

5.9: Determining a Chemical Formula from Experimental Data

In the previous section, we discussed the relationship between the bulk mass of a substance and the number of atoms or molecules it contains (moles). Given the chemical formula of the substance, we were able to determine the amount of the substance (moles) from its mass, and vice versa. But what if the chemical formula of a substance is unknown? In this section, we will explore how to apply these very same principles in order to derive the chemical formulas of unknown substances from experimental mass measurements.

Derivation of Molecular Formulas

Recall that empirical formulas are symbols representing the *relative* numbers of a compound's elements. Determining the *absolute* numbers of atoms that compose a single molecule of a covalent compound requires knowledge of both its empirical formula and its molecular mass or molar mass. These quantities may be determined experimentally by various measurement techniques. Molecular mass, for example, is often derived from the mass spectrum of the compound (see discussion of this technique in the previous chapter on atoms and molecules). Molar mass can be measured by a number of experimental methods, many of which will be introduced in later chapters of this text.

Molecular formulas are derived by comparing the compound's molecular or molar mass to its empirical formula mass. As the name suggests, an empirical formula mass is the sum of the average atomic masses of all the atoms represented in an empirical formula. If we know the molecular (or molar) mass of the substance, we can divide this by the empirical formula mass in order to identify the number of empirical formula units per molecule, which we designate as n :

$$\frac{\text{molecular or molar mass} \left(\text{amu or } \frac{\text{g}}{\text{mol}} \right)}{\text{empirical formula mass} \left(\text{amu or } \frac{\text{g}}{\text{mol}} \right)} = n \text{ formula units/molecule} \quad (5.9.1)$$

The molecular formula is then obtained by multiplying each subscript in the empirical formula by n , as shown by the generic empirical formula A_xB_y :

$$(A_xB_y)_n = A_{nx}B_{ny} \quad (5.9.2)$$

For example, consider a covalent compound whose empirical formula is determined to be CH_2O . The empirical formula mass for this compound is approximately 30 amu (the sum of 12 amu for one C atom, 2 amu for two H atoms, and 16 amu for one O atom). If the compound's molecular mass is determined to be 180 amu, this indicates that molecules of this compound contain six times the number of atoms represented in the empirical formula:

$$\frac{180 \text{ amu/molecule}}{30 \frac{\text{amu}}{\text{formula unit}}} = 6 \text{ formula units/molecule} \quad (5.9.3)$$

Molecules of this compound are then represented by molecular formulas whose subscripts are six times greater than those in the empirical formula:



Note that this same approach may be used when the molar mass (g/mol) instead of the molecular mass (amu) is used. In this case, we are merely considering one mole of empirical formula units and molecules, as opposed to single units and molecules.

Determination of the Molecular Formula for Nicotine

Nicotine, an alkaloid in the nightshade family of plants that is mainly responsible for the addictive nature of cigarettes, contains 74.02% C, 8.710% H, and 17.27% N. If 40.57 g of nicotine contains 0.2500 mol nicotine, what is the molecular formula?

Solution

Determining the molecular formula from the provided data will require comparison of the compound's empirical formula mass to its molar mass. As the first step, use the percent composition to derive the compound's empirical formula. Assuming a convenient, a 100-g sample of nicotine yields the following molar amounts of its elements:

$$(74.02 \text{ g C}) \left(\frac{1 \text{ mol C}}{12.01 \text{ g C}} \right) = 6.163 \text{ mol C} \quad (5.9.5)$$

$$(8.710 \text{ g H}) \left(\frac{1 \text{ mol H}}{1.01 \text{ g H}} \right) = 8.624 \text{ mol H} \quad (5.9.6)$$

$$(17.27 \text{ g N}) \left(\frac{1 \text{ mol N}}{14.01 \text{ g N}} \right) = 1.233 \text{ mol N} \quad (5.9.7)$$

Next, we calculate the molar ratios of these elements.

The C-to-N and H-to-N molar ratios are adequately close to whole numbers, and so the empirical formula is $\text{C}_5\text{H}_7\text{N}$. The empirical formula mass for this compound is therefore 81.13 amu/formula unit, or 81.13 g/mol formula unit.

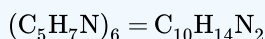
We calculate the molar mass for nicotine from the given mass and molar amount of compound:

$$\frac{40.57 \text{ g nicotine}}{0.2500 \text{ mol nicotine}} = \frac{162.3 \text{ g}}{\text{mol}}$$

Comparing the molar mass and empirical formula mass indicates that each nicotine molecule contains two formula units:

$$\frac{162.3 \text{ g/mol}}{81.13 \frac{\text{g}}{\text{formula unit}}} = 2 \text{ formula units/molecule}$$

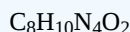
Thus, we can derive the molecular formula for nicotine from the empirical formula by multiplying each subscript by two:



Exercise 5.9.5

What is the molecular formula of a compound with a percent composition of 49.47% C, 5.201% H, 28.84% N, and 16.48% O, and a molecular mass of 194.2 amu?

