Pearson

4.11: Determining a Chemical Formula from Experimental Data

In Section 4.10, we calculated mass percent composition from a chemical formula. Can we also do the reverse? Can we calculate a chemical formula from mass percent composition? This question is important because many laboratory analyses of compounds give the relative masses of each element present in the compound. For example, if we decompose water into hydrogen and oxygen in the laboratory, we can measure the masses of hydrogen and oxygen produced. Can we arrive at a chemical formula from this kind of data? The answer is a qualified yes. We can determine a chemical formula, but it is an empirical formula (not a molecular formula). To get a molecular formula, we need additional information, such as the molar mass of the compound.

Suppose we decompose a sample of water in the laboratory and find that it produces 0.857 g of hydrogen and 6.86 g of oxygen. How do we determine an empirical formula from these data? We know that an empirical formula represents a ratio of atoms or a ratio of moles of atoms, *not a ratio of masses*. So the first thing we must do is convert our data from mass (in grams) to amount (in moles). How many moles of each element are present in the sample? To convert to moles, we divide each mass by the molar mass of that element.

$$\begin{aligned} \text{moles H} &= 0.857 \text{ g H} \times \frac{1 \text{ mol H}}{1.01 \text{ g H}} = 0.849 \text{ mol H} \\ \text{moles O} &= 6.86 \text{ g O} \times \frac{1 \text{ mol O}}{16.00 \text{ g O}} = 0.429 \text{ mol O} \end{aligned}$$

From these data, we know there are 0.849 mol H for every 0.429 mol O. We can now write a pseudoformula for water.

$$H_{0.849}O_{0.429}$$

To get the smallest whole-number subscripts in our formula, we divide all the subscripts by the smallest one, in this case 0.429.

$$H_{\frac{0.849}{0.429}}O_{\frac{0.429}{0.429}} = H_{1.98}O = H_2O$$

Our empirical formula for water, which also happens to be the molecular formula, is H_2O. You can use the procedure in Examples 4.14 and 4.15 to obtain the empirical formula of any compound from experimental data giving the relative masses of the constituent elements. The left column outlines the procedure, and the center and right columns contain two examples of how to apply the procedure.

Example 4.14 Obtaining an Empirical Formula from Experimental Data

PROCEDURE FOR Obtaining an Empirical Formula from Experimental Data

A compound containing nitrogen and oxygen is decomposed in the laboratory and produces 24.5 g nitrogen and 70.0 g oxygen. Find the empirical formula of the compound.

1. Write down (or calculate) as *given* the masses of each element present in a sample of the compound. If you are given mass percent composition, assume a 100-g sample and calculate the masses of each element from the given percentages.

GIVEN: 24.5 g N, 70.0 g O

FIND: empirical formula

2. Convert each of the masses from Step 1 to moles by using the appropriate molar mass for each element as a conversion factor.

$$24.5 \text{ g N} \times \frac{1 \text{ mol N}}{14.01 \text{ g N}} = 1.75 \text{ mol N}$$
$$70.0 \text{ g O} \times \frac{1 \text{ mol O}}{16.00 \text{ g O}} = 4.38 \text{ mol O}$$

3. Write down a pseudoformula for the compound using the number of moles of each element (from Step 2) as subscripts.

$$N_{1.75}O_{4.38}$$

4. Divide all the subscripts in the formula by the smallest subscript.

$$N_{\frac{1.75}{1.75}}O_{\frac{4.38}{1.75}} \rightarrow N_1O_{2.5}$$

5. If the subscripts are not whole numbers, multiply all the subscripts by a small whole number (see table) to determine whole-number subscripts.

Fractional Subscript	Multiply by This
0.20	5
0.25	4
0.33	3
0.40	5
0.50	2
0.66	3
0.75	4
0.80	5

$$N_1O_{2.5} \times 2 \rightarrow N_2O_5$$

FOR PRACTICE 4.14 A sample of a compound is decomposed in the laboratory and produces 165 g carbon, 27.8 g hydrogen, and 220.2 g oxygen. Calculate the empirical formula of the compound.

Example 4.15 Obtaining an Empirical Formula from Experimental Data

PROCEDURE FOR Obtaining an Empirical Formula from Experimental Data

A laboratory analysis of aspirin determined the following mass percent composition:

C 60.00 %
H 4.48 %
O 35.52 %

Find the empirical formula of aspirin.

1. Write down (or calculate) as *given* the masses of each element present in a sample of the compound. If you are given mass percent composition, assume a 100-g sample and calculate the masses of each element from the given percentages.

