Chapter 3

Mass Relationships in Chemical Reactions
In this chapter, Chemical structure and formulas in studying the mass relationships of atoms and molecules.

To explain the composition of compounds and the ways in which composition changes.
The mass of an atom depends on the number of electrons, protons, and neutrons it contains. Knowledge of an atom’s mass is important in laboratory work.

Atomic mass (atomic weight) is the mass of an atom in atomic mass units (amu).

By definition:
1 atom $^{12}$C “weighs” 12 amu

On this scale
$^1$H = 1.008 amu
$^{16}$O = 16.00 amu
The *average atomic mass* is the weighted average of all of the naturally occurring isotopes of the element.

\[
\text{average atomic mass of natural carbon} = (0.9890)(12.00000 \text{ amu}) + (0.0110)(13.00335 \text{ amu})
\]

\[
= 12.01 \text{ amu}
\]
Atomic Mass: Average Atomic Mass

Naturally occurring lithium is:

7.42% $^6\text{Li}$ (6.015 amu)

92.58% $^7\text{Li}$ (7.016 amu)

Average atomic mass of lithium:

$$\frac{7.42 \times 6.015 + 92.58 \times 7.016}{100} = 6.941 \text{ amu}$$
# Atomic Mass: Average Atomic Mass

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- **Metals**
- **Metalloids**
- **Nonmetals**
Copper, a metal known since ancient times, is used in electrical cables and pennies, among other things. The atomic masses of its two stable isotopes, $^{63}_{29}\text{Cu}$ (69.09 percent) and $^{65}_{29}\text{Cu}$ (30.91 percent), are 62.93 amu and 64.9278 amu, respectively. Calculate the average atomic mass of copper. The relative abundances are given in parentheses.

**Strategy** Each isotope contributes to the average atomic mass based on its relative abundance. Multiplying the mass of an isotope by its fractional abundance (not percent) will give the contribution to the average atomic mass of that particular isotope.

**Solution** First the percents are converted to fractions: 69.09 percent to 69.09/100 or 0.6909 and 30.91 percent to 30.91/100 or 0.3091. We find the contribution to the average atomic mass for each isotope, then add the contributions together to obtain the average atomic mass.

\[
(0.6909)(62.93 \text{ amu}) + (0.3091)(64.9278 \text{ amu}) = 63.55 \text{ amu}
\]

**Check** The average atomic mass should be between the two isotopic masses; therefore, the answer is reasonable. Note that because there are more $^{63}_{29}\text{Cu}$ than $^{65}_{29}\text{Cu}$ isotopes, the average atomic mass is closer to 62.93 amu than to 64.9278 amu.

**Practice Exercise** The atomic masses of the two stable isotopes of boron, $^{10}\text{B}$ (19.78 percent) and $^{11}\text{B}$ (80.22 percent), are 10.0129 amu and 11.0093 amu, respectively. Calculate the average atomic mass of boron.
The **mole (mol)**: A unit to count numbers of particles

Dozen = 12

Pair = 2

The **mole (mol)** is the amount of a substance that contains as many elementary entities as there are atoms in exactly 12.00 grams of $^{12}$C

This number is expressed by the Avogadro’s number ($N_A$)

$$1 \text{ mol} = N_A = 6.0221367 \times 10^{23}$$
Avogadro's Number and the Molar Mass of an Element

**Molar mass** ($M$) is the mass of 1 mole of atoms in grams.

1 mole $^{12}$C atoms = $6.022 \times 10^{23}$ atoms = 12.00 g

1 $^{12}$C atom = 12.00 amu

1 mole $^{1}$H atoms = $6.022 \times 10^{23}$ atoms = 1.00 g

1 $^{1}$H atom = 1.00 amu

For any element

atomic mass (amu) = molar mass (grams)
Avogadro's Number and the Molar Mass of an Element

• Unit is the amu mass.
  • atomic unit
  • 1 amu = $1.66 \times 10^{-24}$ g

• We define the masses of atoms in terms of atomic mass units
  • 1 Carbon atom = 12.01 amu,
  • 1 Oxygen atom = 16.00 amu
  • 1 $O_2$ molecule = 2(16.00 amu) = 32.00 amu
Avogadro's Number and the Molar Mass of an Element

One Mole of:

- C
- S
- Cu
- Hg
- Fe
For example:

Molar mass of $^{12}\text{C}$ is $12.01 \text{ g}$ and there are $6.022 \times 10^{23} \ ^{12}\text{C}$ atoms in 1 mole of the substance;

The mass of one $^{12}\text{C}$ atom is given by

$$\frac{12.00 \text{ g} \ ^{12}\text{C} \text{ atoms}}{6.022 \times 10^{23} \ ^{12}\text{C} \text{ atoms}} = 1.993 \times 10^{-23} \text{ g}$$
Avogadro's Number and the Molar Mass of an Element

**Avogadro’s number can be used to convert from the atomic mass units to mass in gram and vice versa.**

The mass of every $^{12}$C atom = 12 amu

The number of atomic mass units equivalent to 1 g is

$$\frac{1 \text{ } ^{12}\text{C atom}}{12 \text{ amu}} \times \frac{12.00 \text{ g}}{6.022 \times 10^{23} \text{ } ^{12}\text{C atoms}} = \frac{1.66 \times 10^{-24} \text{ g}}{1 \text{ amu}}$$

1 amu = 1.66 x 10^{-24} g \hspace{1cm} \text{or} \hspace{1cm} 1 \text{ g} = 6.022 \times 10^{23} \text{ amu}

**Diagram:**

- **Mass of element (m)**
- **Number of moles of element (n)**
- **Number of atoms of element (N)**

\[ m = \frac{m}{M} \]

\[ n = \frac{n}{N/A} \]

\[ N = \frac{N}{N_A} \]

\[ M = \text{molar mass in g/mol} \]

\[ N_A = \text{Avogadro’s number} \]
Avogadro's Number and the Molar Mass of an Element

EXAMPLE 3.2

Helium (He) is a valuable gas used in industry, low-temperature research, deep-sea diving tanks, and balloons. How many moles of He atoms are in 6.46 g of He?

