Tutorial 5-1
Percent Mass and Empirical Formulas

Tutorial 5-1 will help you with the following:

1. Determine percent composition of a compound by mass, given the molecular formula.
2. Calculate the mass of an element contained in a given mass of a compound.
3. Empirical or “simplest” formulas for compounds and what they mean.
4. Determine the empirical formula for a compound from composition or percent composition by mass.
5. Determine the molecular formula from the molecular mass and the empirical formula.

So get out your calculator, periodic table, pencil and paper and let’s rock and roll (as they used to say about 25 years ago).

Finding Percent Composition

Sometimes it is desirable to know the percentage mass of each element in a compound. One example is in fertilizers where percent nitrogen, phosphorus etc. is important in order to know what compounds to use with certain plants and soils. Another place where this comes in handy is in later Chemistry courses and of course for the Unit 5 test.

Let’s start with an example and I’ll go over it in typical step by step fashion. Have your periodic table right beside you. I will use the table that expresses the atomic masses to 1 decimal place. Make sure you have the same one.

eg.) Find the **percent of carbon** by mass in the compound ethane (C_2H_6).

Step 1: Find the molar mass of C_2H_6 (*The mass of one mole of C_2H_6 molecules*)

Molar Mass = 2(12.0) + 6(1.0) = 30.0 g/mol .

Step 2: Find the total mass of all the carbon atoms in one mole of the compound. To do this, multiply the *atomic mass* of carbon by the *subscript* of carbon in the formula.(C_2...)

Mass of carbon = 12.0 g/mol x 2 mol = 24.0 g of carbon

Step 3: Divide the *mass of carbon* by the *molar mass* and multiply by 100 to get percent mass.

$$\text{Percent mass of carbon} = \frac{24.0\text{ g}}{30.0\text{ g}} \times 100\% = 80.0\ \%\ \text{C}$$

You may also be asked to find the percent of hydrogen by mass in the same compound (C_2H_6). Let's do that:

Since it is the same compound (C_2H_6), step 1 is already done.

Step 2: Find the total mass of all the hydrogen atoms in one mole of the compound. To do this, multiply the *atomic mass* of hydrogen by the *subscript* of hydrogen in the formula. (...H_6)

Mass of hydrogen = 1.0 g/mol x 6 mol = 6.0 g of hydrogen

(NOTICE that we use the *atomic* mass of "H", **not** the molar mass of "H_2". We are talking about *atoms* of H, not molecules of H_2 gas)

Step 3: Divide the *mass of hydrogen* by the *molar mass of* C_2H_6 and multiply by 100% to get percent mass.

$$\text{Percent mass of hydrogen} = \frac{6.0\text{ g}}{30.0\text{ g}} \times 100\% = 20.0\ \%\ \text{H}$$

Notice that when you add up the percent Carbon (80%) and the percent Hydrogen (20%), you get 100%. The percent mass of all the elements in a compound should always add up to 100%. Sometimes, you won't get **exactly** 100% due to rounding off. (99% would be alright, but something like 97% would be too far off!)

NOTE. When they ask you to find the "Percent Composition", you have to find the percent of each element in the compound by mass.

Let's do another example:

Find the *percent composition* by mass of potassium dichromate ($K_2Cr_2O_7$).

Step 1: Find the molar mass of $K_2Cr_2O_7$ (*The mass of one mole of $K_2Cr_2O_7$ molecules*)

Molar Mass = 2(39.1) + 2(52.0) + 7(16.0) = 294.2 g/mol .

