Empirical Formulas

6.7

In the previous section you read about the *Phoenix* Mars Lander's search for signs of life. You also learned that researchers use combustion analysis to determine the percentage composition of unknown compounds. Percentage composition gives the percentage, by mass, of the elements in a compound. However, many compounds have the same percentage composition. Methanal, CH_2O, and ethanoic acid, $C_2H_4O_2$, for example, both contain 40.0 % carbon, 6.7 % hydrogen, and 53.3 % oxygen, by mass. However, these compounds have very different properties and applications (**Figure 1**).

Figure 1 (a) Solutions of methanal (formaldehyde) are used to preserve biological specimens, such as this sheep fetus. (b) Vinegar is a solution of ethanoic (acetic) acid and other substances dissolved in water.

The best way to identify an unknown compound is to determine its chemical formula. The subscripts in a chemical formula describe the number of atoms or ions of each element in the formula. How do you convert mass data to numbers of atoms in a molecule, or the number of ions in a formula unit? Earlier, you learned how to determine the number of entities, in moles, from the mass of the sample. Let's consider a compound that is 40.0 % carbon, 6.7 % hydrogen, and 53.3 % oxygen, by mass.

This compound has the same percentage of each element whatever the mass of your sample. So, we will imagine a convenient mass of the compound: 100.0 g. This sample contains 40.0 g of carbon, 6.5 g of hydrogen, and 53.5 g of oxygen. We can then determine the amount of each element (in moles) by dividing each element's mass by its molar mass (**Table 1**).

Table 1 Determining the Amount of Each Element in a 100.0 g Sample of a Compound

Amount of carbon (mol)	Amount of hydrogen (mol)	Amount of oxygen (mol)
$n_C = \dfrac{40.0\ \text{g}}{12.01\ \dfrac{\text{g}}{\text{mol}}}$ $= (40.0\ \cancel{\text{g}})\left(\dfrac{1\ \text{mol}}{12.01\ \cancel{\text{g}}}\right)$ $= 3.33\ \text{mol}$	$n_H = \dfrac{6.5\ \text{g}}{1.01\ \dfrac{\text{g}}{\text{mol}}}$ $= (6.5\ \cancel{\text{g}})\left(\dfrac{1\ \text{mol}}{1.01\ \cancel{\text{g}}}\right)$ $= 6.4\ \text{mol}$	$n_O = \dfrac{53.5\ \text{g}}{16.00\ \dfrac{\text{g}}{\text{mol}}}$ $= (53.5\ \cancel{\text{g}})\left(\dfrac{1\ \text{mol}}{16.00\ \cancel{\text{g}}}\right)$ $= 3.34\ \text{mol}$

Note that the ratio of the amounts of carbon and oxygen is essentially 1:1. The amount of hydrogen is almost double this value. Therefore, the ratio of carbon to hydrogen to oxygen atoms in the compound is 1:2:1. We can express this ratio as the chemical formula $C_1H_2O_1$ or CH_2O.

LEARNING **TIP**

Determining Ratios
One way to determine the ratios of entities is to divide each amount by the smallest amount. The smallest amount becomes "1." The other amounts have higher values, relative to 1.

Distinguishing between Empirical Formula and Molecular Formula

empirical formula a formula that shows the simplest whole-number ratio of elements in a compound

molecular formula a formula that shows the element symbols and exact number of each type of atom in a molecular compound

CH_2O is an example of an empirical formula. The **empirical formula** gives the simplest whole-number ratio of atoms or ions in a compound. Both methanal and ethanoic acid have the same empirical formula: CH_2O. A **molecular formula** gives the exact number of each type of atom in a compound. A methanal molecule contains 1 carbon atom, 2 hydrogen atoms, and 1 oxygen atom (**Table 2**). Therefore, its empirical and molecular formulas are identical. However, an ethanoic acid molecule contains twice the number of atoms given in its empirical formula. As a result, its molecular formula is $C_2H_4O_2$.

