Empirical Formulae:

Let's start off this section with a couple definitions. A molecular formula, if you haven't figured it our already, is a shorthand way of writing down what elements, and how many atoms or moles of each of those elements, are present in a compound. An empirical formula is a molecular formula with all of the subscripts reduced to lowest form. Think of fractions. 4/10 is reduced to 2/5, 3/9 is reduced to 1/3, 10/2 is reduced to 5/1 or just 5. 11/3 stays 11/3 because it is already in lowest terms. Empirical formulae work the same way. Here are some examples:

Examples:

a) molecular formula: H_2O_2 empirical formula: HO

b) molecular formula: $C_{12}H_{14}O_2$ empirical formula: C_6H_7O

c) molecular formula: $Al(OH)_3$ empirical formula: $Al(OH)_3$

Okay, that isn't, or shouldn't be, such a hard subject. Here is where it gets a little trickier. You can easily do this type of problem; it will just take a little practice. Remember, the ultimate goal here is to determine the ratio of moles of each element in the compound (i.e. the subscripts), so keep in mind that you are looking more the number of moles of each element no matter what information you are given. You can be given several percentages in these problems. The percentages represent the percent composition of each element in the compound. You could also be given masses of each element or volumes and densities of each element or some other information, but whatever you are given, you need to get to moles:

1) Convert whatever information you are given about each element into moles of that element. If percentages are given all of the elements in a compound, you can assume that you have a 100 gram sample of the compound.
2) Divide each of the numbers of moles by the SMALLEST of them. This is the step that everyone forgets, so consider yourselves warned! Sometimes this step gives a numbers that is not whole number. In these cases, you will need to do some rounding. When deciding where to round to, keep the following in mind. Round to what ever is the closest of the following: .00, .25, .33, .50, .66, .75, or up to the next whole number. If the number you have is .78, round to .75, if it is .95, round up to the next whole number.
3) At this point, you need to multiply the values obtained in step 3 by a number that will get rid of any decimals. If the value is 1.25 you need to multiply ALL of the values from step 3 by 4 (1.25*4 = 5). If the value from step 3 has a decimal close to .66, (like 2.66) then multiply ALL of the values by 3 (2.66*3 = 8). If there are no decimals, you can skip this step.

The results of step 3 are the subscripts for each element in the empirical formula.

Examples:

a) A sample of a compound is 28.56% carbon, 4.80% hydrogen, and 66.63% nitrogen. What is the compounds empirical formula?

First step, is find the number of grams of each element in the compound. Because you are given percentages, you can assume that the sample size was 100 grams:

$$0.2856 \times 100\ \boldsymbol{g} = 28.56\ \boldsymbol{g}\ \mathbf{C} \qquad 0.0480 \times 100\ \boldsymbol{g} = 4.80\ \boldsymbol{g}\ \mathbf{H} \qquad 0.6663 \times 100\ \boldsymbol{g} = 66.63\ \boldsymbol{g}\ \mathbf{N}$$

Next step is to multiply each mass by the elements atomic weight to get the number of moles of each element:

$$28.56\ \boldsymbol{g}\ \mathbf{C} \times \frac{1\ \boldsymbol{mol}\ \mathbf{C}}{12.0112\ \boldsymbol{g}\ \mathbf{C}} = 2.378\ \boldsymbol{mol}\ \mathbf{C} \qquad 4.80\ \boldsymbol{g}\ \mathbf{H} \times \frac{1\ \boldsymbol{mol}\ \mathbf{H}}{1.00797\ \boldsymbol{g}\ \mathbf{H}} = 4.76\ \boldsymbol{mol}\ \mathbf{H}$$

$$66.63\ \boldsymbol{g}\ \mathbf{N} \times \frac{1\ \boldsymbol{mol}\ \mathbf{N}}{14.0067\ \boldsymbol{g}\ \mathbf{N}} = 4.757\ \boldsymbol{mol}\ \mathbf{N}$$

Now divide each number of moles by the smallest of them, which in this case is 0.305:

$$\mathbf{C} = \frac{2.378}{2.378} = 1 \qquad \mathbf{H} = \frac{4.76}{2.378} = 2.002 \approx 2 \qquad \mathbf{N} = \frac{4.757}{2.378} = 2.004 \approx 2$$

This now gives you the ratio of carbon to hydrogen to nitrogen. For every 1 carbon atom, the molecule contains 2 hydrogen atoms and 2 nitrogen atoms. This means that the empirical formula of the molecule is $\mathbf{CH_2N_2}$. Done!

b) A compound contains 14.6% carbon, 39.0% oxygen, and 46.3% fluorine. Give the empirical formula.

