Calculating Chemical Composition

A Directed Learning Activity for Hartnell College Chemistry 1

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Student Learning Objectives

This tutorial will help you to:
1. Convert between molecular and empirical formulas &
2. Convert between percent composition of chemical compounds and molecular or empirical formulas
Getting Started

- This set of Power Point slides will lead you through a series of short lessons and quizzes on the topics covered by this Directed Learning Activity tutorial.

- Move through the slideshow at your own pace. There are several hyperlinks you can click on to take you to additional information, take quizzes, get answers to quizzes, and to skip to other lessons.

- You can end this slide show at any time by hitting the “ESC” key on your computer keyboard.

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Table of Topics

- What You Should Already Know
- Molecular & Empirical Formulas
- Using Molecular Mass
- Percent Composition
What You Should Already Know

- How to use the periodic table to find the atomic masses of elements
- The relationship between atomic masses and molecular formula masses
- Calculate the formula mass from a chemical formula
- Understand the concept of the “mole”

If you are a little unsure of these concepts, please review your textbook.

Click here to begin
Molecular & Empirical Formula Definitions

- A **molecular formula** gives you the kind and number of atoms in a compound.  
  Example: $\text{C}_6\text{H}_{12}\text{O}_6$  
  This molecular formula tells you there are 6 carbon atoms, 12 hydrogen atoms, and 6 oxygen atoms in each molecule of this compound.

- An **empirical formula** gives the smallest whole number ratio between the different atoms in a compound.  
  Example: $\text{CH}_2\text{O}$  
  This empirical formula tells us that the ratio of carbon atoms to hydrogen atoms to oxygen atoms is 1:2:1  
  Note that this would be the empirical formula for the molecular formula presented in the first example.
Comparing Empirical and Molecular Formulas

So, looking at the example of C\textsubscript{6}H\textsubscript{12}O\textsubscript{6} – we can see that the molecular formula is six times the empirical formula of CH\textsubscript{2}O.

In general, we can say that:

\[
molecular\, formula = n \times (empirical\, formula) \quad \text{or}\quad n = \frac{molecular\, formula}{empirical\, formula}
\]

where \(n\) is a whole number from 1 to whatever is needed.

Let's look at some more examples of how empirical and molecular formulas compare.

Next
<table>
<thead>
<tr>
<th>Compound</th>
<th>Empirical Formula</th>
<th>$n$</th>
<th>Molecular Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon monoxide</td>
<td>CO</td>
<td>1</td>
<td>CO</td>
</tr>
<tr>
<td>Nitrogen dioxide</td>
<td>NO$_2$</td>
<td>1</td>
<td>NO$_2$</td>
</tr>
<tr>
<td>Acetylene</td>
<td>CH</td>
<td>2</td>
<td>C$_2$H$_2$</td>
</tr>
<tr>
<td>Oxalic acid</td>
<td>HCO$_2$</td>
<td>2</td>
<td>H$_2$C$_2$O$_4$</td>
</tr>
<tr>
<td>Dinitrogen tetraoxide</td>
<td>NO$_2$</td>
<td>2</td>
<td>N$_2$O$_4$</td>
</tr>
<tr>
<td>Benzene</td>
<td>CH</td>
<td>6</td>
<td>C$_6$H$_6$</td>
</tr>
</tbody>
</table>

Notice how for nitrogen dioxide and dinitrogen tetraoxide the empirical formulas are the same, but the value for $n$ and the molecular formulas are different. Can you see which other two compounds have a similar relationship? (Acetylene & benzene)

Go to Quiz
Quiz Question 1

Hydrogen peroxide is a chemical that is used to whiten teeth. What is the empirical formula for hydrogen peroxide, which has a molecular formula of $H_2O_2$?

Click [here](#) to review this lesson.

Click [here](#) to check your answer.
Quiz Question 2

Xylene is an industrial solvent. What is the empirical formula for xylene, which has a molecular formula of C$_8$H$_{10}$?

Click here to review this lesson.

Click here to check your answer.
Answer to Quiz Question 1

The ratio of hydrogen atoms to oxygen atoms in this molecule is 2:2. However, the simplest whole number ratio would be 1:1. Therefore, the empirical formula for hydrogen peroxide would be HO.

How did you do? If you missed this question, click here to review the examples and take the quiz again.

Click here to go on to the next question.
Answer to Quiz Question 2

The ratio of carbon atoms to hydrogen atoms in this molecule is 8:10. However, the simplest whole number ratio would be 4:5. Therefore, the empirical formula for xylene would be C₄H₅.

How did you do? If you missed this question, click here to review the examples and take the quizzes again.

