Chem 170

Stoichiometric Calculations

Module Three

Characterizing Compounds Using Mass Percents and Empirical Formulas

Introduction to Module Three

Have you ever been to a lawn and garden store and seen bags of fertilizer labeled with numbers such as “5-10-5”? These numbers identify the percentages, by weight, of three essential nutrients: 5% nitrogen as N, 10% phosphorous as P_2O_5, and 5% potassium as K_2O. A “5-10-5” fertilizer, therefore, contains

$$\frac{5 \text{ g N}}{100 \text{ g fertilizer}} \qquad \frac{10 \text{ g } P_2O_5}{100 \text{ g fertilizer}} \qquad \frac{5 \text{ g } K_2O}{100 \text{ g fertilizer}}$$

These percentages, which are also known as mass percents, are a convenient way to indicate the composition of a fertilizer mixture, and to compare brands of fertilizer.

Mass percents are also a useful way to characterize compounds. Every molecule of ascorbic acid (vitamin C), for example, is 40.92% carbon, by mass. If we synthesize a batch of ascorbic acid and find, upon analysis, that it is 41.35% carbon by mass, then we know it isn’t completely pure. In this module you will learn how to find the mass percent of an element or other species in a compound. More important, you will learn how experimentally determined mass percents can be used to determine a compound’s empirical formula.

Objectives for Module Three

In completing this module you will master the following objectives:

- to calculate the mass percent of each element in a compound
- to calculate the mass percent of any structural unit in a compound
- to use mass percent information to calculate the amount of an element or structural unit in a given amount of compound
- to determine a compound’s empirical formula using information about the mass percent of each element in the compound
- to determine a compound’s empirical formula using chemical reactivity and the conservation of mass
- to determine a compound’s molecular formula from its empirical formula and molar mass

Determining a Compound's Percent Composition

Earlier we claimed that ascorbic acid is 40.92% carbon, by mass. How can we verify that this is true? The skills you learned in Module 2 can be put to use here. If we assume that we have exactly 1 g of ascorbic acid, then

$$1 \text{ g } C_6H_8O_6 \times \frac{1 \text{ mole } C_6H_8O_6}{176.12 \text{ g } C_6H_8O_6} \times \frac{6 \text{ mol C}}{\text{mol } C_6H_8O_6} \times \frac{12.01 \text{ g C}}{\text{mol C}} \times 100 = 40.92\% \text{ C}$$

Look carefully at this equation and note that we can generalize and simplify it to

$$\text{mass \% of element} = \frac{n \times \text{molar mass of element}}{\text{molar mass of compound}} \times 100$$

where n is the moles of element per mole of compound. For ascorbic acid we have

$$\text{mass \% C} = \frac{6 \times 12.01 \text{ g/mol}}{176.12 \text{ g/mol}} \times 100 = 40.92\% \text{ C}$$

Example 1. Cinnamic alcohol is a fragrant compound used in soaps. Its molecular formula is $C_9H_{10}O$. Calculate the mass percent for each element in cinnamic alcohol.

Solution. Cinnamic alcohol's molar mass is 134.17 g/mol. The mass percent for each element is

$$\text{mass \% C} = \frac{9 \times 12.01 \text{ g/mol}}{134.17 \text{ g/mol}} \times 100 = 80.56\% \text{ C}$$

$$\text{mass \% H} = \frac{10 \times 1.008 \text{ g/mol}}{134.17 \text{ g/mol}} \times 100 = 7.513\% \text{ H}$$

$$\text{mass \% C} = \frac{1 \times 16.00 \text{ g/mol}}{134.17 \text{ g/mol}} \times 100 = 11.93\% \text{ O}$$

Adding together the mass percents gives a total of 100.00%.

The calculation of mass percent is not restricted to a single element, but can be extended to a larger "piece" or structural unit of a compound. For instance, many compounds exist as hydrates, meaning that they incorporate water molecules into their structure. One example is barium hydroxide, $Ba(OH)_2$, which incorporates eight moles of water into each mole of the compound. We show this in the compound's formula by writing it as $Ba(OH)_2{\bullet}8H_2O$ where the "•" indicates that the water is present as a hydrate.[†]

Example 2. Find the mass percent for H_2O in $Ba(OH)_2{\bullet}8H_2O$.