Step 2: Find the total mass of all the potassium atoms in one mole of the compound.
To do this, multiply the *atomic mass* of potassium by the *subscript* of potassium in the formula.($K_{2...}$)

Mass of potassium = 39.1 g/mol x 2 mol = 78.2 g of potassium

Step 3: Divide the *mass of potassium* by the *molar mass of $K_2Cr_2O_7$* and multiply by 100% to get percent mass.

$$\text{Percent mass of potassium} = \frac{78.2\text{ g}}{294.2\text{ g}} \times 100\% = 26.6\ \%\ \text{K}$$

Step 4: Find the total mass of all the chromium atoms in one mole of the compound.
To do this, multiply the *atomic mass* of chromium by the *subscript* of chromium in the formula.($...Cr_{2...}$)

Mass of chromium = 52.0 g/mol x 2 mol = 104 g of chromium

Step 5: Divide the *mass of chromium* by the *molar mass of $K_2Cr_2O_7$* and multiply by 100% to get percent mass.

$$\text{Percent mass of chromium} = \frac{104\text{ g}}{294.2\text{ g}} \times 100\% = 35.4\ \%\ \text{Cr}$$

Step 6: Find the total mass of all the oxygen atoms in one mole of the compound.
To do this, multiply the *atomic mass* of oxygen by the *subscript* of oxygen in the

formula.($...O_7$)

Mass of oxygen = 16.0 g/mol x 7 mol = 112 g of oxygen

Step 7: Divide the *mass of oxygen* by the *molar mass of* $K_2Cr_2O_7$ and multiply by 100% to get percent mass.

$$\text{Percent mass of oxygen} = \frac{112\text{ g}}{294.2\text{ g}} \times 100\% = 38.1\%\ O$$

Now, we can summarize the percent composition by mass of $K_2Cr_2O_7$.

$K_2Cr_2O_7$ is 26.6% potassium, 35.4% chromium and 38.1% oxygen by mass.

Adding these three percentages up gives a total of 100.1%. This is close enough to 100. In all the calculations above, the percentage was rounded to 3 significant digits, as justified by the atomic masses on the table. When rounding is done, the total isn't always exactly 100%.

Here's an example for you to try.

<u>Question 1</u>. Find the percent composition by mass of sodium phosphate, Na_3PO_4.

After you have done this, turn to **Tutorial 5-1 Help** and for the solution. Check your answers. If you don't understand the solution, see the teacher for help!

CAUTION:

It is very important to use care when working with formulas with brackets.

For example, let's say you were asked to determine the percent composition of the compound ammonium phosphate. The formula is $(NH_4)_3PO_4$.

When you are going through the steps, you must remember that in this formula there are:

(3x1)= **3** "N"s, (3x4)= **12** "H"s, **1** "P" and **4** "O"s

<u>Question 2</u> Find the percent composition by mass of the compound ammonium phosphate, $(NH_4)_3PO_4$.

When you are finished, check the solution for this question on Tutorial 5-1 Help.

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Finding Mass of an Element in a Given Mass of Compound

Sometimes you need to know the mass of a certain element which is contained in a sample of a compound. One way of analyzing hydrocarbons (compounds containing carbon and hydrogen) is to burn them, producing CO_2 and H_2O. The mass of carbon in an original hydrocarbon sample can be found by knowing the mass of CO_2 which is formed. Let's do an example.

Find the mass of carbon contained in a 25.0 gram sample of carbon dioxide (CO_2).

We can make ourselves a **conversion factor**:

We know that there is 1 mole of C atoms in 1 mole of CO_2 molecules (*the subscript on C is "1"*)

We know that the mass of 1 mole of C atoms = 12.0 grams (*it's atomic mass*)

We know that the mass of 1 mole of CO_2 molecules is 44.0 grams (*it's molar mass or 12.0 + 2(16.0)*)

So from this we can make the conversion factor: $\dfrac{12.0 \text{ g of C}}{44.0 \text{ g of } CO_2}$

We can use this conversion factor to find the answer to the question:

$$25.0 \text{ g of } CO_2 \times \frac{12.0 \text{ g of C}}{44.0 \text{ g of } CO_2} = \underline{\mathbf{6.82 \text{ g of C}}}$$

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Let's do another example: Find the mass of potassium contained in 450.0 g of K_2CO_3.

