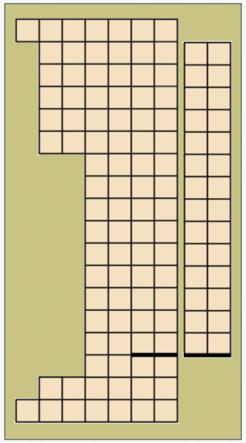
Chapter 3
Stoichiometry



Chapter Objectives:

- Learn how to use the atomic mass of an element and the molecular weight of a compound to relate grams, moles, and the number of formula units.
- Learn how to balance chemical equations.
- Learn how to use the mole concept to relate amounts of chemicals to each other (stoichiometry), and how to find the theoretical yield in limiting reactant problems.
- Learn how to use percent compositions to find empirical and molecular formulas.
- Learn how to use molarity to perform calculations involving solution stoichiometry.

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The Mole Concept

Counting By Weighing

- If the total mass of a sample of small objects is known, and the average mass of the small objects is known, the number of objects in the sample can be determined:

$$\frac{\text{mass of jellybeans (g)}}{\text{average mass of a jellybean (g/jellybean)}} = \text{number of jellybeans}$$

- The same logic works for counting atoms or molecules in a sample, but first we have to figure out how to weigh an atom.

The Mole Concept

- It is not possible to count the number of atoms or molecules involved in chemical reactions, since the molecules are so small, and so many are involved, even in a very small-scale reaction.
- Instead, it is necessary to measure amounts of molecules by using their mass.
- The relationship between sub-microscopic quantities like atoms and molecules, and macroscopic quantities like grams, is made using the **mole concept**.
- Using moles allows us to *count* particles by *weighing* them.

The Mole

- The **mole** (abbreviated **mol**) is the SI unit for *amount of substance*.
- A **mole** is defined as *the amount of a substance that contains the same number of entities as there are atoms in exactly 12 g of carbon-12*.
- 12 g of carbon-12 contains 6.022×10^{23} atoms. This number is known as **Avogadro's number, N_A**, in honor of Amedeo Avogadro (1776-1856, who first proposed the concept, and who also coined the word "molecule").

1 mole = $\mathbf{6.022\times10^{23}}$ units (*Avogadro's number, N_A*)

1 mol carbon-12	contains	6.022×10^{23} atoms
1 mol H_2O	contains	6.022×10^{23} molecules
1 mol NaCl	contains	6.022×10^{23} formula units

The Molar Mass of an Element

- The **molar mass ($\mathcal{M}$ or MM) of an element** is the mass in grams of one mole of atoms of the element. It is numerically equal to the atomic mass of the element in amu's:

molar mass in g/mol = atomic mass in amu

- 1 Fe atom has a mass of 55.847 amu.

  1 mole of Fe atoms has a mass of 55.847 grams.

- 1 O atom has a mass of 15.9994 amu.

  1 mole of O atoms has a mass of 15.9994 grams.

- 1 mole Al = 26.98 g Al = 6.022×10^{23} atoms Al

- 1 mole He = 6.022×10^{23} atoms He = 4.003 g He

The Molar Mass of a Compound

- The **formula mass** or **molar mass of a compound** is the mass in grams of one mole of molecules or formula units of the compound. It is numerically equal to the mass of the compound in amu's:

molar mass in g/mol	**=**	**sum of the atomic masses of the atoms in the molecule/formula unit**

  – For molecular compounds, this is often referred to as the *molecular mass* or *molecular weight*.

$$\text{Molar mass } H_2O = (2\times\text{atomic mass H}) + (1\times\text{atomic mass O})$$
$$= (2\times1.00794) + (1\times15.9994)$$
$$= 18.02$$

- 1 H_2O molecule has a mass of 18.02 amu.

  1 mole of H_2O molecules has a mass of 18.02 grams.