Solution. The molar mass for $Ba(OH)_2{\bullet}8H_2O$, including the molar mass for the eight water molecules, is 315.5 g/mol. We also need the molar mass of H_2O, which is 18.02 g/mol. Proceeding as in Example 1, we obtain

$$\text{mass \% } H_2O = \frac{8 \times 18.02 \text{ g/mol}}{315.5 \text{ g/mol}} \times 100 = 45.69\% \; H_2O$$

One advantage of using mass percents is that they allow for a quick comparison between compounds (remember the "5-10-5" fertilizer?). Example 3 shows how calculating mass percent aids in selecting a source of nitrogen to use as a fertilizer.

Example 3. Several fertilizers are available for adding nitrogen to soil, including: urea, $(NH_2)_2CO$; ammonium nitrate, NH_4NO_3; guanidine, $HNC(NH_2)_2$; and ammonia, NH_3. Which is the best source of nitrogen if we wish to use the smallest amount of compound?

Solution. To solve we need to find the mass percent of nitrogen in each compound, as shown here

$$\text{Urea:} \text{mass \% N} = \frac{2 \times 14.01 \text{ g/mol}}{60.06 \text{ g/mol}} \times 100 = 46.65\% \text{ N}$$
$$\text{Ammonium Nitrate:} \text{mass \% N} = \frac{2 \times 14.01 \text{ g/mol}}{80.05 \text{ g/mol}} \times 100 = 35.00\% \text{ N}$$
$$\text{Guanidine:} \text{mass \% N} = \frac{3 \times 14.01 \text{ g/mol}}{59.08 \text{ g/mol}} \times 100 = 71.14\% \text{ N}$$
$$\text{Ammonia} \text{mass \% N} = \frac{1 \times 14.01 \text{ g/mol}}{17.03 \text{ g/mol}} \times 100 = 82.27\% \text{ N}$$

Ammonia is the best choice because it provides more nitrogen per gram of compound; thus, we need less mass of ammonia to achieve a obtain a desired amount of nitrogen.

[†] Unlike the other stoichiometric coefficients in a compound, which are always listed as whole numbers (see Module 2), the stoichiometric coefficient for a hydrate may be a fraction. For example, copper sulfate is often found as $CuSO_4{\bullet}1/2H_2O$. The reason for writing it this way, instead of $Cu_2(SO_4)_2{\bullet}H_2O$, is to emphasize that the compound consists of both copper sulfate and water. Indeed, the water can be removed with heat, leaving anhydrous copper sulfate, or $CuSO_4$.

In Module 2, you learned to convert the mass of a compound into the mass of a particular element in that compound. For example, we used the following calculation to show that there are 3.92×10^3 g of N in 16.8 kg of urea, $(NH_2)_2CO$

$$16.8 \text{ kg urea} \times \frac{1000 \text{ g urea}}{\text{kg urea}} \times \frac{1 \text{ mol urea}}{60.06 \text{ g urea}} \times \frac{2 \text{ mol N}}{\text{mol urea}} \times \frac{14.01 \text{ g N}}{\text{mol}} = 7.84 \times 10^3 \text{ g N}$$

If you look closely, you will see that part of this calculation

$$\frac{1 \text{ mol urea}}{60.06 \text{ g urea}} \times \frac{2 \text{ mol N}}{\text{mol urea}} \times \frac{14.01 \text{ g N}}{\text{mol}}$$

is equivalent to the mass percent of nitrogen in urea. Knowing that urea is 46.65% N by mass makes the calculation somewhat easier and more direct.

$$16.8 \text{ kg urea} \times \frac{1000 \text{ g urea}}{\text{kg urea}} \times \frac{46.65 \text{ g N}}{100 \text{ g urea}} = 7.84 \times 10^3 \text{ g N}$$

Example 4. Mining engineers know that the mineral cryolite is 12.85% aluminum, by mass. How many grams of aluminum can be obtained from 12.8 tons of cryolite?

