The Empirical Formula of a Compound

6.2

Section Preview/ Specific Expectations

In this section, you will

- **perform** an experiment to determine the percentage composition and the empirical formula of a compound
- **calculate** the empirical formula of a compound using percentage composition
- **communicate** your understanding of the following terms: *empirical formula, molecular formula*

As part of his atomic theory, John Dalton stated that atoms combine with one another in simple whole number ratios to form compounds. For example, the molecular formula of benzene, C_6H_6, indicates that one molecule of benzene contains 6 carbon atoms and 6 hydrogen atoms. The **empirical formula** (also known as the simplest formula) of a compound shows the lowest whole number ratio of the elements in the compound. The **molecular formula** (also known as the actual formula) describes the number of atoms of each element that make up a molecule or formula unit. Benzene, with a molecular formula of C_6H_6, has an empirical formula of CH. Table 6.1 shows the molecular formulas of several compounds, along with their empirical formulas.

Table 6.1 Comparing Molecular Formulas and Empirical Formulas

Name of compound	Molecular (actual) formula	Empirical (simplest) formula	Lowest ratio of elements
hydrogen peroxide	H_2O_2	HO	1:1
glucose	$C_6H_{12}O_6$	CH_2O	1:2:1
benzene	C_6H_6	CH	1:1
acetylene (ethyne)	C_2H_2	CH	1:1
aniline	C_6H_7N	C_6H_7N	6:7:1
water	H_2O	H_2O	2:1

Language LINK

The word "empirical" comes from the Greek word *empeirikos*, meaning, roughly, "by experiment." Why do you think the simplest formula of a compound is called its empirical formula?

It is possible for different compounds to have the same empirical formula, as you can see in Figure 6.6. For example, benzene and acetylene both have the empirical formula CH. Each, however, is a unique compound. Benzene, C_6H_6, is a clear liquid with a molar mass of 78 g/mol and a boiling point of 80°C. Acetylene, C_2H_2, has a molar mass of 26 g/mol. It is a highly flammable gas, commonly used in a welder's torch. There is, in fact, no existing compound with the molecular formula CH. The empirical formula of a compound shows the lowest whole number ratio of the atoms in the compound. It does not express the composition of a molecule.

Many compounds have molecular formulas that are the same as their empirical formulas. One example is ammonia, NH_3. Try to think of three other examples.

Figure 6.6 **The same empirical formula can represent more than one compound. These two compounds are different—at room temperature, one is a gas and one is a liquid. Yet they have the same empirical formula.**

Math LINK

In mathematics, you frequently need to reduce an expression to lowest terms. For example, $\frac{4x^2}{x}$ is equivalent to $4x$. A ratio of 5:10 is equivalent to 1:2. In chemistry, however, the "lowest terms" version of a chemical formula is not equivalent to its "real" molecular formula. Why not?

The relationship between the molecular formula of a compound and its empirical formula can be expressed as

Molecular formula subscripts = $n \times$ Empirical formula subscripts, where $n = 1, 2, 3...$

This relationship shows that the molecular formula of a compound is the same as its empirical formula when $n = 1$. What information do you need in order to determine whether the molecular formula of a compound is the same as its empirical formula?

Determining a Compound's Empirical Formula

In the previous section, you learned how to calculate the percentage composition of a compound from its chemical formula. Now you will do the reverse. You will use the percentage composition of a compound, along with the concept of the mole, to calculate the empirical formula of the compound. Since the percentage composition can often be determined by experiment, chemists use this calculation when they want to identify a compound.

The following Sample Problem illustrates how to use percentage composition to obtain the empirical formula of a compound.

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How do the molar masses of C_6H_6 and C_2H_2 compare with the molar mass of their empirical formula? How does the molar mass of water compare with the molar mass of its empirical formula? Describe the relationship between the molar mass of a compound and the molar mass of the empirical formula of the compound.

Sample Problem

Finding a Compound's Empirical Formula from Percentage Composition: Part A

Problem

Calculate the empirical formula of a compound that is 85.6% carbon and 14.4% hydrogen.

What Is Required?

You need to find the empirical formula of the compound.

What Is Given?

You know the percentage composition of the compound. You have access to a periodic table.