You'll notice that in this problem, you are not given a mass of the sample, so you assume that you have 100 grams of the compound. Step one is to find the mass of each element in the sample.

$$0.146 \times 100.\ \boldsymbol{g} = 14.6\ \boldsymbol{g}\ \mathbf{C} \qquad 0.390 \times 100.\ \boldsymbol{g} = 39.0\ \boldsymbol{g}\ \mathbf{O} \qquad 0.463 \times 100.\ \boldsymbol{g} = 46.3\ \boldsymbol{g}\ \mathbf{F}$$

Step 2:

$$14.6\ \boldsymbol{g}\ \mathbf{C} \times \frac{1\ \boldsymbol{mol}\ \mathbf{C}}{12.0112\ \boldsymbol{g}\ \mathbf{C}} = 1.216\ \boldsymbol{mol}\ \mathbf{C} \qquad 39.0\ \boldsymbol{g}\ \mathbf{O} \times \frac{1\ \boldsymbol{mol}\ \mathbf{O}}{15.9994\ \boldsymbol{g}\ \mathbf{O}} = 2.438\ \boldsymbol{mol}\ \mathbf{O}$$

$$46.3\ \boldsymbol{g}\ \mathbf{F} \times \frac{1\ \boldsymbol{mol}\ \mathbf{F}}{18.9984\ \boldsymbol{g}\ \mathbf{F}} = 2.437\ \boldsymbol{mol}\ \mathbf{F}$$

Now divide each number of moles by the smallest of them, which in this case is 1.216:

$$\mathbf{C} = \frac{1.216}{1.216} = 1 \qquad \mathbf{O} = \frac{2.438}{1.216} \approx 2 \qquad \mathbf{F} = \frac{2.437}{1.216} \approx 2$$

The last step is to make them all whole numbers. In this case, they already ARE all whole numbers, so C=1, O=2, and F=2. This gives the empirical formula of **CO_2F_2**.

c) A sulfide of cobalt contains 55.06% cobalt and 44.94% sulfur. What is the empirical formula?
Go through all the same steps, but this time I am not going to hold your hand so much.

$$55.06\ \boldsymbol{g}\ \mathbf{Co} \times \frac{1\ \boldsymbol{mol}\ \mathbf{Co}}{58.93\ \boldsymbol{g}\ \mathbf{Co}} = 0.9343\ \boldsymbol{mol}\ \mathbf{Co} \qquad 44.94\ \boldsymbol{g}\ \mathbf{S} \times \frac{1\ \boldsymbol{mol}\ \mathbf{S}}{32.07\ \boldsymbol{g}\ \mathbf{S}} = 1.401\ \boldsymbol{mol}\ \mathbf{S}$$

$$\mathbf{Co} = \frac{0.9343}{0.9343} = 1 \qquad \mathbf{S} = \frac{1.401}{0.9343} = 1.49 \approx 1.5$$

In this case, step three yields one value that has a decimal (S = 1.5) In order to fix this, multiply both Co and S by 2 to get them both to be whole numbers and you have Co=2 and S=3. The empirical formula is **Co_2S_3**.

d) You analyze a compound and find that it is 119.0g rhodium, 180.4g chromium, and 194.3g oxygen. What is the empirical formula of the compound?