We see by the formula that there are 2 atoms of K in one molecule of K_2CO_3
(or 2 moles of K atoms in one mole of K_2CO_3)

So the mass of K in one mole of K_2CO_3 is 2 x 39.1 (*2 x the atomic mass of K*) = 78.2 g

The mass of one mole of K_2CO_3 is it's molar mass (*2(39.1) + 12.0 + 3(16.0)*) = 138.2 g

So our conversion factor this time is: $\dfrac{78.2 \text{ g of K}}{138.2 \text{ g of } K_2CO_3}$

We can now do the question. We wanted to know the mass of K in 450.0 g of K_2CO_3.

$$450.0 \text{ g of } K_2CO_3 \times \frac{78.2 \text{ g of K}}{138.2 \text{ g of } K_2CO_3} = \underline{\mathbf{255 \text{ g of K}}}$$

To find the mass of oxygen in 450.0 g of K_2CO_3 we could make the conversion factor:

$$\frac{3(16.0) \text{ g of O}}{138.2 \text{ g of } K_2CO_3} = \frac{48.0 \text{ g of O}}{138.2 \text{ g of } K_2CO_3} \begin{array}{l} \text{< --(3 x the atomic mass of "O")} \\ \text{< --(the molar mass of } K_2CO_3\text{)} \end{array}$$

To finish the question we write down:

$$450.0 \text{ g of } K_2CO_3 \times \frac{48.0 \text{ g of O}}{138.2 \text{ g of } K_2CO_3} = \underline{\mathbf{156 \text{ g of "O"}}}$$

Here's an example for you. Make sure you try it!

Question 3

Find the mass of Na in 568 g of Na_3PO_4

Do this in your notebook showing all units and conversion factors.

Check your answer on Tutorial 5-1 HELP.

What is Meant by the *Empirical* Formula of a Compound?

We know that the molecular formula of a compound tells the number of each kind of atom in the compound.

For example the *molecular formula* for the compound octane is $\mathbf{C_8H_{18}}$.

This means that in one molecule of octane there are 8 "C" atoms and 18 "H" atoms.

Empirical Formula means the *simplest* formula. This formula gives the *simplest whole number ratio* of atoms in the molecule.

So the ***molecular formula*** of octane is C_8H_{18} & the ***empirical formula*** of octane is C_4H_9

The molecular formula of hydrogen peroxide is H_2O_2. You can hopefully see that the empirical formula (*simplest formula*) of hydrogen peroxide is HO. (*both subscripts are divided by 2*,)

Quite often the molecular formula of a compound is the simplest formula to begin with (*You can't divide all subscripts by any whole number*) In these cases, the empirical formula (*simplest formula*) is the same as the molecular formula.

An example would be a compound with the *molecular formula* C_3H_8O.

The *empirical formula* for this compound would also be C_3H_8O.

Question 4

Given the following molecular formulas, find the empirical formulas.

Molecular Formula	Empirical Formula
P_4O_{10}	
$C_{10}H_{22}$	
$C_6H_{18}O_3$	
$C_5H_{12}O$	
N_2O_4	

Check the answers on Tutorial 5-1 HELP.

Finding Empirical Formulas From Masses of Elements in a Sample

You have probably been wondering, "What is the Point? Why do we need to bother with empirical formulas (simplest formulas) when the molecular formula tells us more about the compound?"
Or you also might be wondering, "Why do we bother with all this Math stuff at all? We just want to blow things up!"

Well, I can answer the first question. When an unknown compound is analyzed and the elements in it are determined, chemists can often find the ***mass*** of each element in a sample. This can be accomplished by burning (combustion analysis) or by decomposition by some other means.

It turns out that the ***empirical*** or *simplest* formula is easy to find once we know the mass of each element. Later, with a little more experimentation, the *molecular mass* can be determined. Then the ***molecular formula*** can be found and we are closer to knowing what the unknown compound is.