Plan Your Strategy

Since you know the percentage composition, it is convenient to assume that you have 100 g of the compound. This means that you have 85.6 g of carbon and 14.4 g of hydrogen. Convert each mass to moles. The number of moles can then be converted into a lowest terms ratio of the elements to get the empirical formula.

Act on Your Strategy

$$\text{Number of moles of C in 100 g sample} = \frac{85.6\ \cancel{\text{g}}}{12.01\ \cancel{\text{g}}/\text{mol}} = 7.13\ \text{mol}$$

$$\text{Number of moles of H in 100 g sample} = \frac{14.4\ \cancel{\text{g}}}{1.01\ \cancel{\text{g}}/\text{mol}} = 14.3\ \text{mol}$$

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Now determine the lowest whole number ratio. Divide both molar amounts by the lowest molar amount.

$C_{\frac{7.13}{7.13}}H_{\frac{14.3}{7.13}} \rightarrow C_{1.00}H_{2.01} \rightarrow CH_2$

Alternatively, you can set up your solution as a table.

Element	Mass percent (%)	Grams per 100 g sample (g)	Molar mass (g/mol)	Number of moles (mol)	Molar amount ÷ lowest molar amount
C	85.6	85.6	12.01	7.13	$\frac{7.13}{7.13} = 1$
H	14.4	14.4	1.01	14.3	$\frac{14.3}{7.13} = 2.01$

The empirical formula of the compound is CH_2.

Check Your Solution

Work backward. Calculate the percentage composition of CH_2.

$$\text{Mass percent of C} = \frac{12.01\ \cancel{\text{g/mol}}}{14.03\ \cancel{\text{g/mol}}} \times 100\%$$
$$= 85.6\%$$

$$\text{Mass percent of H} = \frac{2 \times 1.01\ \cancel{\text{g/mol}}}{14.03\ \cancel{\text{g/mol}}} \times 100\%$$
$$= 14.0\%$$

The percentage composition calculated from the empirical formula closely matches the given data. The formula is reasonable.

Practice Problems

9. A compound consists of 17.6% hydrogen and 82.4% nitrogen. Determine the empirical formula of the compound.

10. Find the empirical formula of a compound that is 46.3% lithium and 53.7% oxygen.

11. What is the empirical formula of a compound that is 15.9% boron and 84.1% fluorine?

12. Determine the empirical formula of a compound made up of 52.51% chlorine and 47.48% sulfur.

PROBLEM TIP

The fact that 2.01 was rounded to 2 in CH_2 is fine. The percentage composition is often determined by experiment, so it is unlikely to be exact.

Tips for Solving Empirical Formula Problems

In the Sample Problem above, the numbers were rounded at each step to simplify the calculation. To calculate an empirical formula successfully, however, you should not round the numbers until you have completed the calculation. Use the maximum number of significant digits that your calculator will allow, throughout the calculation. Rounding too soon when calculating an empirical formula may result in getting the wrong answer.

Table 6.2 Converting Subscripts in Empirical Formulas

When you see this decimal...	Try multiplying all subscripts by...
$x.80$ ($\frac{4}{5}$)	5
$x.75$ ($\frac{3}{4}$)	4
$x.67$ ($\frac{2}{3}$)	3
$x.60$ ($\frac{3}{5}$)	5
$x.40$ ($\frac{2}{5}$)	5
$x.50$ ($\frac{1}{2}$)	2
$x.33$ ($\frac{1}{3}$)	3
$x.25$ ($\frac{1}{4}$)	4
$x.20$ ($\frac{1}{5}$)	5
$x.17$ ($\frac{1}{6}$)	6

Often only one step is needed to determine the number of moles in an empirical formula. This is not always the case, however. Since you must divide by the lowest number of moles, initially one of your ratio terms will always be 1. If your other terms are quite close to whole numbers, as in the last Sample Problem, you can round them to the closest whole numbers. If your other terms are not close to whole numbers, you will need to do some additional steps. This is because empirical formulas do not always contain the subscript 1. For example, Fe_2O_3 contains the subscripts 2 and 3.

Decimals such as 0.95 to 0.99 can be rounded up to the nearest whole number. Decimals such as 0.01 to 0.05 can be rounded down to the nearest whole number. Other decimals require additional manipulation. What if you have the empirical formula $C_{1.5}H_3O_1$? To convert all subscripts to whole numbers, multiply each subscript by 2. This gives you the empirical formula $C_3H_6O_2$. Thus, a ratio that involves a decimal ending in 0.5 must be doubled. What if a decimal ends in 0.45 to 0.55? Round the decimal so that it ends in .5, and then double the ratio.