GIVEN: In a 100-g sample: 60.00 g C, 4.48 g H, 35.52 g O

FIND: empirical formula

2. Convert each of the masses from Step 1 to moles by using the appropriate molar mass for each element as a conversion factor.

$$60.00\text{ g C} \times \frac{1\text{ mol C}}{12.01\text{ g C}} = 4.996\text{ mol C}$$
$$4.48\text{ g H} \times \frac{1\text{ mol H}}{1.008\text{ g H}} = 4.44\text{ mol H}$$
$$35.52\text{ g O} \times \frac{1\text{ mol O}}{16.00\text{ g O}} = 2.220\text{ mol O}$$

3. Write down a pseudoformula for the compound using the number of moles of each element (from Step 2) as subscripts.

$$C_{4.996}H_{4.44}O_{2.220}$$

4. Divide all the subscripts in the formula by the smallest subscript.

$$C_{\frac{4.996}{2.220}}H_{\frac{4.44}{2.220}}O_{\frac{2.220}{2.220}} \rightarrow C_{2.25}H_2O_1$$

5. If the subscripts are not whole numbers, multiply all the subscripts by a small whole number (see table) to determine whole-number subscripts.

Fractional Subscript	Multiply by This
0.20	5
0.25	4
0.33	3
0.40	5
0.50	2
0.66	3
0.75	4
0.80	5

$$C_{2.25}H_2O_1 \times 4 \rightarrow C_9H_8O_4$$

The correct empirical formula is $C_9H_8O_4$.

FOR PRACTICE 4.15

Ibuprofen has the following mass percent composition:

C 75.69%, H 8.80%, O 15.51%.

What is the empirical formula of ibuprofen?

Interactive Worked Example 4.15 Obtaining an Empirical Formula from Experimental Data

Calculating Molecular Formulas for Compounds

We can determine the molecular formula of a compound from the empirical formula if we also know the molar mass of the compound. Recall from Section 4.3 that the molecular formula is always a whole-number multiple of the empirical formula.

$$\text{molecular formula} = \text{empirical formula} \times n, \text{ where } n = 1, 2, 3, \ldots$$

Suppose we want to find the molecular formula for fructose (a sugar found in fruit) from its empirical formula, CH_2O, and its molar mass, 180.2 g/mol. We know that the molecular formula is a whole-number multiple of CH_2O.

$$\begin{aligned} \text{molecular formula} &= (CH_2O) \times n \\ &= C_nH_{2n}O_n \end{aligned}$$

We also know that the molar mass is a whole-number multiple of the **empirical formula molar mass**, the sum of the masses of all the atoms in the empirical formula.

$$\text{molar mass} = \text{empirical formula molar mass} \times n$$

For a particular compound, the value of n in both cases is the same. Therefore, we can find n by calculating the ratio of the molar mass to the empirical formula molar mass.

$$n = \frac{\text{molar mass}}{\text{empirical formula molar mass}}$$

For fructose, the empirical formula molar mass is:

empirical formula molar mass

$$= 12.01 \text{ g/mol} + 2(1.01 \text{ g/mol}) + 16.00 \text{ g/mol} = 30.03 \text{ g/mol}$$

Therefore, n is:

$$n = \frac{180.2 \text{ g/mol}}{30.03 \text{ g/mol}} = 6$$

We can then use this value of n to find the molecular formula.

$$\text{molecular formula} = (CH_2O) \times 6 = C_6H_{12}O_6$$

Example 4.16 Calculating a Molecular Formula from an Empirical Formula and Molar Mass

Butanedione—a main component responsible for the smell and taste of butter and cheese—contains the elements carbon, hydrogen, and oxygen. The empirical formula of butanedione is C_2H_3O, and its molar mass is 86.09 g/mol. Find its molecular formula.

SORT You are given the empirical formula and molar mass of butanedione and asked to find the molecular formula.

GIVEN: empirical formula = C_2H_3O
molar mass = 86.09 g/mol

FIND: molecular formula

STRATEGIZE A molecular formula is always a whole-number multiple of the empirical formula. Divide the molar mass by the empirical formula mass to determine the whole number.

molecular formula = empirical formula × n

$$n = \frac{\text{molar mass}}{\text{empirical formula molar mass}}$$

SOLVE Calculate the empirical formula mass.

Divide the molar mass by the empirical formula mass to find n. Multiply the empirical formula by n to obtain the molecular formula.

$$\text{empirical formula molar mass}$$
$$= 2(12.01\ \text{g/mol}) + 3(1.008\ \text{g/mol}) + 16.00\ \text{g/mol} = 43.04\ \text{g/mol}$$
$$n = \frac{\text{molar mass}}{\text{empirical formula mass}} = \frac{86.09\ \text{g/mol}}{43.04\ \text{g/mol}} = 2$$
$$\text{molecular formula} = C_2H_3O \times 2 = C_4H_6O_2$$

CHECK Check the answer by calculating the molar mass of the formula as follows:

$$4(12.01\ \text{g/mol}) + 6(1.008\ \text{g/mol}) + 2(16.00\ \text{g/mol}) = 86.09\ \text{g/mol}$$

The calculated molar mass is in agreement with the given molar mass.

