Calculations Involving Empirical Formulas

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Meaning of Empirical Formula

The empirical formula of a compound is a chemical formula that indicates the ***smallest whole number ratio*** of the number of atoms of the constituent elements present in one molecule of the compound.
To make the picture a little clearer, let's take a look at the molecular as well as the empirical formulas of some compounds:

Name of Compound	**Molecular Formula**	Ratio of number of atoms of constituent elements present	**Empirical Formula**
Hydrogen Peroxide	H_2O_2	2 : 2 or 1 : 1	**HO**
Water	H_2O	2 : 1	H_2O
Glucose	$C_6H_{12}O_6$	6 : 12 : 6 or 1 : 2 : 1	CH_2O
Benzene	C_6H_6	6 : 6 or 1 : 1	**CH**
Butane	C_4H_{10}	4 : 10 or 2 : 5	C_2H_5

As we can see, the empirical formula of a compound is different from its molecular formula. While the molecular formula of a compound tells us the number of atoms of each element that is present in one molecule of the compound, its empirical formula expresses the smallest whole number ratio of the number of atoms of the various elements that are present in one molecule of the compound. For example, $C_6H_{12}O_6$ ***(the molecular formula of glucose)*** tells us that in one molecule of glucose, there are 6 atoms of carbon, 12 atoms of hydrogen, and 6 atoms of oxygen. Whereas, CH_2O ***(the empirical formula of glucose)*** tells us that in one molecule of glucose, the smallest whole number ratio of the number of atoms of carbon to hydrogen to oxygen is 1:2:1.

In some cases, the molecular as well as the empirical formula of a compound can be identical if the ratio of the number of atoms of the constituent elements in its molecular formula cannot be simplified any further without giving rise to decimal fractions. Examples include H_2O, CO_2, C_3H_8, N_2O_5 .

How to Determine the Empirical Formula of a Compound Based on the Information Given about the Composition of the Elements that Makes it up

Generally, the information about the chemical composition of a particular compound can be presented in 3 ways:

(1) The **Number of Moles** of each of the constituent elements making up the compound.

(2) The **Mass (in grams)** of each of the constituent elements making up the compound.

(3) The **Percent Composition** of each of the constituent elements in the compound.

Subsequently, the empirical formula of a compound can also be calculated based on the format by which these information are presented.

Determination of Empirical Formula of Compound if Number of Moles of Constituent Elements are Given.

Sample Question:

Determine the empirical formula of a compound, if a pure sample of the compound contains 7.7 moles of Carbon, 15 moles of Hydrogen, and 7.3 moles of Oxygen.

Steps to Follow:

(1) Create a table with columns and rows and place each element in each of the columns, starting by placing the first element in the second column of the first row of the table that you have created.

(2) Write down the number of moles of each element below its symbol.

(3) Now, identify the **smallest number of moles** in the listing, and then divide all the number of moles in the listing by this number (the smallest number of moles).

(4) Write down the results in the next row.

(5) Now, round off each of the results to the nearest integer (whole number).

(6) What you now have is the ratio of the number of atoms of each of the elements present in one molecule of the compound.

(7) Write out the empirical formula of the compound based on the ratio that you have obtained.

And that's it.

Sample Calculations:

Symbol of element	C	H	O
Number of moles	7.7	15	7.3
Divide through by the smallest # of moles	$\frac{7.7}{7.3} = 1.05$	$\frac{15}{7.3} = 2.05$	$\frac{7.3}{7.3} = 1.00$
Results (ratio of moles)	1.05	2.05	1.00
Round off to the nearest integer	1	2	1
Ratio	1: 2:1		
Empirical Formula	CH_2O		

Determination of Empirical Formula of Compound if Mass (in grams) of the Constituent Elements are Given

Sample Question:

What is the empirical formula of a compound, if an analysis of 51 grams of a pure sample of a compound reveals that the compound contains 20.4 grams of Carbon, 3.40 grams of Hydrogen, and 27.2 grams of Oxygen?

Steps to Follow:

(1) Create a table with columns and rows and place each element in each of the columns, starting by placing the first element in the second column of the first row of the table that you have created.

(2) Write down the mass (in grams) of each of the elements below its symbol.

(3) Find out the number of moles of each element by dividing the mass of each element by its atomic mass.

(4) Write down the number of moles of each element below its symbol.

(5) Now, identify the **smallest number of moles** in the listing, and then divide all the number of moles in the listing by this number (the smallest number of moles).

(6) Write down the results in the next row.

(7) Now, round off each of the results to the nearest integer (whole number).

(8) What you now have is the ratio of the number of atoms of each of the elements present in one molecule of the compound.