Solution. Beginning with the tons of cryolite we find that there are

$$12.8 \text{ tons cryolite} \times \frac{2000 \text{ lb cryolite}}{\text{ton cryolite}} \times \frac{453.6 \text{ g cryolite}}{\text{lb cryolite}} \times \frac{12.85 \text{ g Al}}{100 \text{ g cryolite}} = 1.49 \times 10^6 \text{ g Al}$$

Empirical Formulas from Mass Percent Data

Suppose that you've synthesized a new compound. Because you're not certain of its identity, you decide to analyze the compound for its percent composition, determining that it is 40.92% C, 4.58% H, and 54.50% O. If it is possible to determine a compound's percent composition from its molecular formula (which we've just done in the preceding section), then you might reasonably expect that the process could be reversed – that is, to find the compound's molecular formula given information about its percent composition. Unfortunately, comparing two mass percents only provides information about the relative amounts of the two elements. Using our example, we can say only that any sample of the compound contains 40.92 g of carbon for every 4.58 g of hydrogen, or 3.407 moles of C for every 4.544 moles of H. Although we can't determine how many carbon atoms are in a single molecule of the compound, we can determine its empirical formula.

Example 5. A newly synthesized compound has a percent composition of 40.92% carbon, 4.58% hydrogen, and 54.50% oxygen. What is the compound's empirical formula?

Solution. The mass percents for carbon, hydrogen, and oxygen add together to give 100%; thus, we know that the compound contains only these elements. If we assume a 100-gram sample, then we have 40.92 g of C, 4.58 g of H, and 54.50 g of O. Using each element's molar mass, we calculate the moles of carbon, n_C, hydrogen, n_H, and oxygen, n_O, in the sample.

$$n_C = 40.92 \text{ g C} \times \frac{1 \text{ mol C}}{12.01 \text{ g C}} = 3.407 \text{ mol C}$$

$$n_H = 4.58 \text{ g H} \times \frac{1 \text{ mol H}}{1.008 \text{ g H}} = 4.544 \text{ mol H}$$

$$n_O = 54.50 \text{ g O} \times \frac{1 \text{ mol O}}{16.00 \text{ g O}} = 3.406 \text{ mol O}$$

Dividing the moles of each element by the smallest number of moles, which in this case is 3.406 mol of O, gives the relative number of moles for each element; thus

$$\frac{n_C}{n_O} = \frac{3.407 \text{ mol C}}{3.406 \text{ mol O}} = \frac{1.00 \text{ mol C}}{1.00 \text{ mol O}}$$

$$\frac{n_H}{n_O} = \frac{4.544 \text{ mol H}}{3.406 \text{ mol O}} = \frac{1.33 \text{ mol H}}{1.00 \text{ mol O}}$$

$$\frac{n_O}{n_O} = \frac{3.406 \text{ mol O}}{3.406 \text{ mol O}} = \frac{1.00 \text{ mol O}}{1.00 \text{ mol O}}$$

Based on these mole ratios, the empirical formula is $C_1H_{1.33}O_1$. Because an empirical formula must have integer subscripts (see module 2), we multiply the subscripts by 3, giving an empirical formula of $C_3H_4O_3$.

Empirical Formulas Using the Conservation of Mass

One of Dalton's hypotheses about atoms is that matter is conserved in a chemical reaction. Because of the conservation of mass, we also can determine a compound's empirical formula if we know the mass of each element used to synthesize the compound. If we know, for example, that 40.92 g of C will react completely with 4.58 g of H and 54.50 g of O, then we can find the empirical formula of the product using the same calculation shown in Example 5. Of course, we must assume that all the carbon, hydrogen, and oxygen end up in a single product, and that none ends up in some other product of the reaction.

Example 6. In synthesizing a compound containing only sulfur and fluorine, a chemist reacts 4.69 g of S with an excess of fluorine, obtaining 15.81 g of product. Assuming that all the sulfur ends up in the product, determine the product's empirical formula.

Solution. Because the mass of sulfur is conserved, we can determine the mass of fluorine in the product by difference

$$\text{mass fluorine} = 15.81 \text{ g product} - 4.69 \text{ g sulfur} = 11.12 \text{ g F}$$

Proceeding as in Example 5, we first find the moles of sulfur and fluorine in the product.

$$n_\mathrm{S} = 4.69 \text{ g S} \times \frac{1 \text{ mol S}}{32.06 \text{ g S}} = 0.1463 \text{ mol S}$$

$$n_\mathrm{F} = 11.12 \text{ g F} \times \frac{1 \text{ mol F}}{19.00 \text{ g F}} = 0.5853 \text{ mol F}$$

This gives a mole ratio of

$$\frac{n_\mathrm{F}}{n_\mathrm{S}} = \frac{0.5853 \text{ mol F}}{0.1463 \text{ mol S}} = \frac{4.00 \text{ mol F}}{1.00 \text{ mol S}}$$

and an empirical formula of SF_4.