Relating Moles, amu's and Grams

Molar mass of $Ca(NO_3)_2$ $= (1 \times Ca) + (2 \times N) + (6 \times O)$

$= (1\times40.08) + (2\times14.0067) + (6\times15.9994)$

$= 164.09$

The molar mass of $Ca(NO_3)_2$ is 164.09 g/mol

- 1 O_2 molecule has a mass of 32.00 amu

  1 mole of O_2 has a mass of 32.00g

- 1 NaCl formula unit has a mass of 58.44 amu

  1 mole of NaCl has a mass of 58.44 g

- 1 mole of $C_6H_{12}O_6$ = 180.16 g

- 1 mole of $Mg(C_2H_3O_2)_2$ = 83.35 g

Just How Large is Avogadro's Number?

Amount of water in the oceans (liters)

Age of the Earth (seconds)

Population of the Earth

602,200,000,000,000,000,000,000

Radius of the Milky Way galaxy (meters)

Distance from the Earth to the Sun (centimeters)

Extinction of the dinosaurs (years)

Average college tuition (U.S. dollars)

- How much is a mole of water molecules?

Using Gram-Mole Conversions

- Thus, the molar mass (g/mol) is a conversion factor between numbers of moles and mass:
  - moles $\times$ molar mass = mass in grams
  - grams $\div$ molar mass = amount in moles
- and Avogadro's number (things/mol) is a conversion factor between numbers of things (molecules, atoms, or formula units) and moles:
  - moles $\times$ N_A = number of things
  - number of things $\div$ N_A = amount in moles

Examples: Gram-Mole Conversions

1. How many moles are present in 4.60 g of silicon?

Answer: 0.164 mol Si

Examples: Gram-Mole Conversions

2. How many g of Si are present in 9.0 mol of Si?

Answer: 250 g Si

Examples: Gram-Mole Conversions

3. How many atoms are in a sample of uranium with a mass of 1.000 μg?

Answer: 2.530×10^{15} atoms U

Examples: Gram-Mole Conversions

4. How many atoms of carbon are in 2.5 mol of C_2H_6O?

Answer: 3.0×10^{24} atoms C

Examples: Gram-Mole Conversions

5. A pure silver ring contains 2.80×10^{22} silver atoms. How many grams of silver atoms does it contain?

Answer: 5.02 g Ag

Examples: Gram-Mole Conversions

6. How many moles of sucrose, $C_{12}H_{22}O_{11}$, are in a tablespoon of sugar that contains 2.85 g?

Answer: 0.00833 mol $C_{12}H_{22}O_{11}$

Examples: Gram-Mole Conversions

7. How many grams are in 0.0626 mol of $NaHCO_3$, the main ingredient in Alka-Seltzer tablets?

Answer: 5.26 g $NaHCO_3$

Examples: Gram-Mole Conversions

8. A sample of glucose, $C_6H_{12}O_6$, contains 1.52×10^{25} molecules. How many kilograms of glucose is this?

Answer: 4.55 kg

Chemical Equations

Chemical Reactions and Chemical Equations

- A **chemical reaction** occurs when atoms of different elements combine and create a new chemical compound, with properties which may be completely unlike those of its constituent elements.
- A chemical reaction is written in a standard format called a **chemical equation**. The **reactants** (starting materials) are written on the left, and the **products** on the right, with an arrow in between to indicate a transformation.
- Equations are the "sentences" of chemistry, just as formulas are the "words" and atomic symbols are the "letters."

$$Zn \quad + \quad S \longrightarrow ZnS$$

reactants *products*

A Chemical Reaction Illustrated

Sodium
(Na)

solid
mp 97.8°C
bp 881.4°C
silvery metallic surface
soft, easily cut
conducts electricity
reacts violently with water

+

Chlorine
(Cl_2)

gas
mp -101°C
bp -34°C
pale, yellow-green gas
poisonous; causes lung damage
does not conduct electricity
dissolves slightly in water

