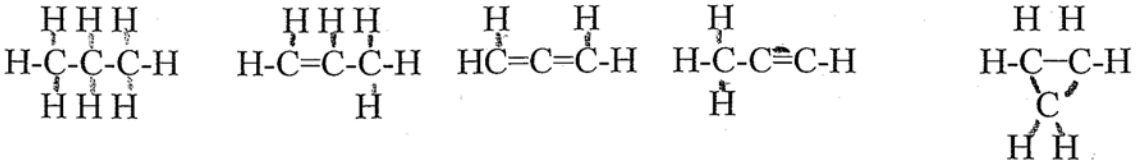
1.6 Predicting the Number of Double Bonds or Rings in a Formula

How do we decide whether we need any double bonds or rings when we are trying to draw structures? We will look at this in some detail and come up with an answer, because it will make life a lot simpler when we are drawing isomers with a given formula.

Compare the formulas for the following structures



C_3H_8 C_3H_6 C_3H_4 C_3H_4 C_3H_6

Note that the addition of a C=C results in a formula with 2 less H atoms than the saturated propane molecule with only single bonds. Putting two double bonds into a structure removes 4 H's. Introducing a triple bond in the structure removes 4 H atoms. The presence of a ring also removes 2 H atoms from the formula compared with the original propane molecule. These observations are true in general, not just for 3 C atoms. We can formulate the following generalizations.

A molecule with only single bonds, no double or triple bonds and no rings, is said to be **saturated**. It has the maximum number of H atoms (or equivalently halogen atoms) that is possible for that number of C atoms. Double bonds, triple bonds and rings all reduce the number of H atoms (or halogens) in the formula and a molecule with double bonds or rings is referred to as unsaturated. A **double bond** removes 2 H atoms and is said to be a **site of unsaturation (or degree of unsaturation)**. A **triple bond** removes 4 H atoms and constitutes **2 sites of unsaturation**. A **ring** removes 2 H atoms and also constitutes a **single site of unsaturation**.

How many H atoms are there in a **saturated** molecule?

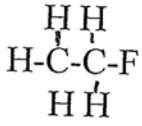
Let's look at the formulas for methane, ethane, propane, butane and pentane:

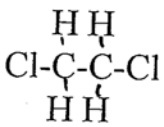
CH_4 C_2H_6 C_3H_8 C_4H_{10} C_5H_{12}

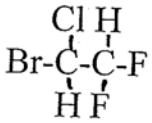
There is a relationship between the number of H atoms and the number of C atoms in each of these saturated molecules. Namely, if there are "n" C atoms in a formula, there will be (2n+2) H atoms in the saturated molecule.

How many H atoms are in a saturated molecule with
8 C atoms? _____ 10 C atoms? _____

Halogen atoms in a formula







C_2H_5F $C_2H_4Cl_2$ $C_2H_2F_2ClBr$

Note that all of these molecules are saturated (no double bonds, rings, or triple bonds) but they will not obey the 2n +2 rule unless we count the halogens (F, Cl, Br, I) in along with H atoms The halogens can substitute for H atoms 1 to 1, so we must include them in our counting along with H atoms. So include ***halogens*** along with ***hydrogen*** in counting the "H" actual molecular formula!

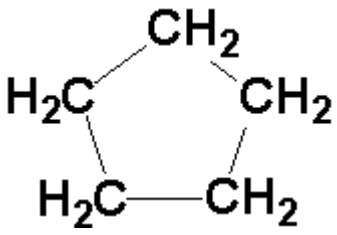
	C_2H_5F	$C_2H_4Cl_2$	$C_2H_2F_2ClBr$
	5H + 1 F	4 H + 2 Cl	2 H + 2 F + 1 Cl + 1 Br
	6 "H's"	6 "H's	6 "H's"
Sites of unsaturation	0	0	0

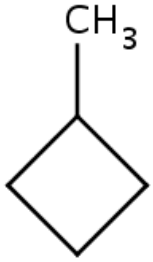
(Halogens were included with H in above calculations.)

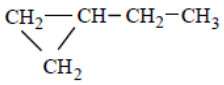
How many sites of unsaturation are in C_5H_{10}?