Answer



Summary

The chemical identity of a substance is defined by the types and relative numbers of atoms composing its fundamental entities (molecules in the case of covalent compounds, ions in the case of ionic compounds). A compound's percent composition provides the mass percentage of each element in the compound, and it is often experimentally determined and used to derive the compound's empirical formula. The empirical formula mass of a covalent compound may be compared to the compound's molecular or molar mass to derive a molecular formula.

Combustion Analysis

When a compound containing carbon and hydrogen is subject to combustion with oxygen in a special combustion apparatus all the carbon is converted to CO_2 and the hydrogen to H_2O (Figure 5.9.2). The amount of carbon produced can be determined by measuring the amount of CO_2 produced. This is trapped by the sodium hydroxide, and thus we can monitor the mass of CO_2 produced by determining the increase in mass of the CO_2 trap. Likewise, we can determine the amount of H produced by the amount of H_2O trapped by the magnesium perchlorate.

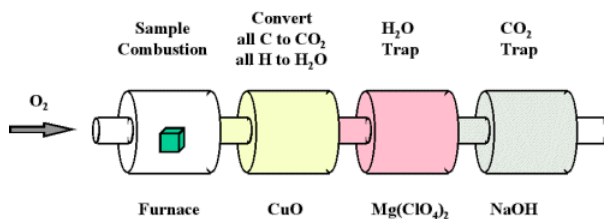


Figure 5.9.2: Combustion analysis apparatus

One of the most common ways to determine the elemental composition of an unknown hydrocarbon is an analytical procedure called combustion analysis. A small, carefully weighed sample of an unknown compound that may contain carbon, hydrogen, nitrogen, and/or sulfur is burned in an oxygen atmosphere. Other elements, such as metals, can be determined by other methods. and the quantities of the resulting gaseous products (CO_2 , H_2O , N_2 , and SO_2 , respectively) are determined by one of several possible methods. One procedure used in combustion analysis is outlined schematically in Figure 5.9.3 and a typical combustion analysis is illustrated in Examples 5.9.3 and 5.9.4.

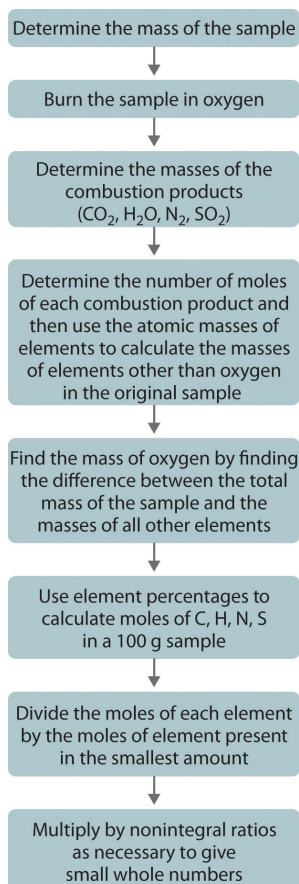


Figure 5.9.3: Steps for Obtaining an Empirical Formula from Combustion Analysis

Example 5.9.3: Combustion of Isopropyl Alcohol

What is the empirical formula for isopropyl alcohol (which contains only C, H and O) if the combustion of a 0.255 grams isopropyl alcohol sample produces 0.561 grams of CO_2 and 0.306 grams of H_2O ?

Solution

From this information quantitate the amount of C and H in the sample.

$$(0.561 \text{ g } \cancel{\text{CO}_2}) \left(\frac{1 \text{ mol } \text{CO}_2}{44.0 \text{ g } \cancel{\text{CO}_2}} \right) = 0.0128 \text{ mol } \text{CO}_2 \quad (5.9.8)$$

Since one mole of CO_2 is made up of one mole of C and two moles of O, if we have 0.0128 moles of CO_2 in our sample, then we know we have 0.0128 moles of C in the sample. How many grams of C is this?

$$(0.0128 \text{ mol } \cancel{\text{C}}) \left(\frac{12.011 \text{ g } \text{C}}{1 \text{ mol } \cancel{\text{C}}} \right) = 0.154 \text{ g } \text{C} \quad (5.9.9)$$

How about the hydrogen?

$$(0.306 \text{ g } \cancel{H_2O}) \left(\frac{1 \text{ mol } H_2O}{18.0 \text{ g } \cancel{H_2O}} \right) = 0.017 \text{ mol } H_2O \quad (5.9.10)$$

Since one mole of H_2O is made up of one mole of oxygen and **two** moles of hydrogen, if we have 0.017 moles of H_2O , then we have $2 \times (0.017) = 0.034$ moles of hydrogen. Since hydrogen is about 1 gram/mole, we must have **0.034 grams of hydrogen** in our original sample.