$\longrightarrow$

Sodium Chloride
($NaCl$)

solid
mp 801°C
bp 1413°C
white crystals or powder
pleasant taste
conducts electricity when
dissolved in water
dissolves freely in water

$$2Na + Cl_2 \rightarrow 2NaCl$$

Balancing Chemical Reactions

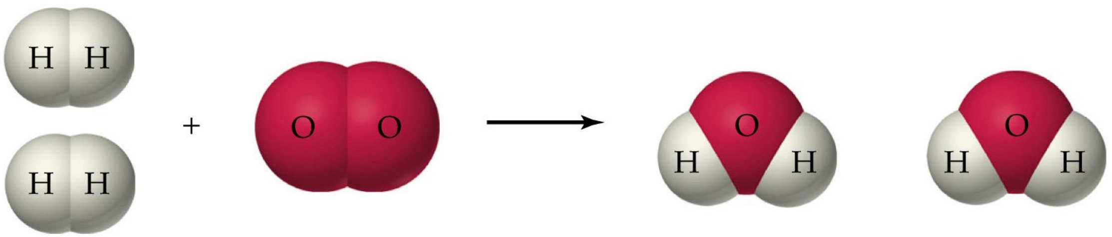
- A chemical equation must be **balanced**: the kinds and numbers of atoms must be the same on both sides of the reaction arrow (conservation of mass).

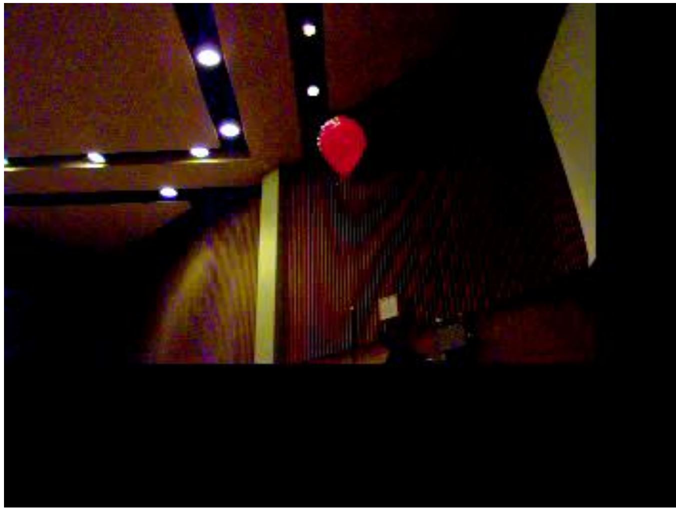
unbalanced: $H_2 + O_2 \rightarrow H_2O$

wrong equation: $H_2 + O_2 \rightarrow H_2O_2$

balanced: $H_2 + \frac{1}{2}O_2 \rightarrow H_2O$

balanced: $2H_2 + O_2 \rightarrow 2H_2O$





Balancing Chemical Reactions

- Equations are balanced by placing a **stoichiometric coefficient** in front of each species, indicating how many units of each compound participate in the reaction.
  - If no coefficient is present, it is assumed to be 1.
  - Usually, we use the smallest whole-number ratios for the coefficients.
  - ***Never*** *balance equations by changing subscripts!* This changes the identity of the species involved in the reaction!
  - In general, it's a good idea to balance the atoms in the most complex substances first, and the atoms in the simpler substances last.

Examples: Balancing Reactions

1. $\_\_\ C(s) + \_\_\ O_2(g) \rightarrow \_\_\ CO_2(g)$

$\_\_\ SO_2(g) + \_\_\ O_2(g) \rightarrow \_\_\ SO_3(g)$

$\_\_\ Fe_2O_3(s) + \_\_\ C(s) \rightarrow \_\_\ Fe(s) + \_\_\ CO_2(g)$

$\_\_\ HCl(aq) + \_\_\ CaCO_3(s) \rightarrow \_\_\ CaCl_2(aq) + \_\_\ H_2O(l) + \_\_\ CO_2(g)$

$\_\_\ N_2(g) + \_\_\ O_2(g) \rightarrow \_\_\ N_2O_5(g)$

$\_\_\ Al(NO_3)_3 + \_\_\ CaSO_4 \rightarrow \_\_\ Al_2(SO_4)_3 + \_\_\ Ca(NO_3)_2$

Examples: Balancing Combustion Reactions

- In a **combustion reaction**, hydrocarbons (containing only H and C) react with molecular oxygen (O_2) to produce carbon dioxide and water. (*Incomplete* combustion can result in other products, such as carbon monoxide and atomic carbon, or soot.)