Another approach to determining a compound's empirical formula is to destroy the compound by a chemical reaction and collect and weigh the reaction's products. As long as all but one of the compound's elements is conserved in a single product, we can determine the compound's empirical formula. The mass of the remaining element is, of course, determined by difference.

The empirical formula of an organic compound containing C, H, and O is often determined by a combustion analysis. In this procedure, a portion of the compound is placed in a tube through which we pass a stream of O_2. Upon heating, the compound reacts with the O_2, forming CO_2 and H_2O as products. The CO_2 and H_2O are collected in traps and weighed. Because the stream of O_2 contains no hydrogen or carbon, all the carbon in CO_2 and all the hydrogen in H_2O comes from the compound. Although the mass of oxygen can't be found directly from the mass of CO_2 or mass of H_2O because some of the oxygen in these compounds comes from the O_2, it can be determined by a conservation of mass.

Example 7. A 0.255-g sample of an organic compound containing only carbon, hydrogen, and oxygen is analyzed by a combustion analysis, producing 0.561 g of CO_2 and 0.306 g of H_2O. What is the compound's empirical formula?

Solution. Because the mass of carbon and hydrogen are conserved, we can find the moles of each in the sample from the masses of CO_2 and H_2O.

$$0.561\text{ g CO}_2 \times \frac{1\text{ mol CO}_2}{44.01\text{ g CO}_2} \times \frac{1\text{ mol C}}{1\text{ mol CO}_2} = 0.01275\text{ mol C}$$

$$0.306\text{ g H}_2\text{O} \times \frac{1\text{ mol H}_2\text{O}}{18.02\text{ g H}_2\text{O}} \times \frac{2\text{ mol H}}{\text{mol H}_2\text{O}} = 0.03396\text{ mol H}$$

To find the moles of O we must first find the masses of C and H in the sample

$$0.01275\text{ mol C} \times \frac{12.01\text{ g C}}{\text{mol C}} = 0.1531\text{ g C} \qquad 0.03396\text{ mol H} \times \frac{1.008\text{ g H}}{\text{mol H}} = 0.0342\text{ g H}$$

and determine the mass of O by difference

$$0.255\text{ g sample} - (0.1531\text{ g C} + 0.0342\text{ g H}) = 0.0677\text{ g O}$$

The moles of O, therefore, are

$$0.0677\text{ g O} \times \frac{1\text{ mol O}}{16.00\text{ g O}} = 0.00423\text{ mol O}$$

The mole ratios of C-to-O and H-to-O are

$$\frac{n_\text{C}}{n_\text{O}} = \frac{0.01275\text{ mol C}}{0.00423\text{ mol O}} = \frac{3.01\text{ mol C}}{1.00\text{ mol O}} \qquad \frac{n_\text{H}}{n_\text{O}} = \frac{0.03396\text{ mol H}}{0.00423\text{ mol O}} = \frac{8.03\text{ mol H}}{1.00\text{ mol O}}$$

giving an empirical formula of C_3H_8O.

As shown in the next example, other forms of chemical reactivity can be used to determine a compound's empirical formula.

Example 8. An organic compound contains only carbon, hydrogen, and chlorine. Combustion of a 1.50-g sample produces 3.52 g of CO_2. In a separate reaction, a 1.00-g sample reacts with Ag^+, producing 1.27 g of AgCl. What is the compound's empirical formula?