FOR PRACTICE 4.16 A compound has the empirical formula CH and a molar mass of 78.11 g/mol. What is its molecular formula?

FOR MORE PRACTICE 4.16

A compound with the percent composition shown here has a molar mass of 60.10 g/mol. Determine its molecular formula.

C, 39.97%
H, 13.41 %
N, 46.62 %

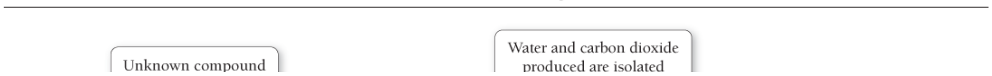
Combustion Analysis

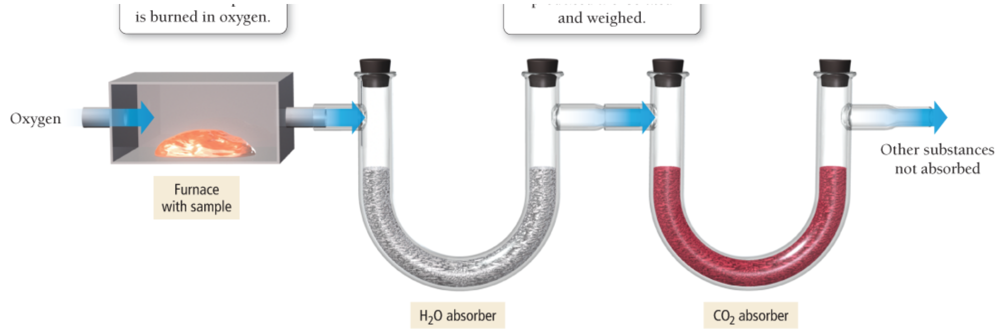
In the previous section, we discussed how to determine the empirical formula of a compound from the relative masses of its constituent elements. Another common (and related) way to obtain empirical formulas for unknown compounds, especially those containing carbon and hydrogen, is **combustion analysis**. In combustion analysis, the unknown compound undergoes combustion (or burning) in the presence of pure oxygen, as shown in Figure 4.11. When the sample is burned, all of the carbon in the sample is converted to CO_2, and all of the hydrogen is converted to H_2O. The CO_2 and H_2O are then weighed. With these masses, we can use the numerical relationships between moles inherent in the formulas for CO_2 and H_2O (1 mol CO_2: 1 mol C and 1 mol H_2O: 2 mol H) to determine the amounts of C and H in the original sample. We can determine the amounts of any other elemental constituents, such as O, Cl, or N, by subtracting the original mass of the sample from the sum of the masses of C and H. Examples 4.17 and 4.18 demonstrate how to perform these calculations for a sample containing only C and H and for a sample containing C, H, and O.

Figure 4.11 Combustion Analysis Apparatus

The sample to be analyzed is placed in a furnace and burned in oxygen. The water and carbon dioxide produced are absorbed into separate containers and weighed.

Combustion Analysis





Combustion is a type of *chemical reaction*. We discuss chemical reactions and their representation in Chapter 7.

Example 4.17 Obtaining an Empirical Formula from Combustion Analysis

PROCEDURE FOR Obtaining an Empirical Formula from Combustion Analysis

Upon combustion, a compound containing only carbon and hydrogen produces 1.83 g CO_2 and 0.901 g H_2O. Determine the empirical formula of the compound.

1. Write down as *given* the masses of each combustion product and the mass of the sample (if given).

GIVEN: 1.83 g CO_2, 0.901 g H_2O

FIND: empirical formula

2. Convert the masses of CO_2 and H_2O from Step 1 to moles by using the appropriate molar mass for each compound as a conversion factor.

$$1.83\text{ g }CO_2 \times \frac{1\text{ mol }CO_2}{44.01\text{ g }CO_2} = 0.0416\text{ mol }CO_2$$

$$0.901\text{ g }H_2O \times \frac{1\text{ mol }H_2O}{18.02\text{ g }H_2O} = 0.0500\text{ mol }H_2O$$

3. Convert the moles of CO_2 and moles of H_2O from Step 2 to moles of C and moles of H using the conversion factors inherent in the chemical formulas of CO_2 and H_2O.

$$0.0416\text{ mol }CO_2 \times \frac{1\text{ mol C}}{1\text{ mol }CO_2} = 0.0416\text{ mol C}$$

$$0.0500\text{ mol }H_2O \times \frac{2\text{ mol H}}{1\text{ mol }H_2O} = 0.100\text{ mol H}$$

4. If the compound contains an element other than C and H, find the mass of the other element by subtracting the sum of the masses of C and H (obtained in Step 3) from the mass of the sample. Finally, convert the mass of the other element to moles.