(9) Write out the empirical formula of the compound based on the ratio that you have obtained.

And that's it.

Sample Calculations:

Symbol of element	**C**	**H**	**O**
Mass in grams	20.40	3.40	27.20
Number of moles	$\frac{20.40}{12.01} = 1.70$	$\frac{3.40}{1.00} = 3.40$	$\frac{27.20}{16.00} = 1.70$
Results (# of moles)	1.70	3.40	1.70
Divide through by smallest # of moles	$\frac{1.70}{1.70} = 1.00$	$\frac{3.40}{1.70} = 2.00$	$\frac{1.70}{1.70} = 2.00$
Results (ratio of moles)	1.00	2.00	1.00
Round off to the nearest integer (whole number)	1	2	1
Ratio of atoms	1 : 2 : 1		
Empirical Formula	CH_2O		

Determination of Empirical Formula of Compound if the Percent Composition of the Constituent Elements are Given

Sample Question:

Calculate the empirical formula of a compound that is composed of 40.0% Carbon, 6.66% Hydrogen, and 53.33% Oxygen.

Steps to Follow:

(1) Create a table with columns and rows and place each element in each of the columns, starting by placing the first element in the second column of the first row of the table that you have created.

(2) Write down the percent composition of each of the elements below its symbol.

Now, we have to make an assumption in order to move to the next step, but before we proceed, let me make a brief illustration:

Let's imagine that we are in an auditorium occupied only by 100 science students that are majoring in their different fields of interest. Let's also assume that 15% of these students are majoring in Biology, 40% are majoring in Nursing, 20% are majoring in Pharmacy while the remaining 25% are Chemistry majors.

Now, it can be clearly observed that: 15% of 100 students is 15 students; 40% of 100 students is 40 students; 20% of 100 students is 20 students; and 25% of 100 students is 25 students.

This therefore implies that in the auditorium, we have 15 students as Biology majors; 40 as Nursing majors; 20 as Pharmacy majors, and 25 as Chemistry majors.

In this next step, we are going to apply the same idea to figure out the empirical formula of a compound if we are given only the percent composition of its constituent elements.

We were told that the compound is 40% Carbon, 6.66% Hydrogen, and 53.33% Oxygen. Since the sum of all the percentages is 100%, this directly implies that if we are given 100 grams of the compound, 40 grams will be Carbon, 6.66 grams will be Hydrogen, while Oxygen will compensate for the remaining 53.33 grams. From here, we can apply the same steps we used to figure out the empirical formula of a compound if we were given the mass (in grams) of its constituent elements.

(3) So, basically, what we have to do next is to assume that we have 100 grams of the compound. And from here, we then copy the respective percent compositions of the constituent elements and then write them down as their masses (in grams) since their respective masses and percent compositions in this kind of situation are indirectly the same.

(4) Since we now have the respective masses of the constituent elements, from here everything is done the same way as calculating the empirical formula from the mass (in grams) of the constituent elements. So:

(5) Write down the assumed mass (in grams) of each of the elements below its percent composition in the compound.

(6) Find out the number of moles of each element by dividing the mass of each element by its atomic mass.

(7) Write down the number of moles of each element below its symbol.

(8) Now, identify the **smallest number of moles** in the listing, and then divide all the number of moles in the listing by this number (the smallest number of moles).

(9) Write down the results in the next row.

(10) Now, round off each of the results to the nearest integer (whole number).

(11) What you now have is the ratio of the number of atoms of each of the elements present in one molecule of the compound.

(12) Write out the empirical formula of the compound based on the ratio that you have obtained.

And that's it.

Sample Calculations:

Symbol of element	**C**	**H**	**O**
Percent composition	40.0%	6.66%	53.33%
Mass in 100 g of compound	40.0 grams	6.66 grams	53.33 grams
Number of moles	$\frac{40.0}{12.01} = 3.33$	$\frac{6.66}{1.00} = 6.66$	$\frac{53.33}{16.00} = 3.33$
Results (# of moles)	3.33	6.66	3.33
Divide through by smallest # of moles	$\frac{3.33}{3.33} = 1.00$	$\frac{6.66}{3.33} = 2.00$	$\frac{3.33}{3.33} = 1.00$
Results (ratio of moles)	1.00	2.00	1.00
Round off to the nearest integer. (nearest whole number)	1	2	1
Ratio of atoms	1 : 2 : 1		

Empirical Formula: CH_2O

Problems with Rounding off Ratio of Moles to the Nearest Integer.