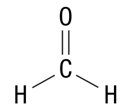
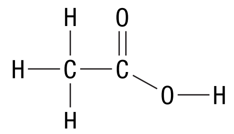
LEARNING TIP

An Analogy for Empirical Formula
Imagine a "compound" that contains exactly 2 thumbs, T, and 8 fingers, F. The molecular formula for this compound is T_2F_8. Since there is 1 thumb for every 4 fingers, the simplest ratio of thumbs to fingers is 1:4. Therefore, the empirical formula of this compound is TF_4.

Molecular formula: T_2F_8

Empirical formula: TF_4

Table 2 Comparing Empirical, Molecular, and Structural Formulas

Compound	Empirical formula	Molecular formula	Structural formula
methanal	CH_2O	CH_2O	
ethanoic acid	CH_2O	$C_2H_4O_2$	

The formula that we write for most ionic compounds is an empirical formula. For example, a tiny grain of sodium chloride (table salt) may contain quadrillions of sodium and chloride ions. Since these ions are in a 1:1 ratio, the empirical formula of sodium chloride is NaCl.

Determining Empirical Formula

Percentage composition gives the proportion of masses of the elements in a compound. The empirical formula gives the proportion of the atoms or ions of each element. If we know the percentage composition of a compound, we can determine the empirical formula. We do this by converting the mass of each of the elements (in grams) into amount (in moles). The ratio of amounts gives the subscripts in the empirical formula.

Tutorial 1 Determining the Empirical Formula from Percentage Composition

When we know the percentage composition of a compound and want to find the empirical formula, it is helpful to consider a 100.0 g sample of the compound.

Sample Problem 1: Determining a Simple Empirical Formula

Find the empirical formula of a compound with percentage composition 35.4 % sodium and the remainder nitrogen.

Given: % Na = 35.4%, remainder is N

Required: empirical formula of compound

Solution:

Step 1. Let's start with a convenient mass of the compound, such as 100.0 g.

Sodium makes up 35.4% of the sample; nitrogen makes up the rest:

$100.0\ g - 35.4\ g = 64.6\ g$

Step 2. Calculate the amount of each element.

$$n_{Na} = (35.4\ \cancel{g})\left(\frac{1\ \text{mol}}{22.99\ \cancel{g}}\right)$$
$$= 1.540\ \text{mol [extra digits carried]}$$
$$n_{N} = (64.6\ \cancel{g})\left(\frac{1\ \text{mol}}{14.01\ \cancel{g}}\right)$$
$$= 4.6110\ \text{mol [extra digits carried]}$$

Step 3. To determine the simplest ratio of the elements in the compound, divide the amount of each element by the smallest amount.

$$\frac{n_{Na}}{n_{Na}} = \frac{\cancel{1.549\ \text{mol}}}{\cancel{1.5459\ \text{mol}}} = 1$$

We assign sodium a value of 1.

$$\frac{n_{N}}{n_{Na}} = \frac{4.6110\ \cancel{\text{mol}}}{1.5459\ \cancel{\text{mol}}} = 2.98$$

According to the calculation, the ratio of sodium to nitrogen is 1:2.98. Since we cannot have a fraction of an element in a compound, the value for nitrogen is rounded off to the nearest whole number. As a result, the simplest whole-number ratio of sodium to nitrogen is 1:3.

Statement: The empirical formula of this compound is NaN_3.

EMPIRICAL FORMULAS WITH FRACTIONS

Determining the simplest ratio of the elements may give whole numbers. However, because you are working with experimental (measured) data, you should expect that your answer may include a fraction. If a number is within 0.05 of a whole number, you can round it up or down to the nearest whole number. But what do you do if one of the values is not close to a whole number? You multiply all the values by the same number to make them all whole numbers. Multiplying the subscripts by the fraction denominator gives whole numbers (**Table 3**). For example

$C_{1 \times 3}H_{1.333 \times 3} = C_3H_4$.

Sample Problem 2 illustrates this procedure.

Table 3 Ratios from Fractions

Decimal/fraction	Whole number	Multiply all subscripts by
$0.25 = \frac{1}{4}$	$4(0.25) = 1$	4
$0.33 = \frac{1}{3}$	$3(0.33) = 1$	3
$0.50 = \frac{1}{2}$	$2(0.5) = 1$	2
$0.67 = \frac{2}{3}$	$3(0.67) = 2$	3
$0.75 = \frac{3}{4}$	$4(0.75) = 3$	4

Sample Problem 2: Determining a More Complex Empirical Formula

Determine the empirical formula of a compound that contains 69.9 % iron and 30.1 % oxygen by mass (**Figure 2**).