The sample contains no elements other than C and H, so proceed to next step.

5. Write down a pseudoformula for the compound using the number of moles of each element (from Steps 3 and 4) as subscripts.

$C_{0.0416}H_{0.100}$

6. Divide all the subscripts in the formula by the smallest subscript. (Round all subscripts that are within 0.1 of a whole number.)

$C_{\frac{0.0416}{0.0416}}H_{\frac{0.100}{0.0416}} \rightarrow C_1H_{2.4}$

7. If the subscripts are not whole numbers, multiply all the subscripts by a small whole number to determine whole-number subscripts.

$C_1H_{2.4} \times 5 \rightarrow C_5H_{12}$ The correct empirical formula is C_5H_{12}.

The subscripts are whole numbers; no additional multiplication is needed. The correct empirical formula is $C_{10}H_{12}O$.

FOR PRACTICE 4.17

Upon combustion, a compound containing only carbon and hydrogen produces 1.60 g CO_2 and 0.819 g H_2O. Find the empirical formula of the compound.

Example 4.18 Obtaining an Empirical Formula from Combustion Analysis

PROCEDURE FOR Obtaining an Empirical Formula from Combustion Analysis

Upon combustion, a 0.8233-g sample of a compound containing only carbon, hydrogen, and oxygen produces 2.445 g CO_2 and 0.6003 g H_2O. Determine the empirical formula of the compound.

1. Write down as *given* the masses of each combustion product and the mass of the sample (if given).

GIVEN: 0.8233-g sample, 2.445 g CO_2, 0.6003 g H_2O

FIND: empirical formula

2. Convert the masses of CO_2 and H_2O from Step 1 to moles by using the appropriate molar mass for each compound as a conversion factor.

$$2.445 \text{ g } CO_2 \times \frac{1 \text{ mol } CO_2}{44.01 \text{ g } CO_2} = 0.05556 \text{ mol } CO_2$$

$$0.6003 \text{ g } H_2O \times \frac{1 \text{ mol } H_2O}{18.02 \text{ g } H_2O} = 0.03331 \text{ mol } H_2O$$

3. Convert the moles of CO_2 and moles of H_2O from Step 2 to moles of C and moles of H using the conversion factors inherent in the chemical formulas of CO_2 and H_2O.

$$0.05556 \text{ mol } CO_2 \times \frac{1 \text{ mol C}}{1 \text{ mol } CO_2} = 0.05556 \text{ mol C}$$

$$0.03331 \text{ mol } H_2O \times \frac{2 \text{ mol H}}{1 \text{ mol } H_2O} = 0.06662 \text{ mol H}$$

4. If the compound contains an element other than C and H, find the mass of the other element by subtracting the sum of the masses of C and H (obtained in Step 3) from the mass of the sample. Finally, convert the mass of the other element to moles.

$$\begin{aligned}
\text{mass C} &= 0.05556 \text{ mol C} \times \frac{12.01 \text{ g C}}{\text{mol C}} \\
&= 0.6673 \text{ g C} \\
\text{mass H} &= 0.06662 \text{ mol H} \times \frac{1.008 \text{ g H}}{\text{mol H}} \\
&= 0.06715 \text{ g H} \\
\text{mass O} &= 0.8233 \text{ g} \\
&- (0.6673 \text{ g} + 0.06715 \text{ g}) \\
&= 0.0889 \text{ g} \\
\text{mol O} &= 0.0889 \text{ gO} \times \frac{\text{mol O}}{16.00 \text{ g O}} \\
&= 0.00556 \text{ mol O}
\end{aligned}$$

5. Write down a pseudoformula for the compound using the number of moles of each element (from Steps 3 and 4) as subscripts.

$C_{0.05556}H_{0.06662}O_{0.00556}$

6. Divide all the subscripts in the formula by the smallest subscript. (Round all subscripts that are within 0.1 of a whole number.)

$C_{\frac{0.05556}{0.00556}}H_{\frac{0.06662}{0.00556}}O_{\frac{0.00556}{0.00556}} \rightarrow C_{10}H_{12}O_{1}$

7. If the subscripts are not whole numbers, multiply all the subscripts by a small whole number to determine whole-number subscripts.

The correct empirical formula is N_2O_5.

FOR PRACTICE 4.18

Upon combustion, a 0.8009-g sample of a compound containing only carbon, hydrogen, and oxygen produces 1.6004 g CO_2 and 0.6551 g H_2O. Find the empirical formula of the compound.

Interactive Worked Example 4.18 **Determining an Empirical Formula from Combustion Analysis**