2. $\_\_\ C_4H_{10} + \_\_\ O_2 \rightarrow \_\_\ CO_2 + \_\_\ H_2O$

$\_\_\ C_2H_6 + \_\_\ O_2 \rightarrow$

$\_\_\ C_3H_8 + \_\_\ O_2 \rightarrow$

$\_\_\ C_2H_5OH + \_\_\ O_2 \rightarrow$

What Do the Coefficients Mean?

- Since **moles combine in the same ratio that atoms or molecules do**, the coefficients in a balanced chemical reaction specify the **relative amounts in moles of the substances** involved in the reaction.

This many **molecules** of H_2	react with this many **molecules** of O_2	to make this many **molecules** of H_2O

$$2\ H_2\ (g)\ +\ 1\ O_2(g)\ \rightarrow\ 2\ H_2O(g)$$

This many **moles** of H_2	react with this many **moles** of O_2	to make this many **moles** of H_2O

Stoichiometry

Stoichiometry: Chemical Arithmetic

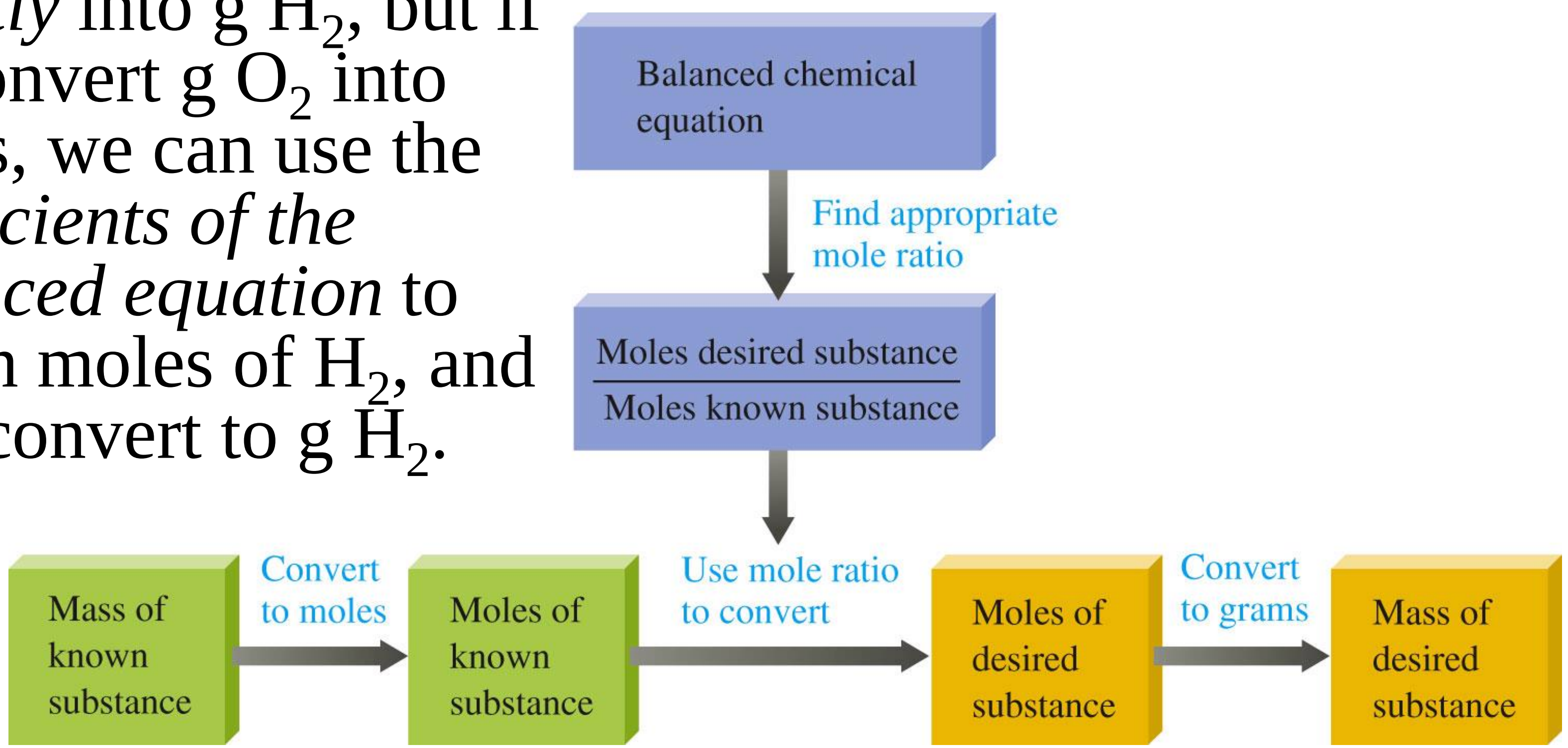
Greek: *stoicheion* + *metron*
element or part   measure

