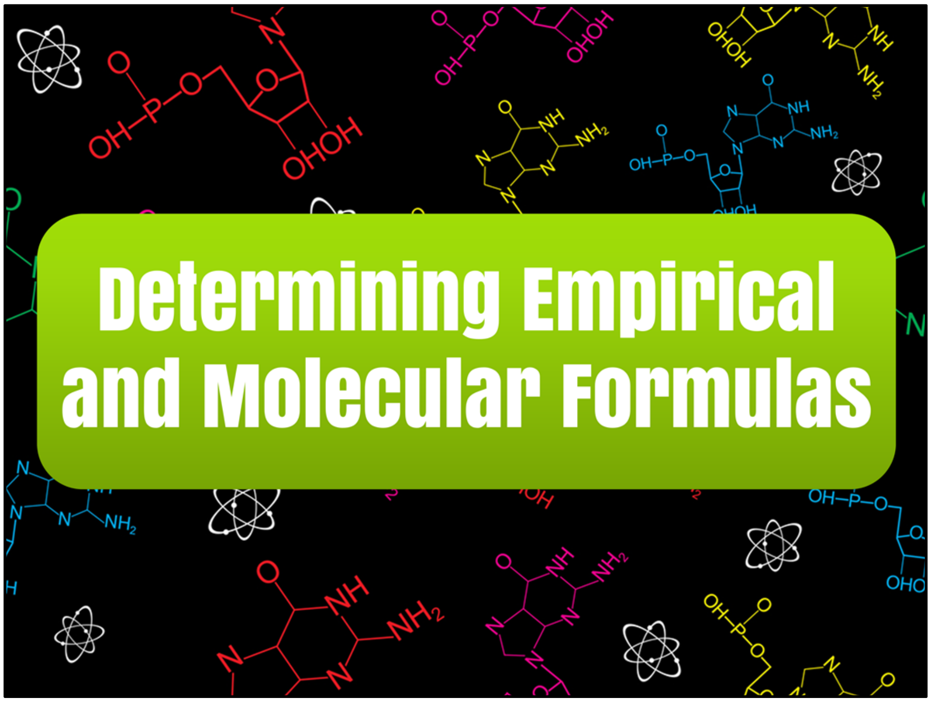
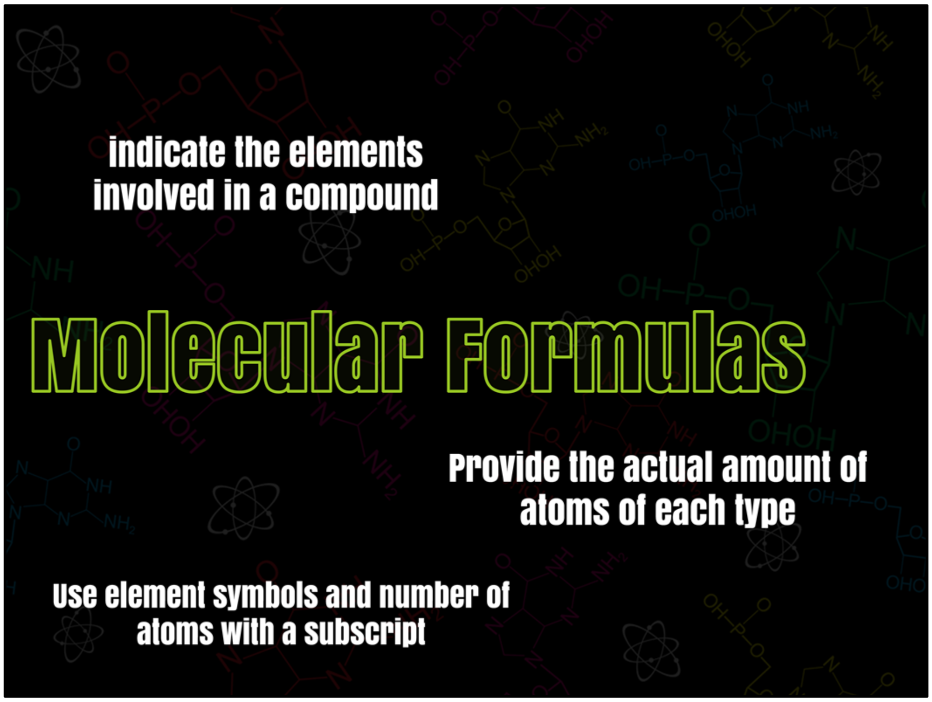
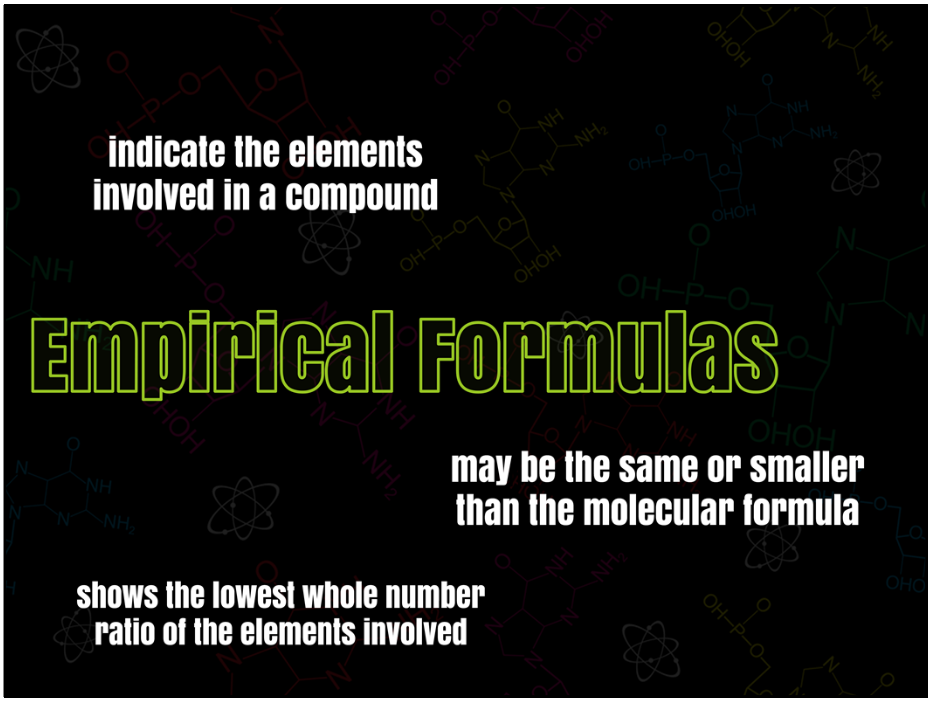
Module 5: Chemical Quantities and Composition
Topic 3 Content: Calculating Empirical Formulas and Molecular Formulas