**Strategy** We are given grams of helium and asked to solve for moles of helium. What conversion factor do we need to convert between grams and moles? Arrange the appropriate conversion factor so that grams cancel and the unit moles is obtained for your answer.

**Solution** The conversion factor needed to convert between grams and moles is the molar mass. In the periodic table (see inside front cover) we see that the molar mass of He is 4.003 g. This can be expressed as

\[ 1 \text{ mol He} = 4.003 \text{ g He} \]

From this equality, we can write two conversion factors

\[ \frac{1 \text{ mol He}}{4.003 \text{ g He}} \quad \text{and} \quad \frac{4.003 \text{ g He}}{1 \text{ mol He}} \]

The conversion factor on the left is the correct one. Grams will cancel, leaving the unit mol for the answer, that is,

\[ 6.46 \text{ g He} \times \frac{1 \text{ mol He}}{4.003 \text{ g He}} = 1.61 \text{ mol He} \]

Thus, there are 1.61 moles of He atoms in 6.46 g of He.

**Check** Because the given mass (6.46 g) is larger than the molar mass of He, we expect to have more than 1 mole of He.

**Practice Exercise** How many moles of magnesium (Mg) are there in 87.3 g of Mg?
EXAMPLE 3.3

Zinc (Zn) is a silvery metal that is used in making brass (with copper) and in plating iron to prevent corrosion. How many grams of Zn are in 0.356 mole of Zn?

**Strategy** We are trying to solve for grams of zinc. What conversion factor do we need to convert between moles and grams? Arrange the appropriate conversion factor so that moles cancel and the unit grams are obtained for your answer.

**Solution** The conversion factor needed to convert between moles and grams is the molar mass. In the periodic table (see inside front cover) we see the molar mass of Zn is 65.39 g. This can be expressed as

$$1 \text{ mol Zn} = 65.39 \text{ g Zn}$$

From this equality, we can write two conversion factors

$$\frac{1 \text{ mol Zn}}{65.39 \text{ g Zn}} \quad \text{and} \quad \frac{65.39 \text{ g Zn}}{1 \text{ mol Zn}}$$

The conversion factor on the right is the correct one. Moles will cancel, leaving unit of grams for the answer. The number of grams of Zn is

$$0.356 \text{ mol Zn} \times \frac{65.39 \text{ g Zn}}{1 \text{ mol Zn}} = 23.3 \text{ g Zn}$$

Thus, there are 23.3 g of Zn in 0.356 mole of Zn.

**Check** Does a mass of 23.3 g for 0.356 mole of Zn seem reasonable? What is the mass of 1 mole of Zn?

**Practice Exercise** Calculate the number of grams of lead (Pb) in 12.4 moles of lead.
Avogadros Number and the Molar Mass of an Element

EXAMPLE 3.4

Sulfur (S) is a nonmetallic element that is present in coal. When coal is burned, sulfur is converted to sulfur dioxide and eventually to sulfuric acid that gives rise to the acid rain phenomenon. How many atoms are in 16.3 g of S?

Strategy The question asks for atoms of sulfur. We cannot convert directly from grams to atoms of sulfur. What unit do we need to convert grams of sulfur to in order to convert to atoms? What does Avogadro’s number represent?

Solution We need two conversions: first from grams to moles and then from moles to number of particles (atoms). The first step is similar to Example 3.2. Because

$$1 \text{ mol } S = 32.07 \text{ g } S$$

the conversion factor is

$$\frac{1 \text{ mol } S}{32.07 \text{ g } S}$$

Avogadro’s number is the key to the second step. We have

$$1 \text{ mol } = 6.022 \times 10^{23} \text{ particles (atoms)}$$

and the conversion factors are

$$\frac{6.022 \times 10^{23} \text{ S atoms}}{1 \text{ mol } S} \quad \text{and} \quad \frac{1 \text{ mol } S}{6.022 \times 10^{23} \text{ S atoms}}$$

The conversion factor on the left is the one we need because it has number of S atoms in the numerator. We can solve the problem by first calculating the number of moles contained in 16.3 g of S, and then calculating the number of S atoms from the number of moles of S:

grams of S → moles of S → number of S atoms

We can combine these conversions in one step as follows:

$$16.3 \text{ g } S \times \frac{1 \text{ mol } S}{32.07 \text{ g } S} \times \frac{6.022 \times 10^{23} \text{ S atoms}}{1 \text{ mol } S} = 3.06 \times 10^{23} \text{ S atoms}$$

Thus, there are $3.06 \times 10^{23}$ atoms of S in 16.3 g of S.

Check Should 16.3 g of S contain fewer than Avogadro’s number of atoms? What mass of S would contain Avogadro’s number of atoms?

Practice Exercise Calculate the number of atoms in 0.551 g of potassium (K).
How many atoms are in 0.551 g of potassium (K)?

\[
\frac{0.551 \text{ g K}}{39.10 \text{ g K}} \times \frac{1 \text{ mol K}}{6.022 \times 10^{23} \text{ atoms K}} = 8.49 \times 10^{21} \text{ atoms K}
\]
**Molecular Mass**

*Molecular mass* (or *molecular weight*) is the sum of the atomic masses (in amu) in a molecule.