Analyzing unknown samples and finding out what they are is a very important part of chemistry called analytical chemistry. This can be much more useful than just blowing things up. It may help us track down a person who did blow something up and put him in jail! ...or find a pesticide residue in vegetables ...or millions of other uses.

The key to finding the empirical or simplest formula is to change the masses into moles of each element. As you know from Tutorial 8, the ratio of *moles of atoms* in a sample of a compound would be the same as the ratio of *single atoms* in one molecule of the compound.

Again, this process is best illustrated by using an example. Read through this ***carefully*** and try to understand each step! Later, as you may have guessed, you will get some of your own to try!

Example: A sample of an unknown compound was analyzed and found to contain 8.4 grams of carbon, 2.1 grams of hydrogen and 5.6 grams of oxygen. Find the empirical (or simplest) formula for this compound.

The first thing we do is change *grams* of each element into *moles of atoms*. To do this we use the **atomic mass** (not the molar mass) of each element. eg. for hydrogen use the **atomic mass** **(**1.0 g/mol), NOT the molar mass for H_2 (2.0 g/mol)

$$8.4 \text{ g of C} \times \frac{1 \text{ mol of C}}{12.0 \text{ g}} = 0.7 \text{ mol of C}$$

$$2.1 \text{ g of H} \times \frac{1 \text{ mol of H}}{1.0 \text{ g}} = 2.1 \text{ mol of H}$$

$$5.6 \text{ g of O} \times \frac{1 \text{ mol of O}}{16.0 \text{ g}} = 0.35 \text{ mol of O}$$

Next what we do is to find the simplest mole ratio. This can usually be done in one step, although sometimes two steps are involved as we will see.

What you do is take the ***smallest number of moles*** and divide the moles of *each* element by this number.

In our example the *smallest number of moles* is **0.35** mol for the oxygen. Dividing each by 0.35, we get:

$$8.4 \text{ g of C} \times \frac{1 \text{ mol of C}}{12.0 \text{ g}} = 0.7 \text{ mol of C} \;\dashrightarrow\; \frac{0.7 \text{ mol of C}}{0.35} = 2 \text{ mol C}$$

$$2.1 \text{ g of H} \times \frac{1 \text{ mol of H}}{1.0 \text{ g}} = 2.1 \text{ mol of H} \;\dashrightarrow\; \frac{2.1 \text{ mol of H}}{0.35} = 6 \text{ mol H}$$

$$5.6 \text{ g of O} \times \frac{1 \text{ mol of O}}{16.0 \text{ g}} = 0.35 \text{ mol of O} \;\dashrightarrow\; \frac{0.35 \text{ mol of O}}{0.35} = 1 \text{ mol O}$$

From this, we can see that the simplest (or empirical) formula would be: $\mathbf{C_2H_6O}$

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This process is easier if we do it in **table** form. It also simplifies it a little bit if we realize that to get **moles of atoms** of an element, we simply *divide* the mass by the atomic mass:

$$\frac{\text{mass (g)}}{\text{atomic mass (g/mol)}} = \text{mol of atoms}$$

In the next example, we will use the table form. It is best if you can ***remember*** the headings for each column of the table and then the process becomes easier - providing you get lots of practice!

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Example:
0.888 grams of a compound made up of carbon, hydrogen and oxygen are analyzed and found to contain 0.576 grams of carbon and 0.120 grams of hydrogen. Determine the empirical (or simplest) formula for this compound.

The first thing we have to do is find the *mass of oxygen* in this compound. (Notice they did not give it to us!)
If the total mass is 0.888 g and it's made up of C, H & O, the mass of **oxygen** must be

[The total mass] - [the mass of C + the mass of H]

= 0.888g - (0.576 g + 0.120 g) = 0.888 g - 0.696 g = **0.192 g of oxygen**

Now, we set up a table with the following headings:

Element	Mass	Atomic Mass	Moles	Moles / Smallest moles	Simplest Whole # Ratio

You would put in a row for each element in your compound. In this example there are three elements: C, H and "O". The calculations are done in the same way as the previous example. Remember that **moles = mass ÷ atomic mass**. In the 5th column, we divide each "moles" by the smallest number of moles. We may get a whole number ratio. If we don't, there should be a simple number (2,3,4 or 5) that we can multiply all the entries by in order to get a whole # ratio. Make sure you **carefully** go over the solution to this problem given in the next table. If you don't understand each step, review the previous example. Ask for help if you need it.