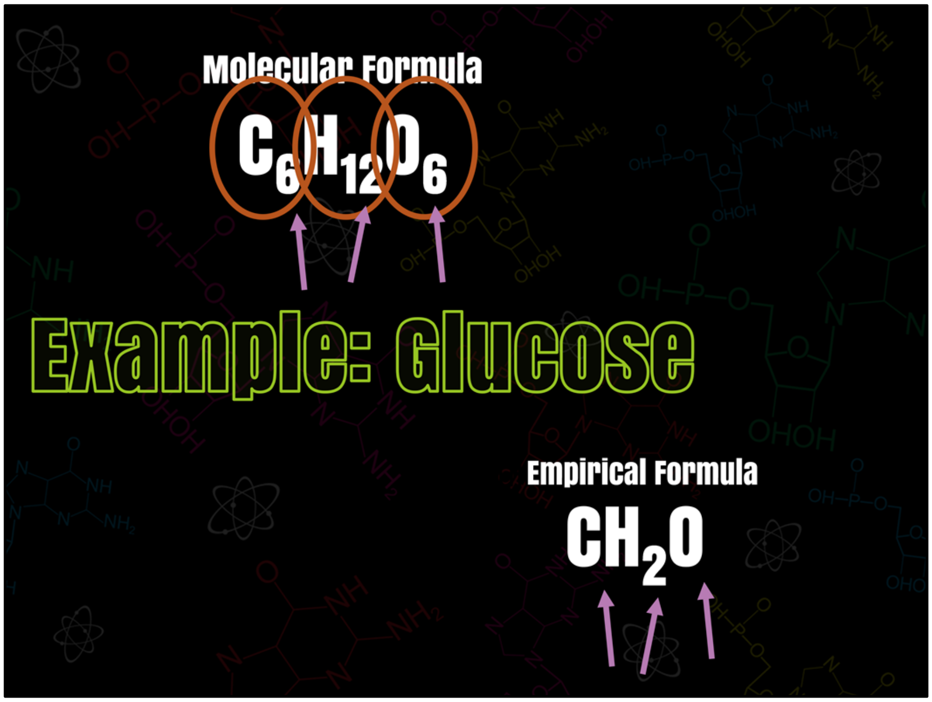
Determining Empirical and Molecular Formulas



Molecular formulas indicate the elements involved in a compound with the element symbols and the number of atoms of each element with a subscript. A molecular formula provides the actual amount of atoms of each type.



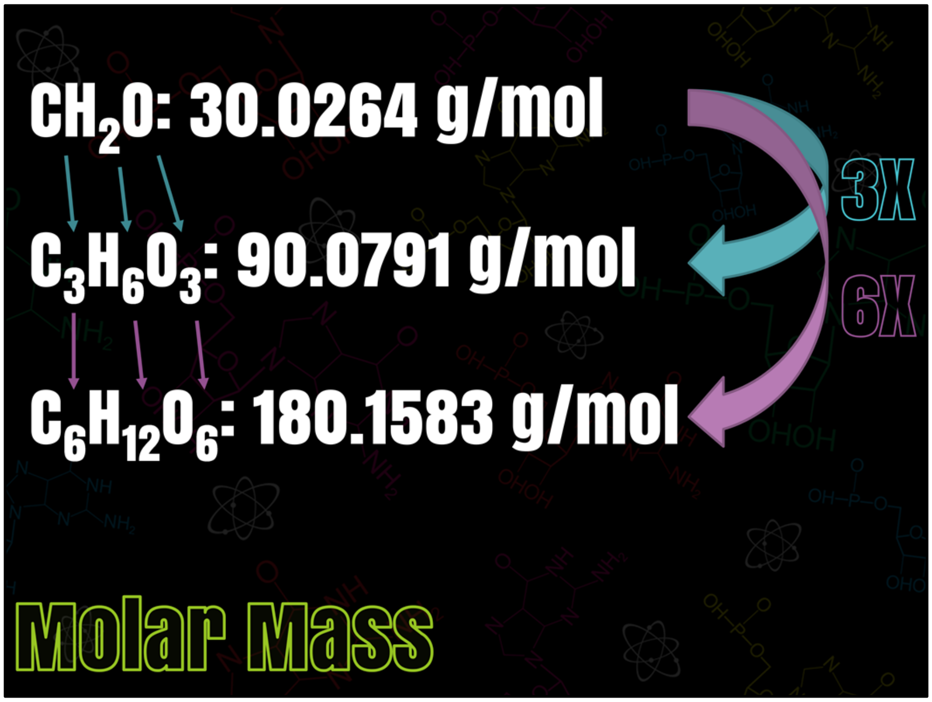
The empirical formula is similar in that it provides the symbols for the elements involved, but the empirical formula shows the lowest whole number ratio of the elements involved. In some cases, the empirical formula and molecular formula are the same. Many times, however, the empirical formula is much smaller.