More often than not, students do encounter a certain degree of difficulty while trying to round off the ratio of moles of the constituent elements to the nearest integer. Generally, as a rule, none of the results of the ratio of moles obtained from dividing through by the smallest number of moles may be rounded off to the nearest integer (whole number), if any of the numbers in the result is far away from its nearest integer by a distance of more than 0.1. That is, the results of the ratio of moles can only be rounded off to the nearest integer, if the distance between the numbers and their closest integer is less than or equal to 0.1.

i.e. the following condition has to be true for all the numbers (the results of the ratio of moles) that are to be rounded off to their nearest integers:

$$| X - N | \leq 0.1$$

where: X is the number to be rounded off

N is its nearest integer

And $| X - N |$ means the distance between the number to be rounded off and its nearest integer.

If this condition cannot be satisfied, that is, if the distance between all the numbers and their nearest integers are not less than or equal to 0.1, all the results for the ratio of moles have to be multiplied by 2 before being rounded off to their nearest integer.

If after the multiplication of all the numbers by 2, the condition is still not satisfied, then all the numbers have to be multiplied by 3.

And if after the multiplication of all the numbers by 3, the condition is still not satisfied, then all the numbers have to be multiplied 4.

And if the condition is still not satisfied, then the process has to be repeated with the next consecutive number 5.

This process has to be repeated with increasing consecutive integers (6, 7, 8, 9 and so on) until the condition is finally satisfied (i.e. until the distance between all the ratio of moles and their nearest integer is less than or equal to 0.1.

To make the picture clearer, let's take a look at a few examples:

Example 1:

If an analysis of a certain hydrocarbon reveals that the compound contain 81.8 g of Carbon and 18.2 g of Hydrogen, what is the empirical formula of the compound?

Solution:

Symbol of element	**C**	**H**
Mass in grams	81.8g	18.2g
Number of moles	$\frac{81.8}{12.01} = 6.81$	$\frac{18.2}{1.00} = 18.2$
Results (# of moles)	6.81	18.2
Divide through by smallest # of moles	$\frac{6.81}{6.81} = 1.00$	$\frac{18.2}{6.81} = 2.67$
Results (ratio of moles)	1.00	2.67

CANNOT BE ROUNDED OFF AT THIS POINT because $| X - N | > 0.1$

Ratio of moles	Bad	1.00	2.67 **$\mid X - N \mid > 0.1$**
Ratio of moles X 2	still bad	2.00	5.34 **$\mid X - N \mid > 0.1$**
Ratio of moles X 3	Now **OK**	3.00	8.01 **$\mid X - N \mid \leq 0.1$**

Initially, since the ratio of moles did not satisfy the condition, the ratio of moles had to be multiplied by 2 and then by 3 until the condition was finally satisfied at 3.

Results (ratio of moles)	3.00	8.01
Round off to the nearest integer. (nearest whole number)	3	8
Ratio of atoms	3 : 8	
Empirical Formula	C_3H_8	

<u>Example 2:</u>
If an analysis of a certain hydrocarbon reveals that the compound contain 83.33 g of Carbon and 16.66 g of Hydrogen, what is the empirical formula of the compound?

Solution:

Symbol of element	**C**	**H**
Mass in grams	83.33g	16.66g
Number of moles	$\frac{83.33}{12.01} = 6.93$	$\frac{16.66}{1.00} = 16.66$
Results (# of moles)	6.93	16.66
Divide through by smallest # of moles	$\frac{6.93}{6.93} = 1.00$	$\frac{16.66}{6.93} = 2.40$
Results (ratio of moles)	1.00	2.40

CANNOT BE ROUNDED OFF AT THIS POINT because $| X - N | > 0.1$

Ratio of moles	Bad	1.00	2.40 $\| X - N \| > 0.1$
Ratio of moles X2	still bad	2.00	4.80 $\| X - N \| > 0.1$
Ratio of moles X 3	still bad	3.00	7.20 $\| X - N \| > 0.1$
Ratio of moles X4	still bad	4.00	9.60 $\| X - N \| > 0.1$
Ratio of moles X3	Now **OK**	5.00	12.00 $\| X - N \| \leq 0.1$

At this point, the ratio of moles can now be rounded off to the nearest whole number, since 12.00 satisfies the condition.

Results (ratio of moles)	5.00	12.00
Round off to the nearest integer. (nearest whole number)	5	12
Ratio of atoms	5 : 12	
Empirical Formula	C_5H_{12}	

If there are any misspellings or misrepresentation of any information in this handout that might result in your misunderstanding or misinterpretation of any of my explanations, please do not hesitate to let me know.

You may contact me by email at **peertutors@yahoo.com** if you have any questions, comments, or suggestions.

The online version of this handout is also available on the internet at:

www.geocities.com/peertutors/lresources.html

Thank you very much for your attention while studying with this piece of information. I hope my work will be of help to you in your studies.

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