Given: % Fe = 69.9 %, % O = 30.1 %

Required: empirical formula of the unknown compound, Fe_xO_y

Solution:

A 100.0 g sample of this compound contains 69.9 g of iron and 30.1 g of oxygen.

$M_{Fe} = 55.85$ g/mol; $M_O = 16.00$ g/mol

Step 1. Calculate the amount of each element in the 100.0 g sample.

$$n_{Fe} = (69.9\ \cancel{g})\left(\frac{1\ \text{mol}}{55.85\ \cancel{g}}\right)$$
$$= 1.2516\ \text{mol [extra digits carried]}$$
$$n_{O} = (30.1\ \cancel{g})\left(\frac{1\ \text{mol}}{16.00\ \cancel{g}}\right)$$
$$= 1.8813\ \text{mol [extra digits carried]}$$

Step 2. Divide the amount of each element by the smallest amount

$$\frac{n_{Fe}}{n_{Fe}} = \frac{\cancel{1.2516\ \text{mol}}}{\cancel{1.2516\ \text{mol}}} = 1$$

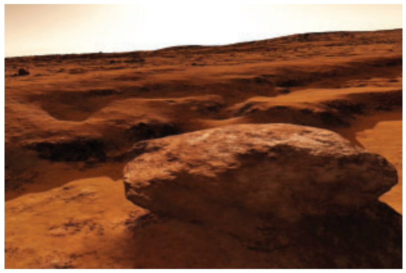


Figure 2 An artist's impression of Mars shows the ground as reddish-orange. Scientists suggest that the rocks are this colour because of their high iron oxide content.

Assign iron a value of 1.

$$\frac{n_O}{n_{Fe}} = \frac{1.8813\ \cancel{mol}}{1.2516\ \cancel{mol}} = 1.50$$

Assign oxygen a value of 1.50, relative to iron.

Step 3. These calculations give an empirical formula of $Fe_1O_{1.5}$. Subscripts in a chemical formula are normally whole numbers. Multiplying both subscripts by 2 gives Fe_2O_3.

Statement: The empirical formula of the compound is Fe_2O_3.

Sample Problem 3: Determining an Empirical Formula with Three Elements

Determine the empirical formula of a compound that contains 52.2 % carbon, 6.15 % hydrogen, and 41.7 % oxygen.

Given: % C = 52.2%, % H = 6.15 %, % O = 41.7 %

Required: empirical formula of compound, $C_xH_yO_z$

Solution:

A 100.0 g sample of this compound contains 52.2 g of carbon, 6.15 g of hydrogen, and 41.7 g of oxygen.

$M_C = 12.01$ g/mol; $M_H = 1.01$ g/mol; $M_O = 16.00$ g/mol

Step 1. Determine the amount of each element in the 100.0 g sample.

$$n_C = (52.2\ \cancel{g})\left(\frac{1\ \text{mol}}{12.01\ \cancel{g}}\right)$$

$$n_C = 4.3464\ \text{mol}\ [2\ \text{extra digits carried}]$$

$$n_H = (6.15\ \cancel{g})\left(\frac{1\ \text{mol}}{1.01\ \cancel{g}}\right)$$

$$n_H = 6.0891\ \text{mol}\ [2\ \text{extra digits carried}]$$

$$n_O = (41.7\ \cancel{g})\left(\frac{1\ \text{mol}}{16.00\ \cancel{g}}\right)$$

$$n_O = 2.6063\ \text{mol}\ [2\ \text{extra digits carried}]$$

Step 2. Divide the amount of each element by the smallest amount.

$$\frac{n_O}{n_O} = \frac{\cancel{2.6063\ mol}}{\cancel{2.6063\ mol}} = 1$$

Assign oxygen a value of 1.

$$\frac{n_C}{n_O} = \frac{4.3464\ \cancel{mol}}{2.6063\ \cancel{mol}} = 1.67$$

Assign carbon a value of 1.67.

$$\frac{n_H}{n_O} = \frac{6.0891\ \cancel{mol}}{2.6063\ \cancel{mol}} = 2.29$$

Assign hydrogen a value of 2.29.