For any molecule

\[
\text{molecular mass (amu)} = \text{molar mass (grams)}
\]

1 molecule \( \text{SO}_2 \) = 64.07 amu
1 mole \( \text{SO}_2 \) = 64.07 g \( \text{SO}_2 \)

*Molecular mass of \( H_2O \) is*

\[
2(\text{atomic mass of H}) + \text{atomic mass of O} = 2(1.008 \text{ amu}) + 16.00 \text{ amu} = 18.02 \text{ amu}
\]
EXAMPLE 3.5

Calculate the molecular masses (in amu) of the following compounds: (a) sulfur dioxide ($\text{SO}_2$) and (b) caffeine ($\text{C}_8\text{H}_{10}\text{N}_4\text{O}_2$).

**Strategy** How do atomic masses of different elements combine to give the molecular mass of a compound?

**Solution** To calculate molecular mass, we need to sum all the atomic masses in the molecule. For each element, we multiply the atomic mass of the element by the number of atoms of that element in the molecule. We find atomic masses in the periodic table (inside front cover).

(a) There are two O atoms and one S atom in $\text{SO}_2$, so that

$$\text{molecular mass of } \text{SO}_2 = 32.07 \text{ amu} + 2(16.00 \text{ amu})$$

$$= 64.07 \text{ amu}$$

(b) There are eight C atoms, ten H atoms, four N atoms, and two O atoms in caffeine, so the molecular mass of $\text{C}_8\text{H}_{10}\text{N}_4\text{O}_2$ is given by

$$8(12.01 \text{ amu}) + 10(1.008 \text{ amu}) + 4(14.01 \text{ amu}) + 2(16.00 \text{ amu}) = 194.20 \text{ amu}$$

**Practice Exercise** What is the molecular mass of methanol ($\text{CH}_4\text{O}$)?
Methane (CH\textsubscript{4}) is the principal component of natural gas. How many moles of CH\textsubscript{4} are present in 6.07 g of CH\textsubscript{4}?

**Strategy** We are given grams of CH\textsubscript{4} and asked to solve for moles of CH\textsubscript{4}. What conversion factor do we need to convert between grams and moles? Arrange the appropriate conversion factor so that grams cancel and the unit moles are obtained for your answer.

**Solution** The conversion factor needed to convert between grams and moles is the molar mass. First we need to calculate the molar mass of CH\textsubscript{4}, following the procedure in Example 3.5:

\[
\text{molar mass of CH}_4 = 12.01 \text{ g} + 4(1.008 \text{ g}) = 16.04 \text{ g}
\]

Because

\[
1 \text{ mol CH}_4 = 16.04 \text{ g CH}_4
\]

the conversion factor we need should have grams in the denominator so that the unit g will cancel, leaving the unit mol in the numerator:

\[
\frac{1 \text{ mol CH}_4}{16.04 \text{ g CH}_4}
\]

We now write

\[
6.07 \text{ g CH}_4 \times \frac{1 \text{ mol CH}_4}{16.04 \text{ g CH}_4} = 0.378 \text{ mol CH}_4
\]

Thus, there is 0.378 mole of CH\textsubscript{4} in 6.07 g of CH\textsubscript{4}.

**Check** Should 6.07 g of CH\textsubscript{4} equal less than 1 mole of CH\textsubscript{4}? What is the mass of 1 mole of CH\textsubscript{4}?

**Practice Exercise** Calculate the number of moles of chloroform (CHCl\textsubscript{3}) in 198 g of chloroform.
EXAMPLE 3.7

How many hydrogen atoms are present in 25.6 g of urea [(NH₂)₂CO], which is used as a fertilizer, in animal feed, and in the manufacture of polymers? The molar mass of urea is 60.06 g.

**Strategy** We are asked to solve for atoms of hydrogen in 25.6 g of urea. We cannot convert directly from grams of urea to atoms of hydrogen. How should molar mass and Avogadro’s number be used in this calculation? How many moles of H are in 1 mole of urea?

**Solution** To calculate the number of H atoms, we first must convert grams of urea to moles of urea using the molar mass of urea. This part is similar to Example 3.2. The molecular formula of urea shows there are four moles of H atoms in one mole of urea molecule, so the mole ratio is 4:1. Finally, knowing the number of moles of H atoms, we can calculate the number of H atoms using Avogadro’s number. We need two conversion factors: molar mass and Avogadro’s number. We can combine these conversions

grams of urea → moles of urea → moles of H → atoms of H

into one step:

\[
25.6 \text{ g } \text{(NH}_2\text{)}_2\text{CO} \times \frac{1 \text{ mol } \text{(NH}_2\text{)}_2\text{CO}}{60.06 \text{ g } \text{(NH}_2\text{)}_2\text{CO}} \times \frac{4 \text{ mol } \text{H}}{1 \text{ mol } \text{(NH}_2\text{)}_2\text{CO}} \times \frac{6.022 \times 10^{23} \text{ H atoms}}{1 \text{ mol } \text{H}}
\]

\[= 1.03 \times 10^{24} \text{ H atoms} \]

**Check** Does the answer look reasonable? How many atoms of H would 60.06 g of urea contain?

**Practice Exercise** How many H atoms are in 72.5 g of isopropanol (rubbing alcohol), C₃H₈O?
How many H atoms are in 72.5 g of C$_3$H$_8$O?