Element	Mass	Atomic Mass	Moles	Moles / Smallest moles	Simplest Whole # Ratio
carbon	0.576 g	12.0 g/mol	0.0480 mol	$\frac{0.0480}{0.0120} = 4$	**4**
hydrogen	0.120 g	1.0 g/mol	0.12 mol	$\frac{0.12}{0.0120} = 10$	**10**
oxygen	0.192 g	16.0 g/mol	0.0120 mol	$\frac{0.0120}{0.0120} = 1$	**1**

From this we can see that the ***empirical formula*** is $C_4H_{10}O$

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Finding Empirical Formulas From Percentage Composition

Empirical formulas can also be found using percentage of each element in a compound. This is probably obvious given the title of this section!

What we do given % composition is just pretend that we have 100.000 grams of the sample. (The significant digits will depend on the data given.)

Let's do another example:

A white powder used in paints, enamels and ceramics has the following composition:
"Ba" 69.58%, "C" 6.090%, and "O" 24.32%. Determine it's empirical formula.

Now, if we had 100.00 grams, we would have 69.58 g of Ba, 6.090 g of C and 24.32 g of "O". We can now use these as "Mass" for each element in our table and do the rest of the calculations:

Element	Mass	Atomic Mass	Moles	Moles / Smallest moles	Simplest Whole # Ratio
barium	69.58 g	137.3 g/mol	0.5068 mol	$\frac{0.5068}{0.5068} = 1$	**1**
carbon	6.090 g	12.0 g/mol	0.5075 mol	$\frac{0.5075}{0.5068} = 1.001$	**1**
oxygen	24.32 g	16.0 g/mol	1.52 mol	$\frac{1.52}{0.5068} = 2.999$	**3**

So the ***empirical*** formula is $\mathbf{BaCO_3}$ and the substance is barium carbonate.

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<u>What to do when the "moles ÷ smallest # of moles" do NOT all come out to whole numbers.</u>

Occasionally when doing an empirical formula, the numbers in column 5 (moles ÷ smallest # of moles) do not come out to nice whole numbers.

If they come out to <u>almost</u> a whole number, round them to that whole number.

For example if you divide the moles of an element by the smallest # of moles and you get an answer like 2.97 → round it to 3. If you get something like 5.04 → round it to 5.

If they come out <u>nowhere near</u> a whole number, use the following guideline:

If the number ends in a decimal of	***Multiply ALL the numbers in this column by***
~.5	**2**
~.33 or ~.66	**3**
~.25 or ~.75	**4**
~.2 or ~.4 or ~.6 or ~.8	**5**

Let's say the values for "moles ÷ smallest # of moles" comes out to the following: (*In the following table the columns for "Mass", "Atomic Mass" and "Moles" are left out just for simplicity. They would not be omitted in a real problem. The symbol "~" means "about"*.)

Element	**$\frac{\text{Moles}}{\text{Smallest moles}}$**	**Simplest Whole # Ratio**	**Final ratio**
carbon	1.01	1 x **3** = 3	**3**
hydrogen	2.66	2.66 x **3** = 7.98	**8**

Look at the table above, the "1.01" for carbon was close enough to a "1" to round it off to the integer "1". However the "2.66" for the hydrogen was not close to any whole number. Referring to the table right above this one, if one of the numbers ends in about .67, multiply ALL the numbers by "3". So we did that. The "1" for the carbon and the "2.66" for the hydrogen are BOTH multiplied by "3". The resulting "7.98" for the hydrogen is close enough to "8" to be rounded to the whole number "8".

