Empirical and Molecular Formulas
Empirical measurements are based on a measurable quantity like mass. Knowing the mass of each element in a compound we can determine it's formula. There are two types of formulas, empirical and molecular.

Empirical Formula: Lowest whole number ratio of the elements in a compound
Molecular Formula: Actual whole number ratio of the elements in a compound.

For salts that do not have homonuclear diatomic ions (like Hg_2^{+2} or O_2^{-2}) the empirical formula is the formula we write to describe the salt. But multiple molecules can have the same empirical formula. For example, benzene (C_6H_6) and acetylene (C_2H_2) both of the empirical formula of CH.

There are two types of problems we will solve, first those from Mass data and second those from mass percent information.

Steps:

1. Obtain Mass of Each Element (in grams)
-if given % composition assume 100 g and convert to mass.
-if given total mass you need the mass of all but one element (sum of masses equals total mass)
-if given % composition you need that of all but one element (sum of percents equals 100 %)

2. Calculate # of moles of each element present from masses and atomic weights
(you do not need to use a huge number of sig figs in atomic weights)
- You now have a formula representing the mole ratio of the elements in the compound and you need to make these integers.

3. Divide # of Moles of each element by the one with the smallest value (forcing it to one and making all other values greater than one).

4. Multiple the results of step 3 by the smallest integer which will convert them all to whole numbers.
Trick: convert decimals to fractions and multiply by lowest common denominator

$$\frac{1}{X} = \text{decimal expresssion} \Rightarrow X = \frac{1}{\text{decimal expression}}$$

Examples:	0.50 = 1/2	0.33 = 1/3	0.67=2/3	0.25 = 1/4	0.75 = 3/4
	0.2 = 1/5	0.4= 2/5	0.6 = 3/5	0.8 = 4/5	0.167 = 1/6

Part A: Empirical Formulas:

A.1 Aspirin contains carbon, hydrogen and oxygen and is 60.0% C and 35.5% O. What is the empirical formula of Aspirin?

Step 1: Calculate the mass of each element for a 100 g sample

$$60.0gC$$

$$35.5gO$$

$$100-60-35.5=4.5gH$$

Step 2: Calculate the moles of each substance present in the 100 gram sample. You can actually write a formula at this point, but it does not have integers.

$$60.0gC\left(\frac{molC}{12.01g}\right)=5$$

$$35.5gO\left(\frac{molO}{16.00g}\right)=2.2187$$

$$4.5gH\left(\frac{molH}{1.007g}\right)=4.4687$$

Step 3: Identify which species has the smallest number of moles and divide all mole values by that number. This makes the smallest value 1 and all others greater than one.

$$60.0gC\left(\frac{molC}{12.01g}\right)=5/2.2187=2.25$$

$$35.5gO\left(\frac{molO}{16.00g}\right)=2.2187/2.2187$$

$$4.5gH\left(\frac{molH}{1.007g}\right)=4.4687/2.2187=2$$

Step 4. Convert any decimals to fractions, and multiply all values by the lowest common denominator of all values.

$$60.0gC\left(\frac{molC}{12.01g}\right)=5/2.2187=2\tfrac{1}{4}=\frac{9}{4}(4)$$

$$35.5gO\left(\frac{molO}{16.00g}\right)=2.2187/2.2187=1=\frac{4}{4}(4)$$

$$4.5gH\left(\frac{molH}{1.007g}\right)=4.4687/2.2187=2=\frac{8}{4}(4)$$

$$C_9O_4H_8$$

Take home problems
A.2. You have a 3.3700 g sample of a salt which contains copper, nitrogen and oxygen. It contains 1.1418 g of copper and 1.7248 g of oxygen.

a. What is the mass nitrogen in the compound?

3.3700-1.1418-1.7248=0.5034

b. What is the empirical formula of the salt?

$$1.1418gCu\left(\frac{molCu}{63.546g}\right)=0.018\Rightarrow 0.018/0.018=1$$

$$1.7248gO\left(\frac{molO}{16.00g}\right)=0.1078\Rightarrow 0.1078/0.018=6$$

$$0.5034gN\left(\frac{molN}{14.007g}\right)=0.036\Rightarrow .036/0.018=2$$

CuN_2O_6

c. Identify the anion of the salt (assume copper was the cation)

If copper(II), than NO_3^- giving $Cu(NO_3)_2$

d. Name the salt

copper(II) nitrate

A.3 What is the empirical formula of a compound that contains 30.43% N and 69.57% O by weight?

$$30.43gN\left(\frac{molN}{14.007g}\right)=2.17\Rightarrow 2.17/2.17=1$$

$$69.57gO\left(\frac{molO}{16.00g}\right)=4.35\Rightarrow 4.35/2.17=2$$

NO_2

A.4 What is the empirical formula of a compound that contains 87.5% N and 12.5% H by weight?

$$87.5gN\left(\frac{molN}{14.007g}\right)=6.25\Rightarrow 6.25/6.25=1$$

$$12.5gH\left(\frac{molH}{1.007g}\right)=12.4\Rightarrow 12.4/6.25=2$$

NH_2

A.5 An unknown compound is made up of C, H, N and O. A 2.402-g sample of this compound contains 1.121 g of N, 0.161 g H, 0.480 g C, and an unspecified amount of oxygen. What is the empirical formula of the unknown compound?