1 mol C$_3$H$_8$O = (3 x 12) + (8 x 1) + 16 = 60 g C$_3$H$_8$O

1 mol C$_3$H$_8$O molecules = 8 mol H atoms

1 mol H = 6.022 x 10$^{23}$ atoms H

\[
\frac{72.5 \text{ g C}_3\text{H}_8\text{O}}{60 \text{ g C}_3\text{H}_8\text{O}} \times \frac{1 \text{ mol C}_3\text{H}_8\text{O}}{1 \text{ mol C}_3\text{H}_8\text{O}} \times \frac{8 \text{ mol H atoms}}{1 \text{ mol C}_3\text{H}_8\text{O}} \times \frac{6.022 \times 10^{23} \text{ H atoms}}{1 \text{ mol H atoms}} =
\]

5.82 x 10$^{24}$ atoms H
Molecular Mass

*Formula mass* is the sum of the atomic masses (in amu) in a formula unit of an ionic compound.

\[
\text{NaCl} = 1\text{Na} + 1\text{Cl} = 22.99 \text{ amu} + 35.45 \text{ amu} = 58.44 \text{ amu}
\]

For any ionic compound

\[
\text{formula mass (amu)} = \text{molar mass (grams)}
\]

1 formula unit NaCl = 58.44 amu

1 mole NaCl = 58.44 g NaCl
What is the formula mass of $\text{Ca}_3(\text{PO}_4)_2$?

1 formula unit of $\text{Ca}_3(\text{PO}_4)_2$

- $3 \text{ Ca} \quad 3 \times 40.08$
- $2 \text{ P} \quad 2 \times 30.97$
- $8 \text{ O} \quad +8 \times 16.00$

$310.18 \text{ amu}$
The **percent composition** by mass is the percent by mass of each element in a compound.

The percent composition of an element is calculated using the formula:

\[
\text{percent composition of an element} = \frac{n \times \text{molar mass of element}}{\text{molar mass of compound}} \times 100\%
\]

where:
- \( n \) is the number of moles of the element in 1 mole of the compound,
- \( \text{molar mass of element} \) is the mass of one mole of the element,
- \( \text{molar mass of compound} \) is the mass of one mole of the compound.

For the compound \( \text{C}_2\text{H}_6\text{O} \):

\[
\begin{align*}
\%C &= \frac{2 \times (12.01 \text{ g})}{46.07 \text{ g}} \times 100\% = 52.14\% \\
\%H &= \frac{6 \times (1.008 \text{ g})}{46.07 \text{ g}} \times 100\% = 13.13\% \\
\%O &= \frac{1 \times (16.00 \text{ g})}{46.07 \text{ g}} \times 100\% = 34.73\%
\end{align*}
\]

\[
52.14\% + 13.13\% + 34.73\% = 100.0\%
\]

This confirms that the percent composition of \( \text{C}_2\text{H}_6\text{O} \) is 100%.
Percent Composition of Compounds

Given the percent composition by mass of a compound, we can determine the empirical formula of the Compound.

1. Mass percent
2. Convert to grams and divide by molar mass
3. Moles of each element
4. Divide by the smallest number of moles
5. Mole ratios of elements
6. Change to integer subscripts
7. Empirical formula
Given the percent composition by mass of a compound, we can determine the empirical formula of the Compound.

Determine the empirical formula of a compound that has the following percent composition by mass: K 24.75, Mn 34.77, O 40.51 percent.

\[
\begin{align*}
n_K &= 24.75 \text{ g K} \times \frac{1 \text{ mol K}}{39.10 \text{ g K}} = 0.6330 \text{ mol K} \\
n_{\text{Mn}} &= 34.77 \text{ g Mn} \times \frac{1 \text{ mol Mn}}{54.94 \text{ g Mn}} = 0.6329 \text{ mol Mn} \\
n_O &= 40.51 \text{ g O} \times \frac{1 \text{ mol O}}{16.00 \text{ g O}} = 2.532 \text{ mol O}
\end{align*}
\]
Percent Composition of Compounds

Percent Composition and Empirical Formulas

\[ n_K = 0.6330, \quad n_{\text{Mn}} = 0.6329, \quad n_O = 2.532 \]

\[ K : \frac{0.6330}{0.6329} \approx 1.0 \]

\[ \text{Mn} : \frac{0.6329}{0.6329} = 1.0 \]

\[ O : \frac{2.532}{0.6329} \approx 4.0 \]

KMnO\textsubscript{4}
Ascorbic acid (vitamin C) cures scurvy. It is composed of 40.92 percent carbon (C), 4.58 percent hydrogen (H), and 54.50 percent oxygen (O) by mass. Determine its empirical formula.

**Strategy** In a chemical formula, the subscripts represent the ratio of the number of moles of each element that combine to form one mole of the compound. How can we convert from mass percent to moles? If we assume an exactly 100-g sample of the compound, do we know the mass of each element in the compound? How do we then convert from grams to moles?