Click here if you are ready to move on to the next lesson.
Using Molecular Mass

If you know the empirical formula of a compound, and if you know the molecular mass for the compound, you can determine the molecular formula.

Example 1:
You are given the empirical formula for a compound as BH$_3$ (one boron to every three hydrogen atoms). You are also given the molecular mass of the compound as 27.66 amu for each molecule of the compound. What is the molecular formula?
Solution to Example 1:

If we calculate the mass of the empirical formula using the atomic masses from the periodic table, we obtain 13.83 amu per empirical formula unit. That means that if we calculate for $n$ (the number of empirical formula units per molecule),

$$n = \frac{\text{molecular formula}}{\text{empirical formula}} = \frac{27.66 \text{ amu}}{13.83 \text{ amu}} = 2$$

Or, $2 \times (\text{BH}_3) = \text{B}_2\text{H}_6$. 

Next example
Example 2:
The empirical formula of a compound is CH\textsubscript{2}. Its molecular mass is 42.08 amu. What is the molecular formula of the compound?

Solution to Example 2:
The empirical formula mass of CH\textsubscript{2} = C + 2H = 12.01 amu + 2(1.008 amu) = 14.03 amu.

\[ n = \frac{\text{molecular mass}}{\text{empirical formula mass}} = \frac{42.08 \text{ amu}}{14.03 \text{ amu}} = 2.999 = 3 \]

Or, the molecular formula is \(3 \times (\text{CH}_2) = \text{C}_3\text{H}_6\).
Quiz Question 3

A colorless liquid has the empirical formula of HO. It has a molecular mass of 34.02 amu. What is the molecular formula of this compound?

Click [here](#) to review the lesson.

Click [here](#) to check your answer.
Quiz Question 4

The empirical formula of a colorless gas is COCl₂. Its molecular mass is 98.9 amu. What is the molecular formula of the compound?

Click here to review the lesson.

Click here to check your answer.
Answer to Quiz Question 3

The empirical formula mass of HO = H + O = 1.008 amu + 16.00 amu = 17.01 amu

n = molecular formula ÷ empirical formula
  = 34.02 amu ÷ 17.01 amu = 2

Molecular formula = 2(HO) = H₂O₂

How did you do? If you missed this question, click here to review the examples and take the quiz again.

Click here to solve quiz question 4.
Answer to Quiz Question 4

The empirical formula mass of COCl$_2$ =
C + O + 2Cl =  
12.01 amu + (16.00 amu) + 2(35.45 amu) = 98.91 amu
The empirical formula mass is the same as the molecular mass of the compound, or $n = 1$. This means the empirical formula and the molecular formula are the same, so the molecular formula = COCl$_2$

How did you do? If you missed this question, click here to review the examples and take the quizzes again.

Click here if you are ready to move on to the next lesson.
Using Percent Composition

To convert from percent composition to an empirical formula:

1. Unless other information is given, presume that you have 100 grams of compound. You can easily convert from the percent composition of each element to the number of grams by multiplying the percent by 100.

2. Calculate the number of moles of each element by dividing the mass you determined in step 1 by the atomic mass of that element.
3. The number of moles become the subscripts in the empirical formula for the compound.

4. If the subscripts are now whole numbers, find the lowest whole number ratio between the moles of the elements to determine the empirical formula.

5. If you also know the molecular mass of the compound, you can determine the molecular formula using the methods you learned in the previous lesson.
Example

This example will put all the ideas together that you have learned in the lessons so far.

The percent composition of borazine is 40.29% boron, 52.21% nitrogen, and 7.50% hydrogen. It has a molecular mass of 80.50 amu.

Using the following atomic masses for the elements, determine the molecular formula for borazine: $B = 10.81$ amu, $N = 14.01$ amu, $H = 1.008$ amu

Click here for the solution to this example.
Example Solution

First determine the number of moles of each element by using steps 1 & 2.

\[ \text{mole } B = \left(40.29 \text{ g } B\right) \times \left(1 \text{ mole } B \div 10.81 \text{ g } B\right) \]
\[ = 3.727 \text{ moles } B \]

\[ \text{mole } N = \left(52.21 \text{ g } N\right) \times \left(1 \text{ mole } N \div 14.01 \text{ g } N\right) \]
\[ = 3.727 \text{ moles } N \]

\[ \text{mole } H = \left(7.50 \text{ g } H\right) \times \left(1 \text{ mole } H \div 1.008 \text{ g } H\right) \]
\[ = 7.44 \text{ moles } H \]
Example Solution (2)

These mole values would give an initial empirical formula of

\[ \text{B}_{3.727}\text{N}_{3.727}\text{H}_{7.44} \]