Step 3. These calculations give an empirical formula of $C_{1.67}H_{2.29}O_1$. Multiplying each of the subscripts by 3 gives $C_5H_7O_3$.

Statement: The empirical formula of the compound is $C_5H_7O_3$.

Practice

SKILLS HANDBOOK **A6.3, A6.5**

1. Write the empirical formulas of compounds with the following percentage compositions: T/I C
   (a) 20.2 % Al, 79.8 % Cl [ans: $AlCl_3$]
   (b) 18.4 % C, 21.5 % N, and the rest K [ans: KCN]
   (c) 52.9 % Al, and the rest O [ans: Al_2O_3]
   (d) 50.85 % C, 8.47 % H, and 40.68 % O [ans: $C_5H_{10}O_3$]

6.7 Summary

- The empirical formula gives the simplest whole-number ratio of the elements in a compound.
- Most chemical formulas for ionic compounds are empirical formulas.
- The empirical formula can be determined from percentage composition data, using molar mass to find the relative amount of each element in the compound.
- The molecular formula gives the exact number of atoms of each element in a molecular compound. The molecular formula is sometimes, but not always, the same as the empirical formula.

6.7 Questions

1. Before you can determine an empirical formula,
   (a) what experimental evidence do you need?
   (b) what researched data do you need? K/U
2. Which of the following are empirical formulas? Explain. K/U

   $C_2H_4O_2$, H_2CO_3, $K_2Cr_2O_7$, $C_3H_6O_3N$
3. Which of the following pairs of compounds have the same empirical formula? Write the empirical formula in each case. T/I C
   (a) NO_2, N_2O_4
   (b) C_3H_6, C_4H_7
   (c) C_2H_2, C_6H_6
   (d) $C_{12}H_{10}O_2$, C_6H_5O
4. Identify the multiplier that converts the subscripts in these formulas into the nearest whole number. Then write the empirical formula of each compound. T/I C
   (a) $CH_{3.5}$
   (b) $C_{0.67}H_{0.67}O$
   (c) $NaSO_{1.5}$
   (d) $C_{1.34}H_{3.66}O$
5. The percentage composition of ascorbic acid (vitamin C) is 40.9 % carbon and 4.55 % hydrogen. The remainder is oxygen. Determine the empirical formula of ascorbic acid. T/I C
6. Nitrogen and oxygen form two different compounds with the following percentage compositions:

   Compound 1: 46.7 % N; 53.3 % O

   Compound 2: 30.4 % N; 69.6 % O

   Determine the empirical formula of each compound. T/I C
7. Nylon-6 is a plastic used to make strings for musical instruments. Nylon-6 consists of 63.68 % carbon, 9.80 % hydrogen, and 12.38 % nitrogen. The remainder is oxygen. Determine the empirical formula of nylon-6. T/I C
8. Aluminum carbide is a hard, abrasive substance used in some high-speed cutting tools. Aluminum makes up 75 % of the mass of this compound and carbon makes up the rest. Determine the empirical formula of aluminum carbide. T/I C
9. A 21.7 g sample of a compound of mercury and oxygen is decomposed into its elements by heating (**Figure 3**). If 20.1 g of mercury is collected, is the empirical formula of the compound HgO or Hg_2O? Why? T/I

Figure 3 Heating a compound of mercury and oxygen leaves a mirror-like coating of mercury lining the test tube.

10. A compound contains an unknown element X. This element forms an oxide with chemical formula X_2O. Experimental tests show that X_2O contains 25.8 % oxygen, by mass. T/I
    (a) What is the percentage of element X in the compound?
    (b) Use this information to identify element X.
11. Glucose and fructose are both examples of sugars. T/I C A
    (a) Research and compare their empirical, molecular, and structural formulas.
    (b) Research the correlation between obesity and these sweeteners in pop. Which sugar appears to be associated with obesity?

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