Solution. Because the two reactions use different amounts of sample we cannot solve this problem in the same way we did in Example 7. Instead, we first find the mass percents of each element. From the masses of CO_2 and AgCl we can find the mass of C in the 1.50-g sample, and the mass of Cl in the 1.00-g sample.

$$3.52 \text{ g } CO_2 \times \frac{1 \text{ mol } CO_2}{44.01 \text{ g } CO_2} \times \frac{1 \text{ mol C}}{1 \text{ mol } CO_2} \times \frac{12.01 \text{ g C}}{\text{mol C}} = 0.9606 \text{ g C}$$

$$1.27 \text{ g AgCl} \times \frac{1 \text{ mol AgCl}}{143.32 \text{ g AgCl}} \times \frac{1 \text{ mol Cl}}{1 \text{ mol AgCl}} \times \frac{35.45 \text{ g Cl}}{\text{mol Cl}} = 0.3141 \text{ g Cl}$$

The mass percents of carbon and chlorine in the two samples are

$$\frac{0.9606 \text{ g C}}{1.50 \text{ g sample}} \times 100 = 64.04\% \text{ C} \qquad \frac{0.3141 \text{ g Cl}}{1.00 \text{ g sample}} \times 100 = 31.41\% \text{ Cl}$$

The mass percent of H is found by difference

$$100\% - (64.04\% \text{ C} + 31.41\% \text{ Cl}) = 4.55\% \text{ H}$$

Finally, proceeding as in Example 5, we calculate the moles of carbon, chlorine and hydrogen.

$$n_C = 64.04 \text{ g C} \times \frac{1 \text{ mol C}}{12.01 \text{ g C}} = 5.332 \text{ mol C}$$

$$n_{Cl} = 31.41 \text{ g Cl} \times \frac{1 \text{ mol Cl}}{35.45 \text{ g Cl}} = 0.886 \text{ mol Cl}$$

$$n_H = 4.55 \text{ g H} \times \frac{1 \text{ mol C}}{1.008 \text{ g H}} = 4.514 \text{ mol H}$$

$$\frac{n_C}{n_{Cl}} = \frac{5.332 \text{ mol C}}{0.886 \text{ mol Cl}} = \frac{6.01 \text{ mol C}}{1.00 \text{ mol Cl}} \qquad \frac{n_H}{n_{Cl}} = \frac{4.514 \text{ mol H}}{0.886 \text{ mol Cl}} = \frac{5.09 \text{ mol H}}{1.00 \text{ mol Cl}}$$

which gives an empirical formula of C_6H_5Cl.

Converting an Empirical Formula to a Molecular Formula

An empirical formula tells us only the relative amounts of each element in a compound. Finding that isopropanol has an empirical formula of C_3H_8O tells us that each molecule of isopropanol has 3 atoms of C for every atom of O. The molecular formula must, therefore, be C_3H_8O or some multiple thereof, such as $C_6H_{16}O_2$ or $C_{30}H_{80}O_{10}$. To find the molecular formula we need only one additional piece of information – the compound's molar mass. Knowing that the molar mass of isopropanol is 60.09 g/mol tells us that isopropanol's molecular formula is C_3H_8O.

Example 9. Fructose is a type of sugar found in fruits and honey. Analysis of a 2.00-g sample shows that it contains 0.80 g of C, 1.06 g of O, and 0.14 g of H. An independent analysis shows that fructose has a molar mass of 180 g/mol. What is the molecular formula for fructose?

Solution. Because the total mass for C, O, and H is the same as sample's mass, we know that fructose contains only these three elements. Converting the masses of C, O, and H to moles gives

$$n_{\text{C}} = 0.80 \text{ g C} \times \frac{1 \text{ mol C}}{12.01 \text{ g C}} = 0.0666 \text{ mol C}$$

$$n_{\text{O}} = 1.06 \text{ g O} \times \frac{1 \text{ mol O}}{16.00 \text{ g O}} = 0.0663 \text{ mol O}$$

$$n_{\text{H}} = 0.14 \text{ g H} \times \frac{1 \text{ mol H}}{1.008 \text{ g H}} = 0.139 \text{ mol H}$$

The empirical formula, therefore, is CH_2O. The apparent molar mass based on this empirical formula is 30 g/mol. Dividing the actual molar mass by the apparent molar mass

$$\frac{\text{Actual Molar Mass}}{\text{Apparent Molar Mass}} = \frac{180 \text{ g/mol}}{30 \text{ g/mol}} = 6$$

tells us that fructose contains 6 units of CH_2O. Multiplying the empirical formula's subscripts by 6, therefore, gives $C_6H_{12}O_6$ as fructose's molecular formula.