Notice that glucose has 6 carbon atoms, 12 hydrogen atoms, and 6 oxygen atoms in each molecule. That is why six, twelve, and six appear as subscripts in its molecular formula.

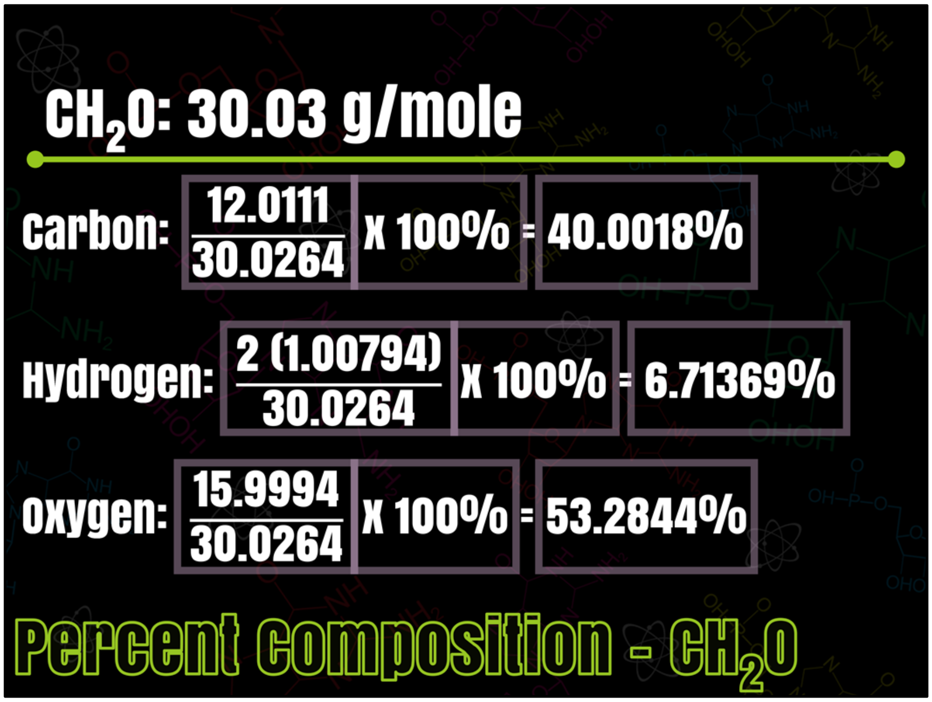
The empirical formula for glucose is reduced to simply one carbon atom for every two hydrogen atoms and one oxygen atom. This ratio has been reduced to its lowest compound. It is possible for many compounds to share the same empirical formula.

Sodium chloride, which is the scientific name for salt, has the empirical formula of NaCl. In this instance, the empirical formula is the same as the molecular formula.

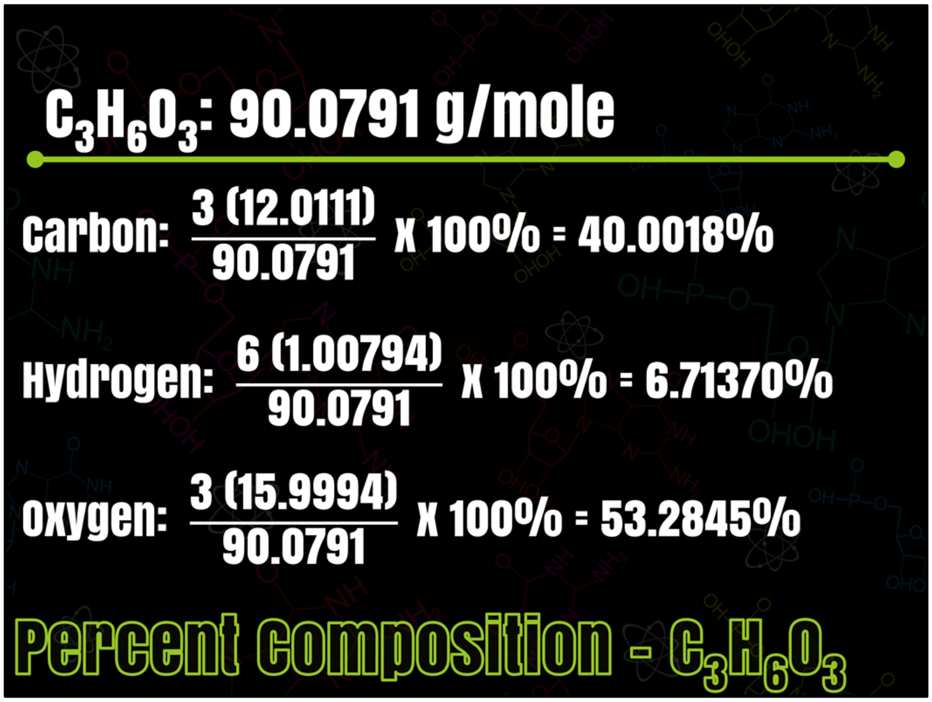


Take a look at the following compounds and their molar masses. The molar mass of CH_2O is 30.0264 grams per mole. The molar mass of lactic acid, or $C_3H_60_3$, is 90.0791 grams per mole. The molar mass of glucose, or $C_6H_{12}O_6$, is 180.1583 grams per mole.

Notice that the molar mass of $C_3H_60_3$ is three times as much as CH_2O, and in $C_3H_60_3$, there are three times as many carbon atoms, three times as many hydrogen atoms, and three times as many oxygen atoms. Similarly, there are six times as many of the individual atoms in $C_6H_{12}O_6$ as there are in CH_2O, and the molar mass of $C_6H_{12}O_6$ is six times larger than CH_2O.