**Solution** If we have 100 g of ascorbic acid, then each percentage can be converted directly to grams. In this sample, there will be 40.92 g of C, 4.58 g of H, and 54.50 g of O. Because the subscripts in the formula represent a mole ratio, we need to convert the grams of each element to moles. The conversion factor needed is the molar mass of each element. Let \( n \) represent the number of moles of each element so that

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

\[
    n_H = \frac{4.58 \text{ g H}}{1.008 \text{ g H}} \times \frac{1 \text{ mol H}}{1 \text{ mol H}} = 4.54 \text{ mol H}
\]

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

Thus, we arrive at the formula \( C_{3.407}H_{4.54}O_{3.406} \), which gives the identity and the mole ratios of atoms present. However, chemical formulas are written with whole numbers.
Percent Composition of Compounds

Percent Composition and Empirical Formulas

Try to convert to whole numbers by dividing all the subscripts by the smallest subscript (3.406):

\[
\begin{align*}
\text{C: } & \quad \frac{3.407}{3.406} \approx 1 \\
\text{H: } & \quad \frac{4.54}{3.406} = 1.33 \\
\text{O: } & \quad \frac{3.406}{3.406} = 1
\end{align*}
\]

where the \( \approx \) sign means “approximately equal to.” This gives \( \text{CH}_{1.33}\text{O} \) as the formula for ascorbic acid. Next, we need to convert 1.33, the subscript for H, into an integer. This can be done by a trial-and-error procedure:

\[
\begin{align*}
1.33 \times 1 &= 1.33 \\
1.33 \times 2 &= 2.66 \\
1.33 \times 3 &= 3.99 \approx 4
\end{align*}
\]

Because \( 1.33 \times 3 \) gives us an integer (4), we multiply all the subscripts by 3 and obtain \( \text{C}_3\text{H}_4\text{O}_3 \) as the empirical formula for ascorbic acid.

**Check** Are the subscripts in \( \text{C}_3\text{H}_4\text{O}_3 \) reduced to the smallest whole numbers?

**Practice Exercise** Determine the empirical formula of a compound having the following percent composition by mass: K: 24.75 percent; Mn: 34.77 percent; O: 40.51 percent.
Percent Composition of Compounds

To know the actual mass of an element in a certain mass of a compound.

**EXAMPLE 3.10**

Chalcopyrite (CuFeS$_2$) is a principal mineral of copper. Calculate the number of kilograms of Cu in $3.71 \times 10^3$ kg of chalcopyrite.

**Strategy** Chalcopyrite is composed of Cu, Fe, and S. The mass due to Cu is based on its percentage by mass in the compound. How do we calculate mass percent of an element?

**Solution** The molar masses of Cu and CuFeS$_2$ are 63.55 g and 183.5 g, respectively. The mass percent of Cu is therefore

$$\%_{\text{Cu}} = \frac{\text{molar mass of Cu}}{\text{molar mass of CuFeS}_2} \times 100\%$$

$$= \frac{63.55 \text{ g}}{183.5 \text{ g}} \times 100\% = 34.63\%$$

To calculate the mass of Cu in a $3.71 \times 10^3$ kg sample of CuFeS$_2$, we need to convert the percentage to a fraction (that is, convert 34.63 percent to $34.63/100$, or 0.3463) and write

$$\text{mass of Cu in CuFeS}_2 = 0.3463 \times (3.71 \times 10^3 \text{ kg}) = 1.28 \times 10^3 \text{ kg}$$

**Check** As a ball-park estimate, note that the mass percent of Cu is roughly 33 percent, so that a third of the mass should be Cu; that is, $\frac{1}{3} \times 3.71 \times 10^3 \text{ kg} \approx 1.24 \times 10^3 \text{ kg}$. This quantity is quite close to the answer.

**Practice Exercise** Calculate the number of grams of Al in 371 g of Al$_2$O$_3$. 
Experimental Determination of Empirical Formulas

Combust 11.5 g ethanol
Collect 22.0 g CO$_2$ and 13.5 g H$_2$O

\[
g \text{ CO}_2 \quad \rightarrow \quad \text{mol CO}_2 \quad \rightarrow \quad \text{mol C} \quad \rightarrow \quad g \text{ C} \quad \quad 6.0 \text{g C} = 0.5 \text{mol C}
\]

\[
g \text{ H}_2\text{O} \quad \rightarrow \quad \text{mol H}_2\text{O} \quad \rightarrow \quad \text{mol H} \quad \rightarrow \quad g \text{ H} \quad \quad 1.5 \text{g H} = 1.5 \text{mol H}
\]

\[
g \text{ of O} = g \text{ of sample} - (g \text{ of C} + g \text{ of H}) \quad \quad 4.0 \text{g O} = 0.25 \text{mol O}
\]

Empirical formula $\text{C}_{0.5}\text{H}_{1.5}\text{O}_{0.25}$

Divide by smallest subscript (0.25)

Empirical formula $\text{C}_2\text{H}_6\text{O}$
Thus, 11.5 g of ethanol contains 6.00 g of carbon and 1.51 g of hydrogen. The remainder must be oxygen, whose mass is

\[
\text{mass of O} = \text{mass of sample} - (\text{mass of C} + \text{mass of H}) \\
= 11.5 \text{ g} - (6.00 \text{ g} + 1.51 \text{ g}) \\
= 4.0 \text{ g}
\]

The number of moles of each element present in 11.5 g of ethanol is

\[
\text{moles of C} = 6.00 \text{ g C} \times \frac{1 \text{ mol C}}{12.01 \text{ g C}} = 0.500 \text{ mol C} \\
\text{moles of H} = 1.51 \text{ g H} \times \frac{1 \text{ mol H}}{1.008 \text{ g H}} = 1.50 \text{ mol H} \\
\text{moles of O} = 4.0 \text{ g O} \times \frac{1 \text{ mol O}}{16.00 \text{ g O}} = 0.25 \text{ mol O}
\]
“empirical” means “based only on observation and measurement.”

Ex: The empirical formula of ethanol is determined from analysis of the compound in terms of its component elements.