Practice Problems

The following problems provide practice in meeting this module's objectives. Answers are provided on the last page. Be sure to seek assistance if you experience difficulty with any of these problems. When you are ready, schedule an appointment for the module's exam.

1. Calculate the mass percent of each element in acetaminophen, which has a molecular formula of $C_8H_9O_2N$.

2. Calculate the mass percent of each element in $Ca_3(PO_4)_2$, a major component of bones.

3. Calculate the mass percent of Fe in each of the following iron ores: (a) Fe_2O_3, (b) FeO, and (c) Fe_3O_4.

4. Calculate the mass percent of H_2O in $CuSO_4{\bullet}5H_2O$.

5. Calculate the mass percent of phosphate ion, PO_4^{3-}, in $Ca_3(PO_4)_2$.

6. Brass is an alloy that is approximately 67% Cu and 33% Zn, by mass. How many grams of Cu and Zn are in a brass doorknocker weighing 2.2 pounds?

7. Ibuprofen, a pain relief medication, is 75.69% C, 8.80% H, and 15.51% O, by mass. What is the empirical formula for ibuprofen?

8. Epinephrine, also known as adrenaline, is 59.0% C, 7.1% H, 26.2% O, and 7.7% N, by mass. What is the empirical formula for epinephrine?

9. One of the principal ores of aluminum is 32.79% Na, 13.02% Al, and 54.19% F, by mass. What is this ore's empirical formula?

10. The active ingredient in photographic fixer solutions contains sodium, Na, sulfur, S, and oxygen, O. Analysis of a sample shows that it contains 0.979 g Na, 1.365 g S, and 1.021 g O. What is the empirical formula for this compound?

11. Menthol, which is present in mentholated cough drops, is an organic compound containing only C, H, and O. When a 0.2010-g sample is analyzed by combustion, 0.5658 g of CO_2 and 0.2318 g of H_2O are obtained. What is the empirical formula of menthol?

12. Eugenol is the compound responsible for the odor of cloves. Analysis of a 0.0188-g sample of eugenol by combustion gives 0.0506 g of CO_2 and 0.0124 g of H_2O. Given that eugenol is known to contain only carbon, hydrogen, and oxygen, what is its empirical formula?

13. Caffeine contains only C, H, N, and O. When a 0.376 g sample is analyzed by combustion, 0.682 g of CO_2, 0.174 g of H_2O, and 0.110 g of N_2 are obtained. What is the empirical formula for caffeine?

14. Lysine, which is an essential amino acid, contains only C, H, N, and O. In one experiment, the complete combustion of 2.175 g of lysine produces 3.93 g of CO_2 and 1.87 g of H_2O. In a separate experiment, 1.873 g of lysine produces 0.436 g of NH_3. What is the empirical formula of lysine?

15. A student synthesizes a compound of nickel known to have the general formula of

$$Ni_a(NH_3)_bCl_c \bullet dH_2O$$

Analysis of the compound shows that it is 29.14% NH_3, 30.33 % Cl, and 25.11% Ni; the remaining mass percent is water. What is the compound's empirical formula?

16. The molar masses for the compounds in problems 11-14 are:

menthol - 156 g/mol

eugenol - 164.2 g/mol

caffeine - 195 g/mol

lysine - 146 g/mol

What are the molecular formulas for these compounds?

Answers to Practice Problems

1. 63.56% C, 6.00% H, 21.17% O, 9.27% N
2. 38.76% Ca, 19.97% P, 41.27% O
3. 69.94% Fe, 77.73% Fe, 72.36% Fe
4. 36.08% H_2O
5. 61.24% PO_4^{3-}
6. 6.7×10^2 g Cu, 3.3×10^2 g Zn
7. $C_{13}H_{18}O_2$
8. $C_9H_{13}O_3N$
9. Na_3AlF_6
10. $Na_2S_2O_3$
11. $C_{10}H_{20}O$
12. C_5H_6O
13. $C_4H_5N_2O$
14. C_3H_7NO
15. $Ni(NH_3)_4Cl_2 \cdot 2H_2O$
16. menthol - $C_{10}H_{20}O$

    eugenol - $C_{10}H_{12}O_2$

    caffeine - $C_8H_{10}N_4O_2$

    lysine - $C_6H_{14}N_2O_2$