$$1.121gN\left(\frac{molN}{14.007g}\right)=0.08\Rightarrow .08/0.04=2$$

$$0.161gH\left(\frac{molH}{1.007g}\right)=0.16\Rightarrow 0.016/0.04=4$$

$$0.480gC\left(\frac{molC}{12.011g}\right)=0.04\Rightarrow 0.04/0.04=1$$

$$(2.402-1.121-0.161-0.480)gO\left(\frac{molO}{16.00g}\right)=0.04\Rightarrow 0.04/0.04=1$$

N_2H_4CO

A.6 A substance was determined to be 49.9% oxygen, 37.5% carbon and 12.6% hydrogen by mass. What is the proper empirical formula for this compound?

$$49.9gO\left(\frac{molO}{16.00g}\right)=3.119\Rightarrow 3.119/3.119=1$$

$$37.5gC\left(\frac{molC}{12.011g}\right)=3.122\Rightarrow 3.122/3.119=1$$

$$12.6gH\left(\frac{molH}{1.007g}\right)=12.5\Rightarrow 12.5/3.119=4$$

CH_4O

A.7 A certain compound was found to contain 67.6% C, 22.5% O, and 9.9% H. What is the empirical formula?

$$22.5gO\left(\frac{molO}{16.00g}\right)=1.4\Rightarrow 1.4/1.4=1$$

$$67.6gC\left(\frac{molC}{12.011g}\right)=5.63\Rightarrow 5.63/1.4=4$$

$$9.9gH\left(\frac{molH}{1.007g}\right)=9.9\Rightarrow 9.9/1.4=7$$

C_4H_7O

B: Molecular Formulas

The empirical formula represents the lowest whole number ratio of the elements in a molecule while the molecular formula represents the actual formula of the molecule. Both Benzene (C_6H_6, molar mass = 78.12g/mol) and acetylene (C_2H_2, molar mass = 26.04g/mol) have the same percent composition (92.24 mass% carbon and 7.76% hydrogen) and the empirical formula, CH. The ratio of the atoms in the actual molecule is an integer multiple of those in the empirical formula (acetylene has twice the number of atoms and benzene has 6 times the number in the empirical formula). Likewise, the molar mass of a molecule will be an integer times that of the formula mass of the empirical formula (n = 1,2,3,4..?, note if these equal, n=1).

Trick: Calculate the formula mass of the empirical formula and divide this into the molar mass of the compound. This will give you the integer which when multiplied by the empirical formula gives you the molar formula.

In class problem

Look at problem A.7: A certain compound was found to contain 67.6% C, 22.5% O, and 9.9% H. If the molecular weight of the compound was found to be approximately 142 g/mol, what is the correct molecular formula for the compound?

C_4H_7O has an empircal weight (EW) of

4(12.01) +7(1.007) + 16.00=71.09g/mol

The molecular formula is an interger time the empircal formula

so the molar mass is an interger times the emprical mass(weight)

$$\text{MW=n(WW) so n=}\frac{\text{MW}}{\text{EW}}=\frac{142g/mol}{71.09g/mol}=2$$

So multiply all coeficients of the empirical formula by 2

the compound is $C_8H_{14}O_2$

B.1. A compound has an empirical formula of C_2HF has a molar mass of 132.06 g/mol. What is the molecular formula for the compound?

$$C_2HF \Rightarrow 44.03g/mol$$
$$n\left(C_2HF\right) \Rightarrow 132.06g/mol$$
$$n = \frac{132.06}{44.03} = 3 \quad \therefore C_6H_3F_3$$

B.2. What is the molecular formula if a 200.0 g sample of an acid with a molar mass of 616.73g/mol contains 171.36 g of carbon, 18.18g of nitrogen and the rest is hydrogen?

$$171.36gC\left(\frac{molC}{12.011g}\right) = 14.27 \Rightarrow 14.27/1.2979 = 11$$
$$18.18gN\left(\frac{molN}{14.007g}\right) = 1.2979 \Rightarrow 1.2979/1.2979 = 1$$
$$(200 - 171.36 - 18.18)gH\left(\frac{molH}{1.007g}\right) = 10.46 \Rightarrow 10.46/1.2979 = 8$$
$$C_{11}NH_8 \Rightarrow 154.173g/mol$$
$$n\left(C_{11}NH_8\right) \Rightarrow 616.73g/mol$$
$$n = \frac{616.73}{154.173} = 4 \quad \therefore C_{44}N_4H_{32}$$

B.3. Strychine has a molar mass of 334 g/mol and percent composition of 75.42%C, 6.63%H and 8.38%N and the rest oxygen. What is the formula of strychine.

$$75.42gC\left(\frac{molC}{12.011g}\right)=6.279\Rightarrow 6.279/0.5983=10.5\Rightarrow\frac{21}{2}$$

$$8.38gN\left(\frac{molN}{14.007g}\right)=0.5983\Rightarrow 0.5983/0.5983=1\Rightarrow\frac{2}{2}$$

$$6.63gH\left(\frac{molH}{1.007g}\right)=6.584\Rightarrow 6.584/0.5983=11\Rightarrow\frac{22}{2}$$

$$(100-75.42-8.386.63)gO\left(\frac{molO}{16.00g}\right)=0.5981\Rightarrow 0.5981/0.5983=1\Rightarrow\frac{2}{2}$$

$$C_{21}N_2H_{22}O_2\Rightarrow 334g/mol$$

$$n\left(C_{11}N_2H_8\right)\Rightarrow 334g/mol$$

$$n=\frac{334}{334}=1\quad\therefore C_{21}N_2H_{22}O_2$$