No knowledge of how the atoms are linked together in the compound is required.
To calculate the actual, molecular formula we must know
- the *approximate* molar mass of the compound
- its empirical formula.
Determination of Molecular Formulas

EXAMPLE 3.11

A sample of a compound contains 1.52 g of nitrogen (N) and 3.47 g of oxygen (O). The molar mass of this compound is between 90 g and 95 g. Determine the molecular formula and the accurate molar mass of the compound.

**Strategy** To determine the molecular formula, we first need to determine the empirical formula. How do we convert between grams and moles? Comparing the empirical molar mass to the experimentally determined molar mass will reveal the relationship between the empirical formula and molecular formula.

**Solution** We are given grams of N and O. Use molar mass as a conversion factor to convert grams to moles of each element. Let $n$ represent the number of moles of each element. We write

\[
  n_N = 1.52 \text{ g N} \times \frac{1 \text{ mol N}}{14.01 \text{ g N}} = 0.108 \text{ mol N}
\]

\[
  n_O = 3.47 \text{ g O} \times \frac{1 \text{ mol O}}{16.00 \text{ g O}} = 0.217 \text{ mol O}
\]

Thus, we arrive at the formula $N_{0.108}O_{0.217}$, which gives the identity and the ratios of atoms present. However, chemical formulas are written with whole numbers. Try to convert to whole numbers by dividing the subscripts by the smaller subscript (0.108). After rounding off, we obtain NO$_2$ as the empirical formula.
Determination of Molecular Formulas

The molecular formula might be the same as the empirical formula or some integral multiple of it (for example, two, three, four, or more times the empirical formula). Comparing the ratio of the molar mass to the molar mass of the empirical formula will show the integral relationship between the empirical and molecular formulas. The molar mass of the empirical formula NO₂ is

\[
\text{empirical molar mass} = 14.01 \text{ g} + 2(16.00 \text{ g}) = 46.01 \text{ g}
\]

Next, we determine the ratio between the molar mass and the empirical molar mass

\[
\frac{\text{molar mass}}{\text{empirical molar mass}} = \frac{90 \text{ g}}{46.01 \text{ g}} \approx 2
\]

The molar mass is twice the empirical molar mass. This means that there are two NO₂ units in each molecule of the compound, and the molecular formula is (NO₂)₂ or N₂O₄.

The actual molar mass of the compound is two times the empirical molar mass, that is, 2(46.01 g) or 92.02 g, which is between 90 g and 95 g.

**Check** Note that in determining the molecular formula from the empirical formula, we need only know the *approximate* molar mass of the compound. The reason is that the true molar mass is an integral multiple (1×, 2×, 3×, . . .) of the empirical molar mass. Therefore, the ratio (molar mass/empirical molar mass) will always be close to an integer.

**Practice Exercise** A sample of a compound containing boron (B) and hydrogen (H) contains 6.444 g of B and 1.803 g of H. The molar mass of the compound is about 30 g. What is its molecular formula?
A process in which one or more substances is changed into one or more new substances is a chemical reaction.

A chemical equation uses chemical symbols to show what happens during a chemical reaction:

**reactants** → **products**

### 3 ways of representing the reaction of H₂ with O₂ to form H₂O

Two hydrogen molecules + One oxygen molecule → Two water molecules

2H₂ + O₂ → 2H₂O
How to “Read” Chemical Equations

2 Mg + O₂ → 2 MgO

2 atoms Mg + 1 molecule O₂ makes 2 formula units MgO

2 moles Mg + 1 mole O₂ makes 2 moles MgO

48.6 grams Mg + 32.0 grams O₂ makes 80.6 g MgO

NOT

2 grams Mg + 1 gram O₂ makes 2 g MgO
1. Write the **correct** formula(s) for the reactants on the left side and the **correct** formula(s) for the product(s) on the right side of the equation.

   Ethane reacts with oxygen to form carbon dioxide and water

   \[ \text{C}_2\text{H}_6 + \text{O}_2 \rightarrow \text{CO}_2 + \text{H}_2\text{O} \]

2. Change the numbers in front of the formulas (**coefficients**) to make the number of atoms of each element the same on both sides of the equation. Do not change the subscripts.

   \[ 2\text{C}_2\text{H}_6 \quad \text{NOT} \quad \text{C}_4\text{H}_{12} \]
3. Start by balancing those elements that appear in only one reactant and one product.

\[ \text{C}_2\text{H}_6 + \text{O}_2 \rightarrow \text{CO}_2 + \text{H}_2\text{O} \]

- Start with C or H but not O
- Multiply CO\(_2\) by 2
- Multiply H\(_2\)O by 3
4. Balance those elements that appear in two or more reactants or products.

\[
\begin{align*}
\text{C}_2\text{H}_6 + \frac{7}{2}\text{O}_2 & \rightarrow 2\text{CO}_2 + 3\text{H}_2\text{O} & \text{multiply } \text{O}_2 \text{ by } \frac{7}{2} \\
\text{2 oxygen on left} & \rightarrow \text{4 oxygen + 3 oxygen = 7 oxygen on right} & \text{of the same element}
\end{align*}
\]

\[
\begin{align*}
\text{C}_2\text{H}_6 + \frac{7}{2}\text{O}_2 & \rightarrow 2\text{CO}_2 + 3\text{H}_2\text{O} & \text{remove fraction} \\
\text{2C}_2\text{H}_6 + 7\text{O}_2 & \rightarrow 4\text{CO}_2 + 6\text{H}_2\text{O} & \text{multiply both sides by 2}
\end{align*}
\]
5. Check to make sure that you have the same number of each type of atom on both sides of the equation.