Table 6.2 gives you some strategies for converting subscripts to whole numbers. The variable x stands for any whole number. Examine the following Sample Problem to learn how to convert the empirical formula subscripts to the lowest possible whole numbers.

Sample Problem

Finding a Compound's Empirical Formula from Percentage Composition: Part B

Problem

The percentage composition of a fuel is 81.7% carbon and 18.3% hydrogen. Find the empirical formula of the fuel.

What Is Required?

You need to determine the empirical formula of the fuel.

What Is Given?

You know the percentage composition of the fuel. You have access to a periodic table.

Plan Your Strategy

Convert mass percent to mass, then to number of moles. Then find the lowest whole number ratio.

Act on Your Strategy

Element	Mass percent (%)	Grams per 100 g sample (g)	Molar mass (g/mol)	Number of moles (mol)	Molar amount ÷ lowest molar amount
C	81.7	81.7	12.0	6.81	$\frac{6.81}{6.81} = 1$
H	18.3	18.3	1.01	18.1	$\frac{18.1}{6.81} = 2.66$

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You now have the empirical formula $C_1H_{2.66}$. Convert the subscript 2.66 ($\frac{8}{3}$) to a whole number. $C_{1\times 3}H_{2.66\times 3} = C_3H_8$.

Check Your Solution

Work backward. Calculate the percentage composition of C_3H_8.

$$\text{Mass percent of C} = \frac{3 \times 12.01\ \cancel{\text{g/mol}}}{44.09\ \cancel{\text{g/mol}}} \times 100\%$$
$$= 81.7\%$$

$$\text{Mass percent of H} = \frac{8 \times 1.008\ \cancel{\text{g/mol}}}{44.09\ \cancel{\text{g/mol}}} \times 100\%$$
$$= 18.3\%$$

The percentage composition calculated from the empirical formula matches the percentage composition given in the problem.

Practice Problems

13. An oxide of chromium is made up of 68.4% chromium and 31.6% oxygen. What is the empirical formula of this oxide?

14. Phosphorus reacts with oxygen to give a compound that is 43.7% phosphorus and 56.4% oxygen. What is the empirical formula of the compound?

15. An inorganic salt is composed of 17.6% sodium, 39.7% chromium, and 42.8% oxygen. What is the empirical formula of this salt?

16. Compound X contains 69.9% carbon, 6.86% hydrogen, and 23.3% oxygen. Determine the empirical formula of compound X.

PROBLEM TIP

Notice that Table 6.2 suggests multiplying by 3 when you obtain a subscript ending in .67, which is very close to .66.

Determining the Empirical Formula by Experiment

In practice, you can determine a compound's empirical formula by analyzing its percentage composition. There are several different ways to do this. One way is to use a synthesis reaction in which a sample of an element with a known mass reacts with another element to form a compound. Since you know the mass of one of the elements and you can measure the mass of the compound produced, you can calculate the percentage composition.

For example, copper reacts with the oxygen in air to form the green compound copper oxide. Many buildings in Canada, such as the Parliament buildings in Ottawa, have green roofs that contain some copper(II) oxide. (See Figure 6.7.) Imagine you have a 5.0 g sample of copper shavings. You allow the copper shavings to react completely with oxygen. If the resulting compound has a mass of 6.3 g, you know that the compound contains 5.0 g copper and 1.3 g oxygen. Although you can use the periodic table to predict that the formula for copper(II) oxide is CuO, the masses help you confirm your prediction. Try converting the masses given above into an empirical formula.

In Investigation 6-A, you will use a synthesis reaction to determine the empirical formula of magnesium oxide by experiment.

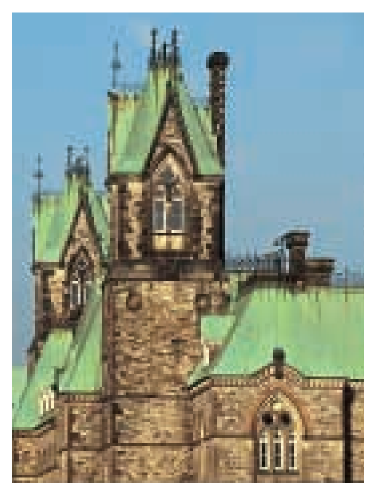


Figure 6.7 Although this green roof may contain some copper(II) oxide, it is mostly composed of basic copper sulfates and carbonates that form when the copper reacts with acid precipitation.