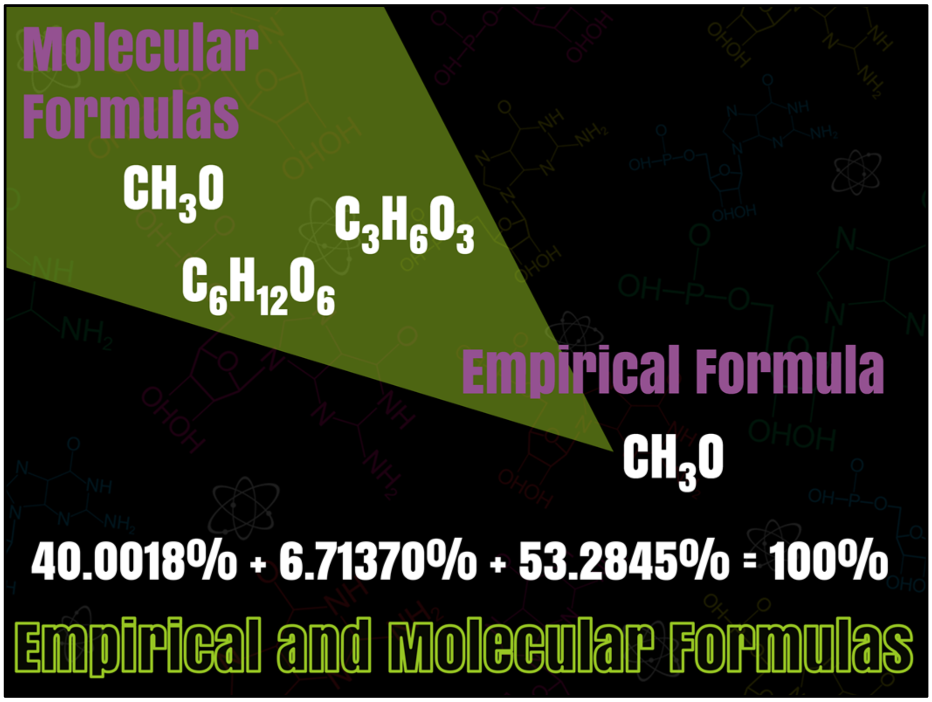
Now, determine the percent composition of each type of element in each of these compounds. To determine the percentage of carbon, divide the mass of carbon, which is 12.0111 grams per mole, by the molar mass of CH_2O, which is 30.0264 grams per mole, and then multiply this figure by 100. This shows that carbon is 40.0018% of CH_2O. To determine the percentage of hydrogen, divide two times 1.00794, the atomic mass of hydrogen, by the molar mass of CH_2O. This shows that hydrogen is 6.71369% of CH_2O. The percent of oxygen is determined by dividing the atomic mass of oxygen, 15.9994 , by 30.0264 to get a percentage of 53.2844% oxygen in the compound.



The percentages for $C_3H_60_3$ are calculated the same way, but with regards to the number of atoms of each element, which will change the molar mass. As shown here, in $C_3H_60_3$, there are three times as many of the individual atoms, and the molar mass has also increased by a factor of three. In $C_3H_60_3$, the percent compositions of carbon, hydrogen, and oxygen are still the same, since the mass of each element was multiplied by three and the molar mass of the compound was also multiplied by three.

In $C_6H_{12}O_6$, there are six atoms of carbon, twelve atoms of hydrogen, and six atoms of oxygen, and the molar mass of the compound is larger since there are more of each type of atom, but the percentages of the elements does not change. That is because they all have the same empirical formula of one carbon atom, two hydrogen atoms, and one oxygen atom, or CH2O. This means that the reverse is true as well. The empirical formula of a substance can be determined from its percent composition.

The percent abundances of the elements should add up to one hundred percent, and in this example, the percents of carbon, hydrogen, and oxygen add up to approximately one hundred percent.