Balancing Chemical Equations

2\text{C}_2\text{H}_6 + 7\text{O}_2 \rightarrow 4\text{CO}_2 + 6\text{H}_2\text{O}

Reactants: 4 \text{C} (2 \times 2) \quad 12 \text{H} (2 \times 6) \quad 14 \text{O} (7 \times 2)

Products: 4 \text{C} \quad 12 \text{H} (6 \times 2) \quad 14 \text{O} (4 \times 2 + 6)
Chemical Reactions and Chemical Equations

Balancing Chemical Equations

**EXAMPLE 3.12**

When aluminum metal is exposed to air, a protective layer of aluminum oxide (Al₂O₃) forms on its surface. This layer prevents further reaction between aluminum and oxygen, and it is the reason that aluminum beverage cans do not corrode. [In the case of iron, the rust, or iron(III) oxide, that forms is too porous to protect the iron metal underneath, so rusting continues.] Write a balanced equation for the formation of Al₂O₃.

**Strategy** Remember that the formula of an element or compound cannot be changed when balancing a chemical equation. The equation is balanced by placing the appropriate coefficients in front of the formulas. Follow the procedure described on p. 96.

**Solution** The unbalanced equation is

\[ \text{Al} + \text{O}_2 \rightarrow \text{Al}_2\text{O}_3 \]

In a balanced equation, the number and types of atoms on each side of the equation must be the same. We see that there is one Al atom on the reactants side and there are two Al atoms on the product side. We can balance the Al atoms by placing a coefficient of 2 in front of Al on the reactants side.

\[ 2\text{Al} + \text{O}_2 \rightarrow \text{Al}_2\text{O}_3 \]

There are two O atoms on the reactants side, and three O atoms on the product side of the equation. We can balance the O atoms by placing a coefficient of \( \frac{3}{2} \) in front of \( \text{O}_2 \) on the reactants side.

\[ 2\text{Al} + \frac{3}{2}\text{O}_2 \rightarrow \text{Al}_2\text{O}_3 \]

This is a balanced equation. However, equations are normally balanced with the smallest set of *whole* number coefficients. Multiplying both sides of the equation by 2 gives whole number coefficients.

\[ 2(2\text{Al} + \frac{3}{2}\text{O}_2 \rightarrow \text{Al}_2\text{O}_3) \]

or

\[ 4\text{Al} + 3\text{O}_2 \rightarrow 2\text{Al}_2\text{O}_3 \]
Chemical Reactions and Chemical Equations

Balancing Chemical Equations

Check  For an equation to be balanced, the number and types of atoms on each side of the equation must be the same. The final tally is

<table>
<thead>
<tr>
<th>Reactants</th>
<th>Products</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al (4)</td>
<td>Al (4)</td>
</tr>
<tr>
<td>O (6)</td>
<td>O (6)</td>
</tr>
</tbody>
</table>

The equation is balanced. Also, the coefficients are reduced to the simplest set of whole numbers.

Practice Exercise  Balance the equation representing the reaction between iron(III) oxide, \( \text{Fe}_2\text{O}_3 \), and carbon monoxide (CO) to yield iron (Fe) and carbon dioxide (CO\(_2\)).
1. Write balanced chemical equation
2. Convert quantities of known substances into moles
3. Use coefficients in balanced equation to calculate the number of moles of the sought quantity
4. Convert moles of sought quantity into desired units
Methanol burns in air according to the equation

$$2\text{CH}_3\text{OH} + 3\text{O}_2 \rightarrow 2\text{CO}_2 + 4\text{H}_2\text{O}$$

If 209 g of methanol are used up in the combustion, what mass of water is produced?

grams CH$_3$OH $\rightarrow$ moles CH$_3$OH $\rightarrow$ moles H$_2$O $\rightarrow$ grams H$_2$O

molar mass
CH$_3$OH

coefficients
chemical equation

molar mass
H$_2$O

$$209 \text{ g CH}_3\text{OH} \times \frac{1 \text{ mol CH}_3\text{OH}}{32.0 \text{ g CH}_3\text{OH}} \times \frac{4 \text{ mol H}_2\text{O}}{2 \text{ mol CH}_3\text{OH}} \times \frac{18.0 \text{ g H}_2\text{O}}{1 \text{ mol H}_2\text{O}} = 235 \text{ g H}_2\text{O}$$
Limiting Reagents

Reactant used up first in the reaction.

\[ 2\text{NO} + \text{O}_2 \rightarrow 2\text{NO}_2 \]

NO is the limiting reagent

O\textsubscript{2} is the excess reagent
In one process, 124 g of Al are reacted with 601 g of Fe\(_2\)O\(_3\).

\[ 2\text{Al} + \text{Fe}_2\text{O}_3 \rightarrow \text{Al}_2\text{O}_3 + 2\text{Fe} \]

Calculate the mass of Al\(_2\)O\(_3\) formed.

\[
\begin{align*}
g \text{Al} & \quad \rightarrow \quad \text{mol Al} \quad \rightarrow \quad \text{mol Fe}_2\text{O}_3 \text{ needed} \quad \rightarrow \quad g \text{ Fe}_2\text{O}_3 \text{ needed} \\
g \text{Fe}_2\text{O}_3 & \quad \rightarrow \quad \text{mol Fe}_2\text{O}_3 \quad \rightarrow \quad \text{mol Al needed} \quad \rightarrow \quad g \text{ Al needed}
\end{align*}
\]

\[
\begin{align*}
124 \text{ g Al} \times \frac{1 \text{ mol Al}}{27.0 \text{ g Al}} \times \frac{1 \text{ mol Fe}_2\text{O}_3}{2 \text{ mol Al}} \times \frac{160. \text{ g Fe}_2\text{O}_3}{1 \text{ mol Fe}_2\text{O}_3} &= 367 \text{ g Fe}_2\text{O}_3 \\
\end{align*}
\]