SKILL FOCUS

Predicting

Performing and recording

Analyzing and interpreting

Communicating results

Investigation 6-A

Determining the Empirical Formula of Magnesium Oxide

When magnesium metal is heated over a flame, it reacts with oxygen in the air to form magnesium oxide, Mg_xO_y:

$$Mg_{(s)} + O_{2(g)} \rightarrow Mg_xO_{y(s)}$$

In this investigation, you will react a strip of pure magnesium metal with oxygen, O_2, in the air to form magnesium oxide. Then you will measure the mass of the magnesium oxide produced to determine the percentage composition of magnesium oxide. You will use this percentage composition to calculate the empirical formula of magnesium oxide. CAUTION **Do not perform this investigation unless welder's goggles are available.**

Question

What is the percentage composition and empirical formula of magnesium oxide?

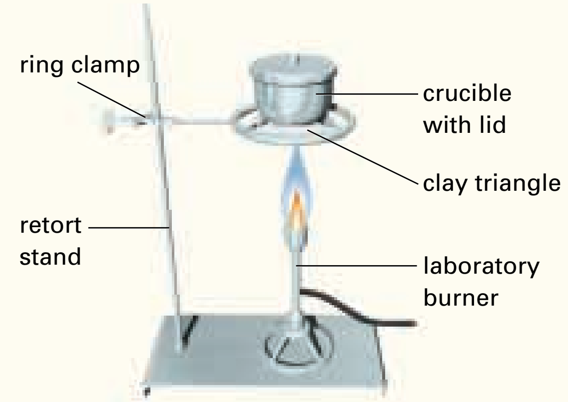
Predictions

Using what you have learned about writing formulas, predict the molecular formula and percentage composition of magnesium oxide.

Materials

electronic balance
small square of sandpaper or emery paper
8 cm strip of magnesium ribbon
laboratory burner
sparker
retort stand
ring clamp
clay triangle
clean crucible with lid
crucible tongs
ceramic pad
distilled water
wash bottle
disposal beaker
welder's goggles

Note: Make sure that the mass of the magnesium ribbon is at least 0.10 g.



Safety Precautions

- Do not look directly at the burning magnesium.
- Do not put a hot crucible on the bench or the balance.

Procedure

1. Make a table like the one below.

Observations

Mass of clean, empty crucible and lid	
Mass of crucible, lid, and magnesium	
Mass of crucible and magnesium oxide	

2. Assemble the apparatus as shown in the diagram.
3. Obtain a strip of magnesium, about 8 cm long, from your teacher. Clean the magnesium strip with sandpaper or emery paper to remove any oxide coating.
4. Measure and record the mass of the empty crucible and lid. Add the strip of cleaned magnesium to the crucible. Record the mass of the crucible, lid, and magnesium.

5. With the lid off, place the crucible containing the magnesium on the clay triangle. Heat the crucible with a strong flame. Using the crucible tongs, hold the lid of the crucible nearby. CAUTION When the magnesium ignites, quickly cover the crucible with the lid. Continue heating for about 1 min.

6. Carefully remove the lid. CAUTION Heat the crucible until the magnesium ignites once more. Again, quickly cover the crucible. Repeat this heating and covering of the crucible until the magnesium no longer ignites. Heat for a further 4 to 5 min with the lid off.

7. Using the crucible tongs, put the crucible on the ceramic pad to cool.

8. When the crucible is cool enough to touch, put it on the bench. Carefully grind the product into small particles using the glass rod. Rinse any particles on the glass rod into the crucible with distilled water from the wash bottle.

9. Add enough distilled water to the crucible to thoroughly wet the contents. The white product is magnesium oxide. The yellowish-orange product is magnesium nitride.

10. Return the crucible to the clay triangle. Place the lid slightly ajar. Heat the crucible gently until the water begins to boil. Continue heating until all the water has evaporated, and the product is completely dry. Allow the crucible to cool on the ceramic pad.

