Unsaturation

All,  
Please see below for a correction and additional information regarding unsaturation  

Unsaturation / Elements of Unsaturation / Degrees of Unsaturation / Index of Hydrogen Deficiency:  
Use the molecular formula to calculate the number of unsaturations (rings or multiple bonds). The degree of unsaturation indicates whether or not the compound has one or more double bonds or rings, or even a triple bond. There are different ways to calculate it.

*Note the following relationship between carbon and hydrogen: alkanes - C\textsubscript{n}H\textsubscript{2n+2}; alkenes and cyclohexane - C\textsubscript{n}H\textsubscript{2n}; alkynes - C\textsubscript{n}H\textsubscript{2n-2}. Try these formulae by analyzing ethane, ethene, and ethyne.

*Always compare to the formula of alkanes, C\textsubscript{n}H\textsubscript{2n+2}, which are the most saturated molecules. Note the following rules when heteroatoms (atoms other than carbon and hydrogen) are present:
  
  Organohalogenes, containing C, H, X where X = F, Cl, Br, I; organooxygen compounds, containing C, H, O; and organonitrogen compounds, containing C, H, N. Of course there are molecules that have all of the above, i.e. C, H, O, X, N.

Take the formula that you are given and

- **Add** the number of halogens to the number of hydrogens  
- **Ignore** the number of oxygens  
- **Subtract (not add)** the number of nitrogens from the number of hydrogens

*For example:*
C\textsubscript{5}H\textsubscript{9}N is equivalent to “C\textsubscript{5}H\textsubscript{8}”. Compare the latter with a fully saturated molecule. According to C\textsubscript{n}H\textsubscript{2n+2} an alkane with 5 carbons should have 12 hydrogens. So, half of the hydrogen difference gives you the element(s) / degree(s) of unsaturation: (12-8) / 2 = 2. Thus, C\textsubscript{5}H\textsubscript{9}N has two degrees of unsaturation and could contain one of the following: a) a triple bond; b) two double bonds or c) one double bond and a ring.

Pyridine has three double bonds and one ring = 4 degrees of unsaturation

*Another Example:*
Consider the formula C5H5N.  
Subtract (not add) one hydrogen for each nitrogen, yielding C5H4.  
Compare it to CnH2n+2.  
This yields, for n=5, the formula C5H12.  
Compare C5H12 with C5H4 and find a difference of 8 hydrogens.  
Divide 8 by 2 and find 4 degrees of unsaturation.  
The example could be pyridine. More than one structure may be possible.

Or take the formula you are given for an unknown and apply it to the equation below:
- **Number of Unsaturations = {2(#C) + 2 - #H - #Hal + #N}/2**

For example: C\textsubscript{5}H\textsubscript{9}N would yield: {2x5 + 2 - 9 - 0 + 1}/2 = 2