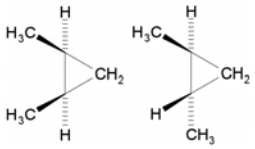
The 2n+2 rule predicts that a 5 C molecule should have 12 H atoms. The actual formula only has 10 H atoms, 2 short of saturation. Therefore there is one site of unsaturation. Any structure with this formula will need to have either a double bond or a ring.

Some of the many possibilities include:
1) a ring. (Ring can have any number of atoms within it.)



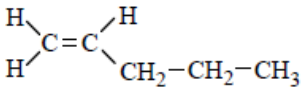


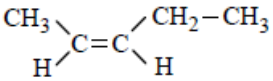


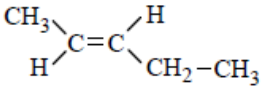


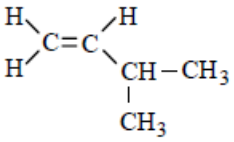
(What type of isomers are the above h molecule?)

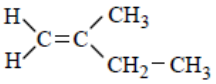
2)Molecules with C=C

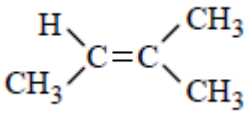












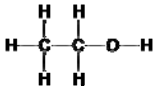
Predict how many sites of unsaturation will be found in the following formulas. Draw at least 3 isomers for each of the formulas.

a)C_6H_{10} b)$C_5H_{10}F_2$

How many sites of unsaturation in $C_3H_6Br_2$? Draw 4 isomers with the formula $C_3H_6Br_2$.

How many sites of unsaturation in $C_4H_8F_2$? Draw 5 isomers with the formula $C_4H_8F_2$:

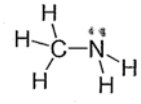
Molecules with O in the formula

If we look at the structural formula for ethanol: 
we see that the formula is C_2H_6O and that there are 6 H atoms for 2 C atoms, just like in the case of ethane(C_2H_6) . Thus, the presence of O does NOT affect the "2n+2" rule and the O atom is NOT included with H atoms like we did with the halogen atoms when determining saturation.

Predict the number of sites of unsaturation in the following examples. Draw two isomers for the each formula.

C_2H_6O $C_2H_4F_2O$ C_2H_2O

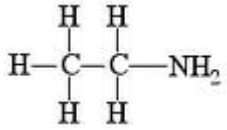
C_2F_2O $C_2H_2Cl_2O$ $C_2H_4F_2O$

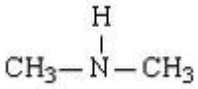
Molecules with N in the formula. Look at the saturated molecule:


If we apply the 2n+2 rule in the above molecule, we predict that we would have 4 H atoms for 1 C atom. The actual formula has 5 H atoms in the structure, 1 more H than predicted for a saturated molecule with 1 C atom We conclude that each N atom in a formula adds one more H atom to

the saturated formula. To calculate the number of H atoms in the saturated molecule with N in the formula we have: 2n+2 + # of N atoms.

a) How many sites of unsaturation are there in C_2H_7N?
A saturated molecule with 2 C atoms and 1 N atom will have
2(2) + 2 + 1= 7 H atoms. Since the above formula has 7 H atoms, it is saturated.
Draw 2 isomers with the formula C_2H_7N.





b) How many sites of unsaturation are there in C_2H_5N?
As calculated above a saturated molecule with 2 C atoms and one N atom will have 7 H atoms. The actual formula has 5 H atoms, 2 H atoms(one site) short of saturation. There is one site of unsaturation: either a double bond or a ring.
Draw 3 isomers with the formula C_2H_5N.

[put in hyperlink with answers here]

c) How many sites of unsaturation are there in C_2H_3N?
Draw 3 isomers with the formula C_2H_3N.

d) How many sites of unsaturation are in C_3H_9N? Draw 4 isomers with formula C_3H_9N

e) How many sites of unsaturation are in C_3H_7N? Draw 4 isomers with formula C_3H_7N.

f) How many sites of unsaturation are in C_3H_5N? Draw 4 isomers with formula C_3H_5N.

g) How many sites of unsaturation are in C_3H_3N? Draw 4 isomers with formula C_3H_3N.