When we add our carbon and hydrogen together we get:

$$0.154 \text{ grams (C)} + 0.034 \text{ grams (H)} = \mathbf{0.188 \text{ grams}}$$

But we know we combusted 0.255 grams of isopropyl alcohol. The 'missing' mass must be from the oxygen atoms in the isopropyl alcohol:

$$0.255 \text{ grams} - 0.188 \text{ grams} = 0.067 \text{ grams oxygen}$$

This much oxygen is how many moles?

$$(0.067 \text{ g } \cancel{O}) \left(\frac{1 \text{ mol } O}{15.994 \text{ g } \cancel{O}} \right) = 0.0042 \text{ mol } O \quad (5.9.11)$$

Overall therefore, we have:

- 0.0128 moles Carbon
- 0.0340 moles Hydrogen
- 0.0042 moles Oxygen

Divide by the smallest molar amount to normalize:

- C = 3.05 atoms
- H = 8.1 atoms
- O = 1 atom

Within experimental error, the most likely empirical formula for propanol would be C_3H_8O

Example 5.9.4: Combustion of Naphthalene

Naphthalene, the active ingredient in one variety of mothballs, is an organic compound that contains carbon and hydrogen only. Complete combustion of a 20.10 mg sample of naphthalene in oxygen yielded 69.00 mg of CO_2 and 11.30 mg of H_2O . Determine the empirical formula of naphthalene.

Given: mass of sample and mass of combustion products

Asked for: empirical formula

Strategy:

- Use the masses and molar masses of the combustion products, CO_2 and H_2O , to calculate the masses of carbon and hydrogen present in the original sample of naphthalene.
- Use those masses and the molar masses of the elements to calculate the empirical formula of naphthalene.

Solution:

A Upon combustion, 1 mol of CO_2 is produced for each mole of carbon atoms in the original sample. Similarly, 1 mol of H_2O is produced for every 2 mol of hydrogen atoms present in the sample. The masses of carbon and hydrogen in the original sample can be calculated from these ratios, the masses of CO_2 and H_2O , and their molar masses. Because the units of molar mass are grams per mole, we must first convert the masses from milligrams to grams:

$$\text{mass of C} = 69.00 \text{ mg } CO_2 \times \frac{1 \text{ g}}{1000 \text{ mg}} \times \frac{1 \text{ mol } CO_2}{44.010 \text{ g } CO_2} \times \frac{1 \text{ mol C}}{1 \text{ mol } CO_2} \times \frac{12.011 \text{ g}}{1 \text{ mol C}} \quad (5.9.12)$$

$$= 1.883 \times 10^{-2} \text{ g C} \quad (5.9.13)$$

$$\begin{aligned} \text{mass of } H &= 11.30 \text{ mg } H_2O \times \frac{1 \text{ g}}{1000 \text{ mg}} \times \frac{1 \text{ mol } H_2O}{18.015 \text{ g } H_2O} \times \frac{2 \text{ mol } H}{1 \text{ mol } H_2O} \times \frac{1.0079 \text{ g}}{1 \text{ mol } H} \\ &= 1.264 \times 10^{-3} \text{ g } H \end{aligned} \quad \begin{aligned} (5.9.14) \\ (5.9.15) \end{aligned}$$

B To obtain the relative numbers of atoms of both elements present, we need to calculate the number of moles of each and divide by the number of moles of the element present in the smallest amount:

$$\text{moles } C = 1.883 \times 10^{-2} \text{ g } C \times \frac{1 \text{ mol } C}{12.011 \text{ g } C} = 1.568 \times 10^{-3} \text{ mol } C \quad (5.9.16)$$

$$\text{moles } H = 1.264 \times 10^{-3} \text{ g } H \times \frac{1 \text{ mol } H}{1.0079 \text{ g } H} = 1.254 \times 10^{-3} \text{ mol } H \quad (5.9.17)$$

Dividing each number by the number of moles of the element present in the smaller amount gives

$$H : \frac{1.254 \times 10^{-3}}{1.254 \times 10^{-3}} = 1.000 \quad C : \frac{1.568 \times 10^{-3}}{1.254 \times 10^{-3}} = 1.250 \quad (5.9.18)$$

Thus naphthalene contains a 1.25:1 ratio of moles of carbon to moles of hydrogen: $C_{1.25}H_{1.0}$. Because the ratios of the elements in the empirical formula must be expressed as small whole numbers, multiply both subscripts by 4, which gives C_5H_4 as the empirical formula of naphthalene. In fact, the molecular formula of naphthalene is $C_{10}H_8$, which is consistent with our results.

Exercise 5.9.4

- Xylene, an organic compound that is a major component of many gasoline blends, contains carbon and hydrogen only. Complete combustion of a 17.12 mg sample of xylene in oxygen yielded 56.77 mg of CO_2 and 14.53 mg of H_2O . Determine the empirical formula of xylene.
- The empirical formula of benzene is CH (its molecular formula is C_6H_6). If 10.00 mg of benzene is subjected to combustion analysis, what mass of CO_2 and H_2O will be produced?

Answer a

The empirical formula is C_4H_5 . (The molecular formula of xylene is actually C_8H_{10} .)

Answer b

33.81 mg of CO_2 ; 6.92 mg of H_2O

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