Therefore, the empirical formula for the compound in this example was $\mathbf{C_3H_8}$.

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Finding the Molecular Formula from the Empirical Formula and Molar Mass

The last task of this tutorial is to show you how to go one step farther and find the actual molecular formula for a compound.

At this point we should quickly review what the empirical and molecular formulas are:

The ***molecular formula*** of a compound tells the **actual number** of each kind of atom in the compound.

For example, the *molecular formula* of octane is C_8H_{18}

Empirical Formula means the **simplest** formula. This formula gives the **simplest whole number ratio** of atoms in the molecule.

For example, the *empirical formula* of octane (*molecular formula* C_8H_{18}) is C_4H_9

You will notice that if you multiply all the subscripts in the empirical formula (*4 & 9*) by "**2**", you will get the subscripts of the molecular formula (*8 & 18*).

The molecular formula is either:

a) the *same* as the empirical formula or

b) a *simple whole number multiple* of the empirical formula (like x 2, x 3 etc.)

If you have the empirical formula and are given the molar mass, it is simple to find the molecular formula.

Let's do an example:
The empirical formula for a compound is CH_2O and the molar mass (*some books call it the molecular mass*) is 60.0 g/mol. Find the molecular formula.

First find the ***mass of the empirical formula***:

C H$_2$ O

↑ ↑ ↑

12.0 + 2(1.0) +16.0 = **30** g/mol is the *mass of the empirical formula*

Now try to find a ***simple whole number*** that you multiply the mass of the empirical formula by to get the molar mass:

mass of the empirical formula x ? = *molar mass*

↑ ↑ ↑

30 x ? = 60

You can see that in this case the simple whole number is "**2**"

Now, multiply all subscripts in the empirical formula by this whole number: ("2" in this case)

Empirical formula x 2 = Molecular Formula

↑ ↑ ↑

CH_2O x 2 = $C_2H_4O_2$

A good thing to do now is to figure out the molecular mass using your molecular formula ($C_2H_4O_2$) and make sure it is the same as the molar mass given (*60.0 g/mol*):

C_2 H_4 O_2

↑ ↑ ↑

2(12.0) + 4(1.0) +2(16.0) = **60** g/mol is the molar *mass.*

So ***$C_2H_4O_2$*** must be the correct molecular formula for this compound.

This is easiest to do using little table:

	Empirical	**Molecular**
Formula	CH_2O $\xrightarrow{\mathbf{x\ 2}}$	**$C_2H_4O_2$**
Mass	30.0 $\xrightarrow{\mathbf{x\ 2}}$	60.0

Now, here's a question for you to try. Make a table like the one above.

<u>Question 5</u>

The empirical formula for a compound is CH_2O and the molar mass is 90.0. Find the molecular formula.

Check Tutorial 5-1 HELP for the solution to this problem.

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<u>Self-Test on Tutorial 5-1</u>

Do all of these questions showing full work and check the answers on Tutorial 5-1 HELP. Show the teacher your work.

1. Determine the ***<u>percent composition</u>*** of the compound calcium nitrate ($Ca(NO_3)_2$)

   (That is, find the % calcium, the % nitrogen and the % oxygen in this compound.)

2. Find the mass of carbon contained in 336.16 grams of CO_2.

3. Find the mass of oxygen contained in 860.0 grams of magnesium nitrate ($Mg(NO_3)_2$)

4. A compound used in photography is called potassium persulphate. A 0.8162 gram sample of the compound was analyzed and found to contain 0.2361 grams of potassium, 0.1936 grams of sulphur and the rest was oxygen.

   a) Find the mass of oxygen in the sample.

   b) Determine the empirical formula for this compound. (Use a table like the one on page 10)

   c) The molar mass of this compound is 270.4 g/mol. Determine the molecular formula. (Use a table like the one on the top of this page.)