But remembering that the empirical formula must have whole numbers, we can divide each subscript by 3.727 and get a proper empirical formula of

\[ \text{BNH}_2 \]

The empirical formula mass would then be

\[ \text{B} + \text{N} + 2\text{H} = \\
10.81 \text{ amu} + 14.01 \text{ amu} + 2(1.008) \text{ amu} = \\
26.84 \text{ amu} \]

Next
Example Solution (3)

If we use the formula we learned earlier:

\[ n = \frac{\text{molecular formula}}{\text{empirical formula}} \]

and substitute in the values for molecular formula and empirical formula masses, we get

\[ n = \frac{80.50 \text{ amu}}{26.84 \text{ amu}} = 2.999 = 3 \]

So the molecular formula of borazine is

\[ 3(\text{BNH}_2) = \text{B}_3\text{N}_3\text{H}_6. \]

Let’s move on to the quiz questions for this lesson. Click here.
Quiz Question 5

An ionic compound contains only chromium and chlorine. The percent composition is Cr = 42.31% and Cl = 57.69%. Calculate the empirical formula using the steps provided earlier in this lesson.

Click here to review the steps and example problem.

Click here to check your answer.
Quiz Question 6

Calculate the empirical formula of a compound that is 63.6% nitrogen and 36.4% oxygen.

Click here to review the steps and example problem.

Click here to check your answer.
Quiz Question 7

The molecular mass of an organic compound is 118.1 amu. Calculate the molecular formula of this compound if its percent composition is 40.68% C, 5.12% H, 54.20% O.

Click here to review the steps and example problem.

Click here to check your answer.
Answer to Quiz Question 5

Solution: \( \text{CrCl}_2 \)

Explanation:
moles Cr = 42.31 g Cr x (1 mole Cr/52.00 g Cr) = 0.8137 mole Cr
moles Cl = 57.69 g Cl x (1 mole Cl/35.45 g Cl) = 1.627 moles Cl
If we take the smaller number of moles and divide into the larger number of moles, we will obtain an empirical formula of \( \text{CrCl}_2 \)

If you missed this question, click here to review this lesson.

If you are ready to move on to the next question, click here.
Answer to Quiz Question 6

Solution: $\text{N}_2\text{O}$

Explanation:

$m\text{ole N} = 63.6 \text{ g N} \times \left( \frac{1 \text{ mole N}}{14.01 \text{ g N}} \right) = 4.54 \text{ moles N}$

$m\text{ole O} = 36.4 \text{ g O} \times \left( \frac{1 \text{ mole O}}{16.00 \text{ g O}} \right) = 2.28 \text{ moles O}$

If we take the smaller number of moles and divide into the larger number of moles, we will obtain an empirical formula of $\text{N}_2\text{O}$.

If you missed this question, click here to review this lesson.

If you are ready to move on to the next question, click here.
Answer to Quiz Question 7

Solution: \( C_4H_6O_4 \)

Explanation:
mole C = 40.68 g C x (1 mole C/12.01 g C) = 3.387 moles C
mole H = 5.12 g H x (1 mole H/1.008 g H) = 5.08 moles H
mole O = 54.20 g O x (1 mole O/16.00 g O) = 3.387 moles O

The initial empirical formula would be

\( C_{3.387}H_{5.08}O_{3.387} \)

Dividing each subscript by 3.387, you obtain

\( C_1H_{1.5}O_1 \)
Answer to Quiz Question 7 (2)

But we need whole numbers in the subscripts. By multiplying the subscripts by 2 to get whole numbers, you obtain

\[ \text{C}_2\text{H}_3\text{O}_2 \]

as the empirical formula.

However, we are also given 118.1 amu as the molecular mass of the compound. The empirical formula mass would be

\[ 2\text{C} + 3\text{H} + 2\text{O} = 2(12.01 \text{ amu}) + 3(1.008 \text{ amu}) + 2(16.00 \text{ amu}) = 59.04 \text{ amu} \]

\[ n = \text{molecular formula ÷ empirical formula} \]

and substituting in the values for molecular formula and empirical formula masses, we get

Next slide
Answer to Quiz Question 7 (3)

\[ n = \frac{118.1 \text{ amu}}{59.04 \text{ amu}} = 2 \]

So the molecular formula is

\[ 2(C_2H_3O_2) = C_4H_6O_4 \]

If you missed this question, click [here](#) to review this lesson.

If you successfully answered this question, click [here](#).
Congratulations!

You have successfully completed this Directed Learning Activity tutorial. We hope that this has helped you to better understand this topic.

Click [here](#) to end.

Click [here](#) to repeat this activity.
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