11. Using the crucible tongs, carry the crucible and lid to the balance. Measure and record the mass of the crucible and lid.

12. Do not put the magnesium oxide in the garbage or in the sink. Put it in the disposal beaker designated by your teacher.

Analysis

1. (a) What mass of magnesium did you use in the reaction?
   (b) What mass of magnesium oxide was produced?
   (c) Calculate the mass of oxygen that reacted with the magnesium.
   (d) Use your data to calculate the percentage composition of magnesium oxide.
   (e) Determine the empirical formula of magnesium oxide. Remember to round your empirical formula to the nearest whole number ratio, such as 1:1, 1:2, 2:1, or 3:3.

2. (a) Verify your empirical formula with your teacher. Use the empirical formula of magnesium oxide to determine the mass percent of magnesium in magnesium oxide.
   (b) Calculate your percent error (PE) by finding the difference between the experimental mass percent (EP) of magnesium and the actual mass percent (AP) of magnesium. Then you divide the difference by the actual mass percent of magnesium and multiply by 100%.

$$PE = \frac{EP - AP}{AP} \times 100\%$$

3. Why did you need to round the empirical formula you obtained to a whole number ratio?

Conclusion

4. Compare the empirical formula you obtained with the empirical formula you predicted.

Applications

5. Write a balanced chemical equation for the reaction of magnesium with oxygen gas, O_2.

6. (a) Suppose that you had allowed some magnesium oxide smoke to escape during the investigation. How would the Mg:O ratio have been affected? Would the ratio have increased, decreased, or remained unchanged? Explain using sample calculations.
   (b) How would your calculated value for the empirical formula of magnesium oxide have been affected if all the magnesium in the crucible had not burned? Support your answer with sample calculations.
   (c) Could either of the situations mentioned in parts (a) and (b) have affected your results? Explain.

Section Wrap-up

In section 6.2, you learned how to calculate the empirical formula of a compound based on percentage composition data obtained by experiment. In section 6.3, you will learn how chemists use the empirical formula of a compound and its molar mass to determine the molecular formula of a compound.

Section Review

1. (a) K/U Why is the empirical formula of a compound also referred to as its simplest formula?

   (b) K/U Explain how the empirical formula of a compound is related to its molecular formula.

2. I Methyl salicylate, or oil of wintergreen, is produced by the wintergreen plant. It can also be prepared easily in a laboratory. Methyl salicylate is 63.1% carbon, 5.31% hydrogen, and 31.6% oxygen. Calculate the empirical formula of methyl salicylate.

3. I Determine the empirical formula of the compound that is formed by each of the following reactions.

   (a) 0.315 mol chlorine atoms react completely with 1.1 mol oxygen atoms

   (b) 4.90 g silicon react completely with 24.8 g chlorine

4. I Muscle soreness from physical activity is caused by a buildup of lactic acid in muscle tissue. Analysis of lactic acid reveals it to be 40.0% carbon, 6.71% hydrogen, and 53.3% oxygen by mass. Calculate the empirical formula of lactic acid.

5. MC Imagine that you are a lawyer. You are representing a client charged with possession of a controlled substance. The prosecutor introduces, as forensic evidence, the empirical formula of the substance that was found in your client's possession. How would you deal with this evidence as a lawyer for the defence?

6. I Olive oil is used widely in cooking. Oleic acid, a component of olive oil, contains 76.54% carbon, 12.13% hydrogen and 11.33% oxygen by mass. What is the empirical formula of oleic acid?

7. I Phenyl valerate is a colourless liquid that is used as a flavour and odorant. It contains 74.13% carbon, 7.92% hydrogen and 17.95% oxygen by mass. Determine the empirical formula of phenyl valerate.

8. I Ferrocene is the common name given to a unique compound that consists of one iron atom sandwiched between two rings containing hydrogen and carbon. This orange, crystalline solid is added to fuel oil to improve combustion efficiency and eliminate smoke. As well, it is used as an industrial catalyst and a high-temperature lubricant.

   (a) Elemental analysis reveals ferrocene to be 64.56% carbon, 5.42% hydrogen and 30.02% iron by mass. Determine the empirical formula of ferrocene.

   (b) Read the description of ferrocene carefully. Does this description provide enough information for you to determine the molecular formula of ferrocene? Explain your answer.