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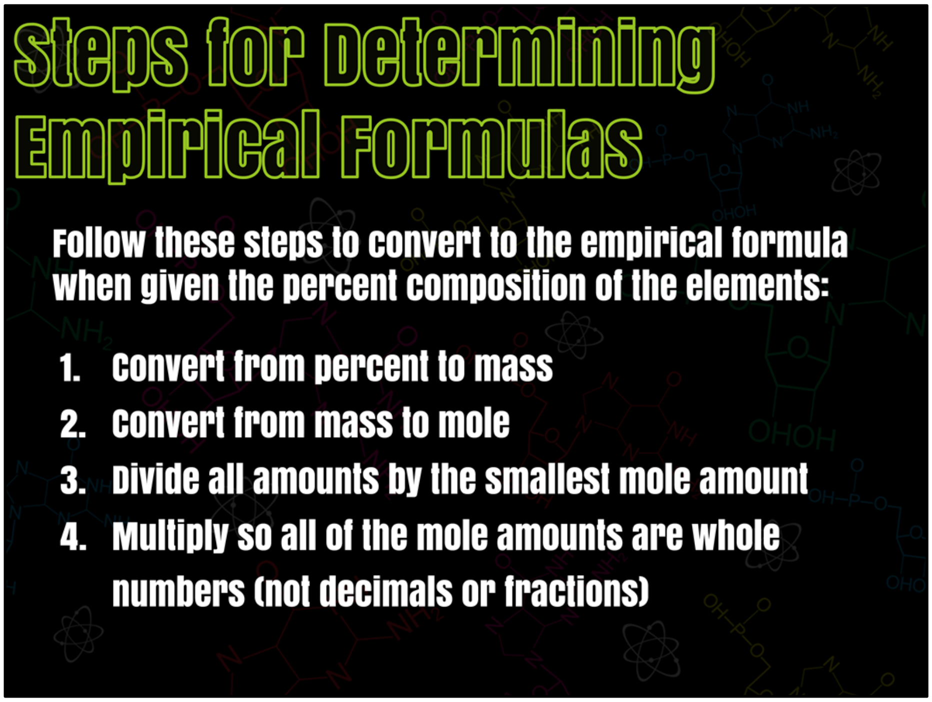
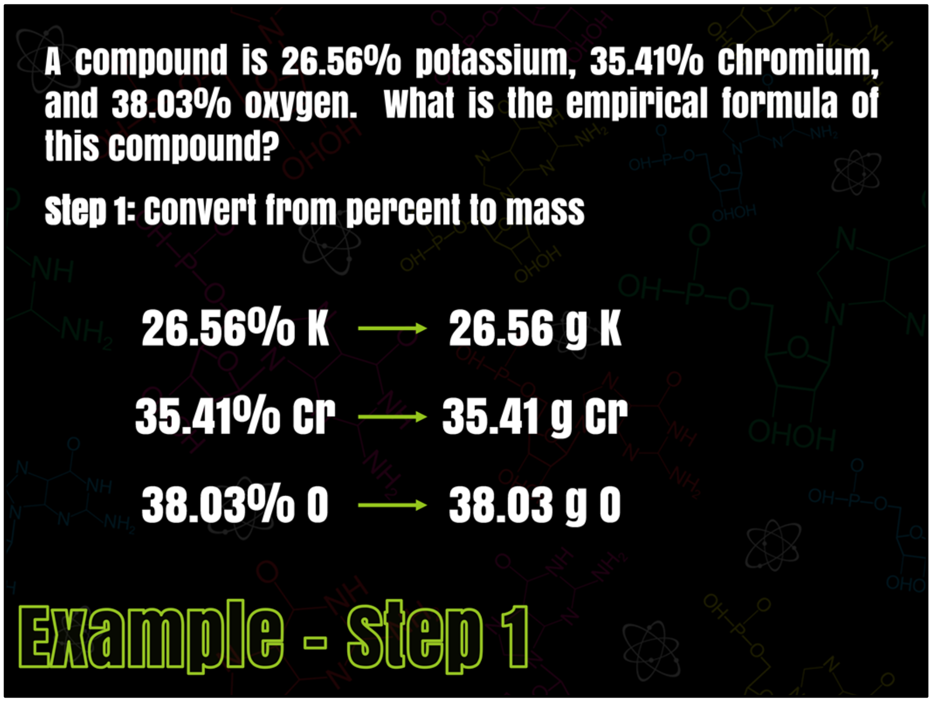
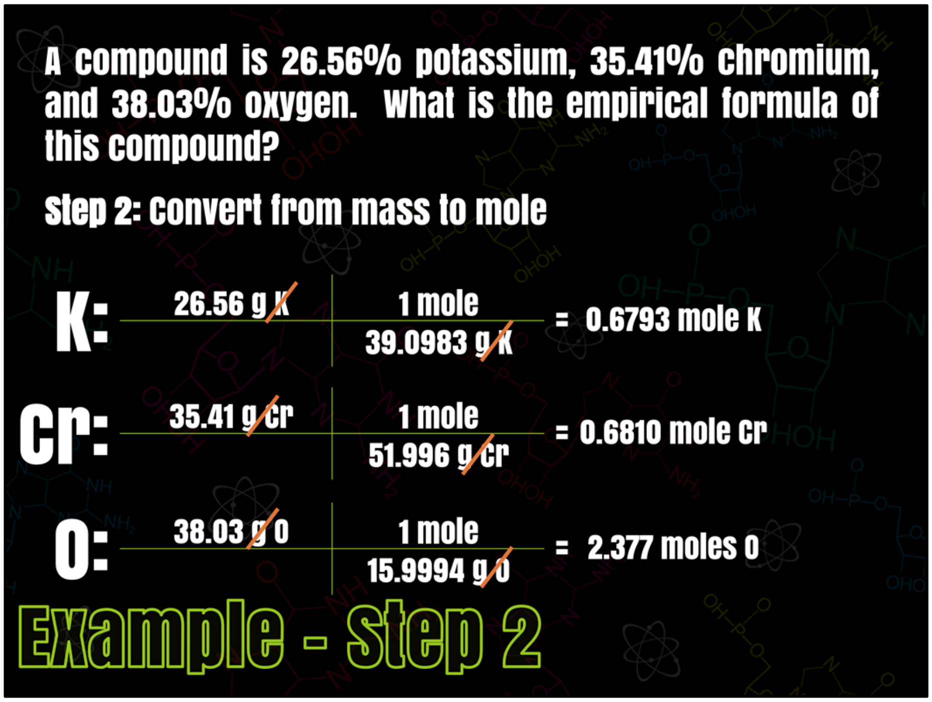


If you are given or have the percent composition of the elements and you need to determine the empirical formula, there are four steps you will need to follow. For the first step, convert from percent to mass by multiplying the percent of the element by the molar mass of the compound. For this step, you can assume you have a 100.0 gram sample. In that instance, if the compound is 33% carbon, then it will have 33.0 grams of carbon in a 100.0 gram sample. The second step is to convert from mass to mole, which is done by using the periodic table to find the molar mass of the element and convert it to moles. Once you have all of the mole amounts calculated, complete the third step by dividing all of the mole amounts by the smallest mole amount that was determined in Step Two. This insures that the mole amounts are at least one. For the last step, make sure all of the mole amounts are whole numbers. If the amounts calculated in the previous step are whole numbers already, then this step is not needed. If they are decimals, however, then they must be multiplied by a value, such as two, three, four, five, or ten, until they are whole.



Practice writing an empirical formula for a compound with this example. A compound has 26.56% potassium, 35.41% chromium, and 38.03% oxygen.

In step one, you assume that you have a 100.0 gram sample of the compound. The percent signs are switched to grams, so 26.56% potassium is converted to 26.56 grams potassium, 35.41% chromium is 35.41 grams chromium, and 38.03% oxygen is switched to 38.03 grams oxygen.

