain oxygen
If degrees of freedom, think carbonyl group
If no degrees of freedom, think alcohol or ether
If < 4 degrees of freedom, think alkene or alkyne
If ≥ 4 degrees of freedom, think benzene
Halogens
Treat halogens as if
there were hydrogens
ex. $C_2H_5Cl = C_3H_6$



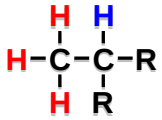
- No neighboring (adjacent) hydrogens

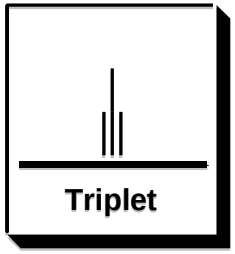




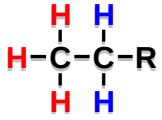


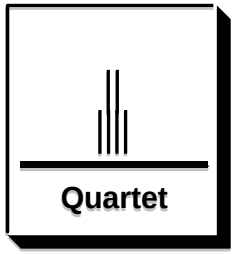
- One neighboring (adjacent) hydrogen



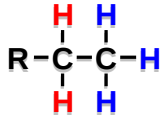


- Two neighboring (adjacent) hydrogens



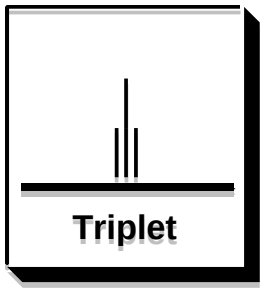


- Three neighboring (adjacent) hydrogens

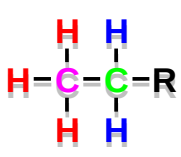


H = Hydrogens that we are interseted in
H = Hydrogens that we use for the n+1 rule

Note: the number of lines in the peak ***does not*** refer to the number of hydrogens; a singlet does not mean 1 hydrogen; a double does not mean 2 hydrogens



All three are equivalent

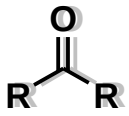


- Pick a specific carbon with hydrogens
- Look at adjacent carbon(s) and count the number of hydrogens...then add 1
- The n + 1 value refers to the peak arising from the carbon with hydrogens you picked

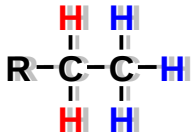
n + 1 = 2 + 1 = 3 (triplet)

In this case, the triplet refers to signal (peak) from the three red hydrogens

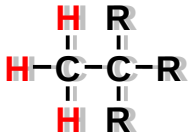
We have 1° of unsaturation and oxygens: carbonyl

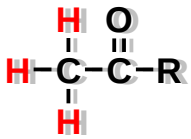


We have a quartet at ~ 4 ppm: these hydrogens must be next to 3 hydrogens

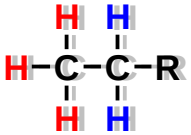


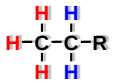
We have a singlet at ~ 2 ppm: these hydrogens are not next to any hydrogens

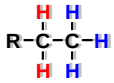


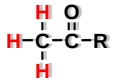


We have a triplet at ~ 1 ppm: these hydrogens must be next to 2 hydrogens

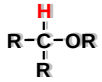






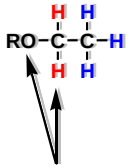


Where does the extra oxygen go? Let's look at our NMR charts:

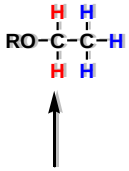


H = 3-4 ppm

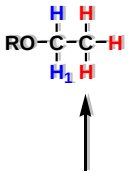
Therefore, we must have:



gives rise to 4 ppm shift

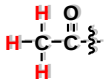


quartet (n+1)

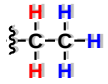


triplet (n+1)

Now, we have used 2 carbons, 5 hydrogens, and one oxygen. All we have left to figure out is the remaining 2 carbons, 3 hydrogens, and 1 oxygen. After our analysis, we know we have a carbonyl and a singlet peak at 2 ppm. Let's see how to put this together:



singlet (n+1)



(from above)