Start with 124 g Al \quad \rightarrow \quad need 367 g Fe\(_2\)O\(_3\)

Have more Fe\(_2\)O\(_3\) (601 g) so Al is limiting reagent
Limiting Reagents

Use limiting reagent (Al) to calculate amount of product that can be formed.

\[
g \text{ Al} \rightarrow \text{ mol Al} \rightarrow \text{ mol Al}_2\text{O}_3 \rightarrow \text{ g Al}_2\text{O}_3
\]

\[
2\text{Al} + \text{Fe}_2\text{O}_3 \rightarrow \text{Al}_2\text{O}_3 + 2\text{Fe}
\]

\[
\begin{align*}
124 \text{ g Al} & \times \frac{1 \text{ mol Al}}{27.0 \text{ g Al}} \times \frac{1 \text{ mol Al}_2\text{O}_3}{2 \text{ mol Al}} \times \frac{102. \text{ g Al}_2\text{O}_3}{1 \text{ mol Al}_2\text{O}_3} = 234 \text{ g Al}_2\text{O}_3
\end{align*}
\]

At this point, all the Al is consumed and \( \text{Fe}_2\text{O}_3 \) remains in excess.
Theoretical Yield is the amount of product that would result if all the limiting reagent reacted.

Actual Yield is the amount of product actually obtained from a reaction.

\[
\text{\% Yield} = \frac{\text{Actual Yield}}{\text{Theoretical Yield}} \times 100\% 
\]
Titanium is a strong, lightweight, corrosion-resistant metal that is used in rockets, aircraft, jet engines, and bicycle frames. It is prepared by the reaction of titanium(IV) chloride with molten magnesium between 950°C and 1150°C:

\[
\text{TiCl}_4(g) + 2\text{Mg}(l) \rightarrow \text{Ti}(s) + 2\text{MgCl}_2(l)
\]

In a certain industrial operation \(3.54 \times 10^7\) g of TiCl\(_4\) are reacted with \(1.13 \times 10^7\) g of Mg. (a) Calculate the theoretical yield of Ti in grams. (b) Calculate the percent yield if \(7.91 \times 10^6\) g of Ti are actually obtained.

**Strategy** Because there are two reactants, this is likely to be a limiting reagent problem. The reactant that produces fewer moles of product is the limiting reagent. How do we convert from amount of reactant to amount of product? Perform this calculation for each reactant, then compare the moles of product, Ti, formed.

**Solution** Carry out two separate calculations to see which of the two reactants is the limiting reagent. First, starting with \(3.54 \times 10^7\) g of TiCl\(_4\), calculate the number of moles of Ti that could be produced if all the TiCl\(_4\) reacted. The conversions are

\[
\text{grams of TiCl}_4 \rightarrow \text{moles of TiCl}_4 \rightarrow \text{moles of Ti}
\]

so that

\[
\text{moles of Ti} = 3.54 \times 10^7 \text{ g TiCl}_4 \times \frac{1 \text{ mol TiCl}_4}{189.7 \text{ g TiCl}_4} \times \frac{1 \text{ mol Ti}}{1 \text{ mol TiCl}_4}
\]

\[
= 1.87 \times 10^5 \text{ mol Ti}
\]

Next, we calculate the number of moles of Ti formed from \(1.13 \times 10^7\) g of Mg. The conversion steps are

\[
\text{grams of Mg} \rightarrow \text{moles of Mg} \rightarrow \text{moles of Ti}
\]

and we write

\[
\text{moles of Ti} = 1.13 \times 10^7 \text{ g Mg} \times \frac{1 \text{ mol Mg}}{24.31 \text{ g Mg}} \times \frac{1 \text{ mol Ti}}{2 \text{ mol Mg}}
\]

\[
= 2.32 \times 10^5 \text{ mol Ti}
\]

Therefore, TiCl\(_4\) is the limiting reagent because it produces a smaller amount of Ti. The mass of Ti formed is

\[
1.87 \times 10^5 \text{ mol Ti} \times \frac{47.88 \text{ g Ti}}{1 \text{ mol Ti}} = 8.95 \times 10^6 \text{ g Ti}
\]
(b) **Strategy**  The mass of Ti determined in part (a) is the theoretical yield. The amount given in part (b) is the actual yield of the reaction.

**Solution**  The percent yield is given by

\[
\% \text{ yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100\%
\]

\[
= \frac{7.91 \times 10^6 \text{ g}}{8.95 \times 10^6 \text{ g}} \times 100\%
\]

\[
= 88.4\%
\]

**Check**  Should the percent yield be less than 100 percent?

**Practice Exercise**  Industrially, vanadium metal, which is used in steel alloys, can be obtained by reacting vanadium(V) oxide with calcium at high temperatures:

\[
5\text{Ca} + \text{V}_2\text{O}_5 \rightarrow 5\text{CaO} + 2\text{V}
\]

In one process, \(1.54 \times 10^3 \text{ g of } \text{V}_2\text{O}_5\) react with \(1.96 \times 10^3 \text{ g of Ca}\). (a) Calculate the theoretical yield of V. (b) Calculate the percent yield if 803 g of V are obtained.