$$119.0\ \boldsymbol{g}\ \mathbf{Rh} \times \frac{1\ \boldsymbol{mol}\ \mathbf{Rh}}{102.905\ \boldsymbol{g}\ \mathbf{Rh}} = 1.156\ \boldsymbol{mol}\ \mathbf{Rh}$$

$$180.4\ \boldsymbol{g}\ \mathbf{Cr} \times \frac{1\ \boldsymbol{mol}\ \mathbf{Cr}}{51.996\ \boldsymbol{g}\ \mathbf{Cr}} = 3.469\ \boldsymbol{mol}\ \mathbf{Cr}$$

$$194.3\ \boldsymbol{g}\ \mathbf{O} \times \frac{1\ \boldsymbol{mol}\ \mathbf{O}}{15.9994\ \boldsymbol{g}\ \mathbf{O}} = 12.14\ \boldsymbol{mol}\ \mathbf{O}$$

$$\mathbf{Rh} = \frac{1.156}{1.156} = 1 \qquad \mathbf{Cr} = \frac{3.469}{1.156} = 3 \qquad \mathbf{O} = \frac{12.14}{1.156} = 10.5$$

Again, the third step yields a decimal, so you need to multiply ALL of them by an number to get rid of the decimal. In this case, you need to multiply by 2 because the decimal is .5. This gives an empirical formula of **$Rh_2Cr_6O_{21}$**

Have fun!!
Determine the empirical formula of each of the following compounds if a sample contains:
1) 57.3 grams and is 31.7% boron and 68.3% nitrogen
2) 69.94% iron and 30.06% oxygen
3) 40.0% carbon, 6.70% hydrogen, and 53.3% oxygen
4) 61.04% tin and 38.96% fluorine and has a mass of 56.301 grams
5) 0.0235 grams and is 87.5% nitrogen and 12.5% hydrogen
6) 32.79% sodium, 13.02% aluminum, and 54.19% fluorine
7) 62.1% carbon, 5.21% hydrogen, 12.1% nitrogen, and 20.7% oxygen
8) 1.56 kg of compound and is 5.2kg carbon, 13.9kg sulfur, and 30.85kg chlorine
9) 43.4g carbon, 19.2g oxygen, and 134.7g fluorine
10) 75.944 % carbon, 3.824% hydrogen, 20.232 % oxygen

You will also be asked to find the molecular formula based on a molecular mass and an empirical formula. This is probably one of the easiest things you will do in this class. You simply add up the formula weight of the empirical formula and divide it by the molecular mass. This will give you a ratio that you then multiply the empirical formula by. The result is the molecular formula.

Examples:

a) The molecular mass of the compound for which you found the empirical formula in example a) above is 126.15 grams per mole. What is the molecular formula?

The empirical formula in example a) was CH_2N_2 which has a formula mass of:

$$12.01\,\boldsymbol{g} \times 1 + 1.01\,\boldsymbol{g} \times 2 + 14.01\,\boldsymbol{g} \times 2 = 42.05\,\boldsymbol{g}$$

Now divide the molecular mass by the formula mass to get a ratio:

$$\frac{126.15}{42.05} = 3$$

The ratio is 3, so multiply the empirical formula by 3 to get the molecular formula:

$$3 \times (\mathbf{CH_2N_2}) = \mathbf{C_3H_6N_6}$$

Therefore the molecular formula is **$C_3H_6N_6$**!

b) The molecular mass of the compound whose empirical formula was found in example b) was found to be 164.02 grams per mole. Find the molecular formula.

Formula mass of CO_2F_2 is 82.01, so:

$$\frac{164.02}{82.01} = 2 \times (\mathbf{CO_2F_2}) = \mathbf{C_2O_4F_4}$$

c) The molecular mass of the compound whose empirical formula was found in example b) was found to be 214.07 grams per mole. Find the molecular formula.

Formula mass of Co_2S_3 is 214.07g/mol. Because the formula mass and the molecular mass are the same, the molecular formula is **Co_2S_3**

Using the empirical formulae you found in 1-10 above, and the molecular masses given, find the molecular formulae.

1) 204.93 g/mol
2) 159.69 g/mol
3) 90.03 g/mol
4) 389.42 g/mol
5) 32.06 g/mol
6) 209.95 g/mol
7) 696.78 g/mol
8) 229.96 g/mol
9) 166.03 g/mol
10) 316.32 g/mol