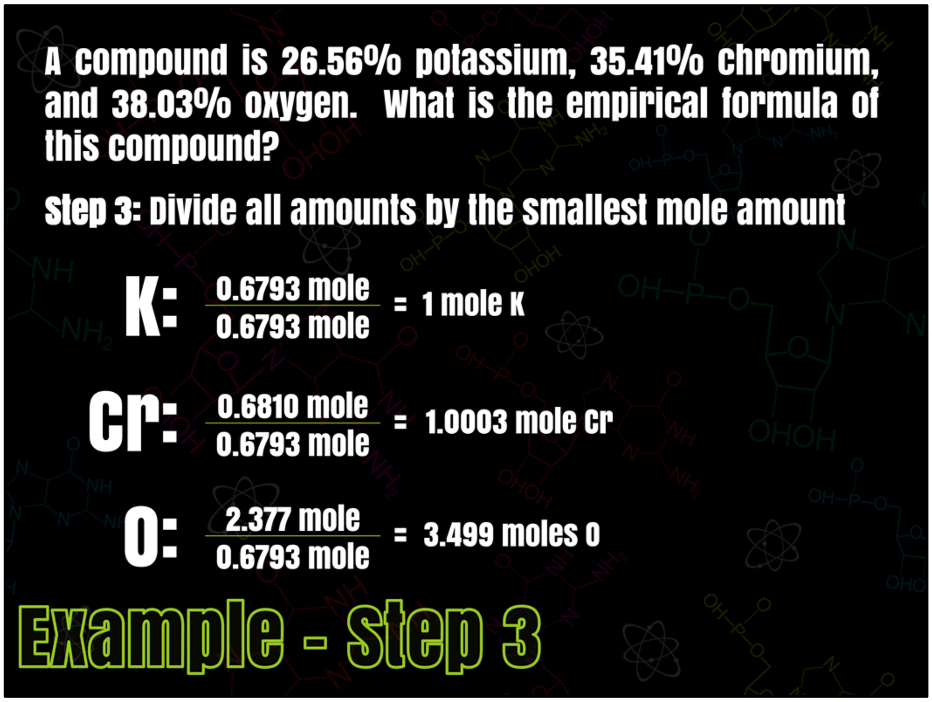


In Step Two, the masses are converted to moles using the molar masses for each element.

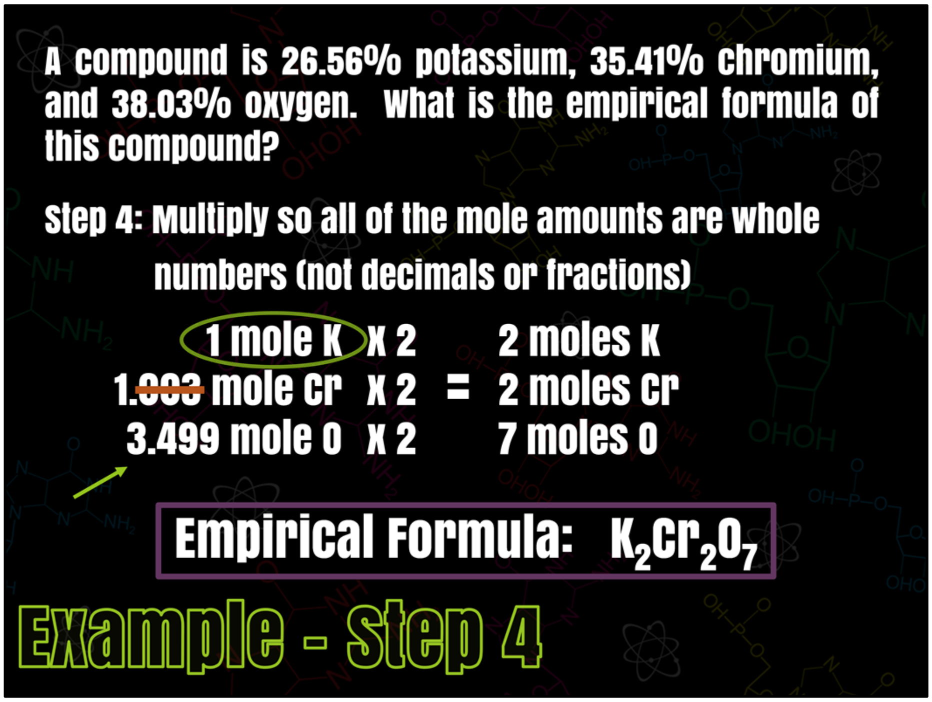
You know that you have 26.56 grams of potassium and that there are 39.0983 grams of potassium per mole, based on potassium's molar mass. Using dimensional analysis, you multiply twenty-six point five six grams of potassium by 1 mole and then divide by 39.0983 to get 0.6793 moles of potassium.

Chromium has a molar mass of 51.996 grams, so 35.41 grams is multiplied by one mole over 51.996 for a result of 0.6810 mole chromium.

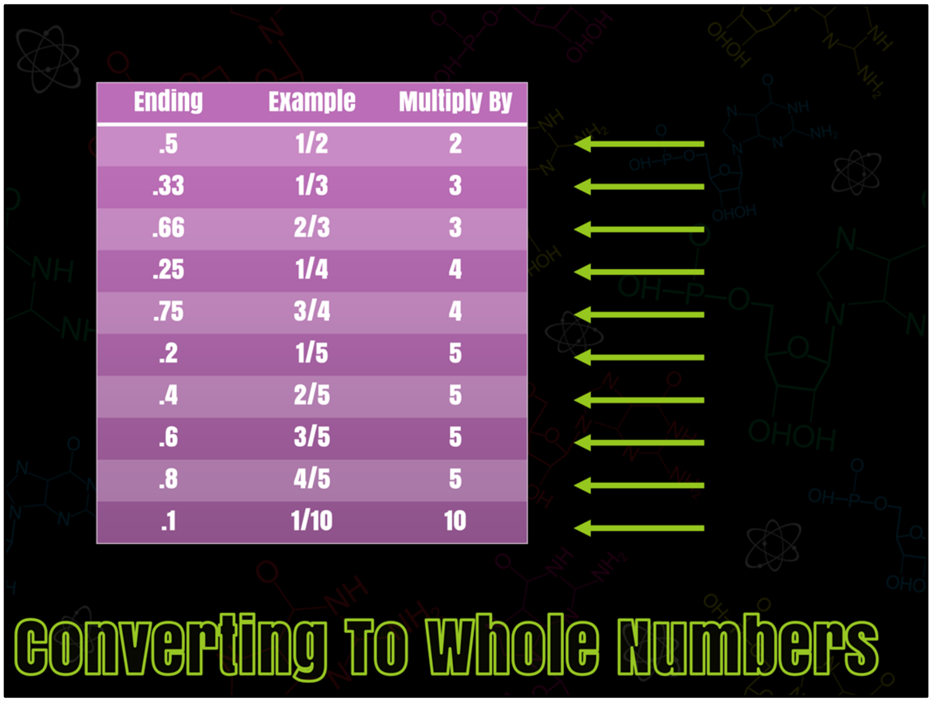
Oxygen has a molar mass of 15.9994 grams, so 38.03 grams of oxygen is multiplied by one mole oxygen and the divided by 15.9994 grams oxygen to get 2.377 moles of oxygen.



In Step Three, the mole amounts from Step Two are divided by the smallest mole amount. So, each quantity is divided by 0.6793, which results in one mole of potassium, 1.003 moles of chromium, and 3.499 moles of oxygen.

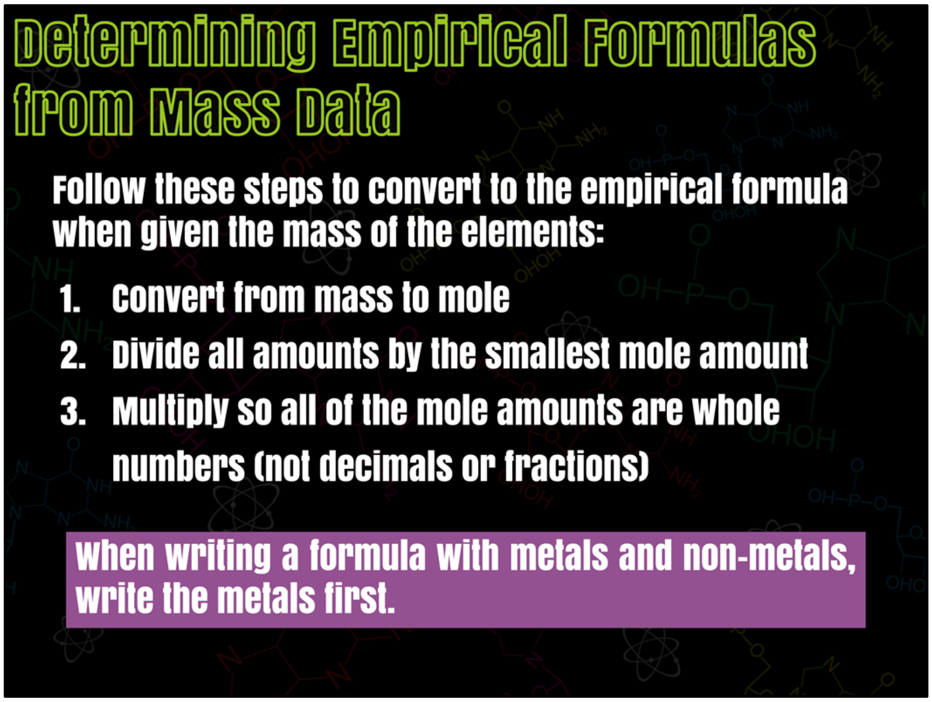


Step Four is where all mole amounts need to be multiplied so all of them are whole numbers. The mole amount of potassium is one mole, which is a whole number. The mole amount for chromium, 1.003, is close enough to one to round to one. The number 3.499 is not close enough to three or four to round. This number is essentially three and a half. That means that by multiplying all of the amounts by two, all numbers will be a whole number ratio. It is important to remember that if one mole amount is doubled, the other ones are doubled as well. The result is two moles of potassium, two moles of chromium, and seven moles of oxygen for an empirical formula of $K_2Cr_2O_7$.



Ending	Example	Multiply By
.5	1/2	2
.33	1/3	3
.66	2/3	3
.25	1/4	4
.75	3/4	4
.2	1/5	5
.4	2/5	5
.6	3/5	5
.8	4/5	5
.1	1/10	10

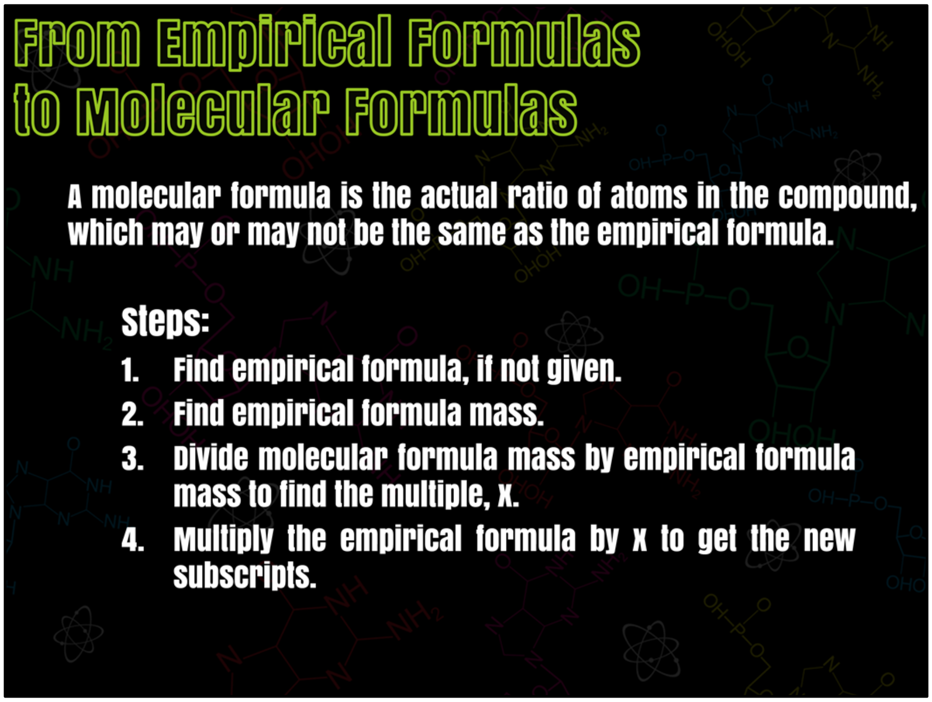
As you just saw, the final step in calculating the empirical formula when given the percent composition of the elements states that the subscripts of the elements must be whole numbers. In other words, the subscripts can not be decimals or fractions. This table shows what numbers to multiply decimals by so all numbers will be whole numbers. If the number ends in point five, this is the same as one-half, so the value should be multiplied by two. For numbers ending in the repeating decimals of 0.33 or 0.66, such as with the fractions one-third or two-thirds, then multiply the number by three. If a number ends in 0.25, such as with one-fourth, or point seven five, as with three-fourth, multiply the number by four. For numbers ending in 0.2 (one-fifth), 0.4 (two-fifth), 0.6 (three-fifth), or 0.8 (four-fifth), multiply by five. If a value ends in 0.1, or one-tenth, then multiply it by ten.



You can also find the empirical formula of a compound when given the mass of the elements. When writing an empirical formula given the mass data, follow the same steps for writing an empirical formula given the percent composition, but the first step of converting the percent to grams is not needed. This means there are three steps when given the mass data, versus four steps when given the percent composition of the elements.

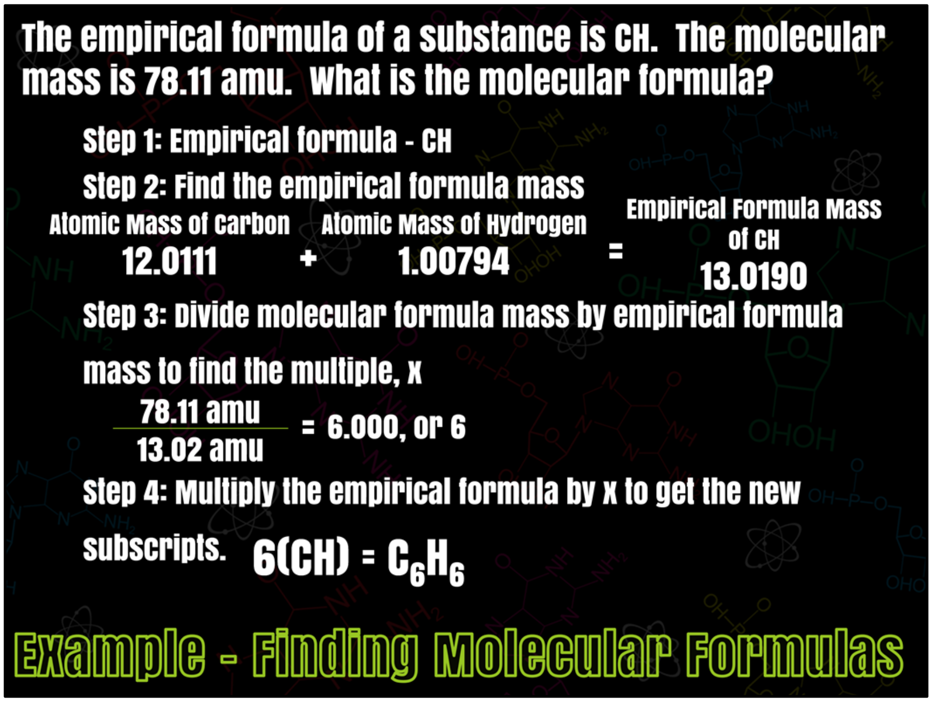
First, convert the gram amounts to moles by using the periodic table to find the molar mass of the element and convert it to moles.
Then, divide each of the mole amounts by the smallest mole amount to find the mole ratio between the elements involved.
For the last step, multiply so that each of the amounts of moles is a whole number.

The mole ratios that result are the subscripts for the elements. When writing a formula that has both metals and non-metals, write the metals first.



A molecular formula is the actual ratio of atoms in the compound. This may or may not be the same as the empirical formula. To find the molecular formula, you must know the empirical formula and the molecular formula mass.

To write the molecular form with the empirical formula, follow these four steps.
First, if the empirical formula is not given, then this will have to be determined.
After the empirical formula is known, find the empirical formula mass.
The third step involves dividing the molecular formula by the empirical formula mass to find the multiple, which can be defined as "x".
The fourth step is to multiply the empirical formula by the multiple, x, to get the subscripts.



For this example, you have been given a substance that has the empirical formula of CH with a molecular formula mass of 78.11 amu. To find the molecular formula, follow these steps:

For Step One, the empirical formula of CH has already been given.

In Step Two, you need to find the empirical formula mass. To do so, add the atomic masses of the elements. The atomic mass of carbon is 12.0111 amu and the atomic mass of hydrogen is 1.00794 amu. The empirical formula mass of CH is 13.0190.

In Step Three, you divide the molecular formula mass by the empirical mass. Then given molecular formula mass is 78.11 amu. This number is divided by the empirical formula mass of 13.0190 to get the multiple, x, which is 6.000, or six.

The final step involves the multiplying the multiple, x, which in this example is six, by the subscripts of the empirical formula, to get the molecular formula. The molecular formula is C_6H_6.