- **Stoichiometry** is the study of the numerical relationships in chemical formulas and reactions.
  - Knowing the stoichiometry of a formula allows us to relate moles and grams for *particular* reactants or products (e.g., that 1 mole of H_2O weighs 18.02 g).
  - Knowing the stoichiometry of a reaction allows us to relate amounts of different substances *to each other*, using the **mole ratios** in the balanced equation, and allows us to predict how much of the products will be formed or how much of the reactants will be needed.

Reaction Stoichiometry: An Example

$$2\ H_2\ (g)\ +\ 1\ O_2(g)\ \rightarrow\ 2\ H_2O(g)$$

- Suppose we have 25.0 g of O_2. How many grams of H_2 will be needed for this reaction? How many grams of H_2O will be produced?
  - We can't convert g O_2 *directly* into g H_2, but if we convert g O_2 into moles, we can use the *coefficients of the balanced equation* to obtain moles of H_2, and then convert to g H_2.



Reaction Stoichiometry: An Example

$$2\,H_2\,(g) \;+\; 1\,O_2(g) \;\rightarrow\; 2\,H_2O(g)$$

Convert g O_2 to mol O_2:

$$25.0\,g\,O_2 \times \frac{1\,mol\,O_2}{32.00\,g\,O_2} = 0.781\,mol\,O_2$$

Convert mol O_2 to mol H_2:

coefficient of what we're interested in

$$0.781\,mol\,O_2 \times \frac{2\,mol\,H_2}{1\,mol\,O_2} = 1.56\,mol\,H_2$$

coefficient of what we're canceling out

Convert mol H_2 to g H_2:

$$1.56\,mol\,H_2 \times \frac{2.016\,g\,H_2}{1\,mol\,H_2} = 3.15\,g\,H_2$$

Reaction Stoichiometry: An Example

$$2\ H_2\ (g)\ +\ 1\ O_2(g)\ \rightarrow\ 2\ H_2O(g)$$

Or we can put everything together:

$$25.0\ \text{g}\ O_2 \times \frac{1\ \text{mol}\ O_2}{32.00\ \text{g}\ O_2} \times \frac{2\ \text{mol}\ H_2}{1\ \text{mol}\ O_2} \times \frac{2.016\ \text{g}\ H_2}{1\ \text{mol}\ H_2} = 3.15\ \text{g}\ H_2$$

How many grams of H_2O will be formed?

$$25.0\ \text{g}\ O_2 \times \frac{1\ \text{mol}\ O_2}{32.00\ \text{g}\ O_2} \times \frac{2\ \text{mol}\ H_2O}{1\ \text{mol}\ O_2} \times \frac{18.02\ \text{g}\ H_2O}{1\ \text{mol}\ H_2O} = 28.2\ \text{g}\ H_2O$$

Examples: Reaction Stoichiometry

$$C_3H_8(g) + 5O_2(g) \rightarrow 3CO_2(g) + 4H_2O(g)$$

1a. How many moles of CO_2 can we make from 2.0 moles of C_3H_8?

1b. How many moles of H_2O can we make from 2.0 moles of C_3H_8?

1c. How many moles of O_2 are needed to react with 2.0 moles of C_3H_8?

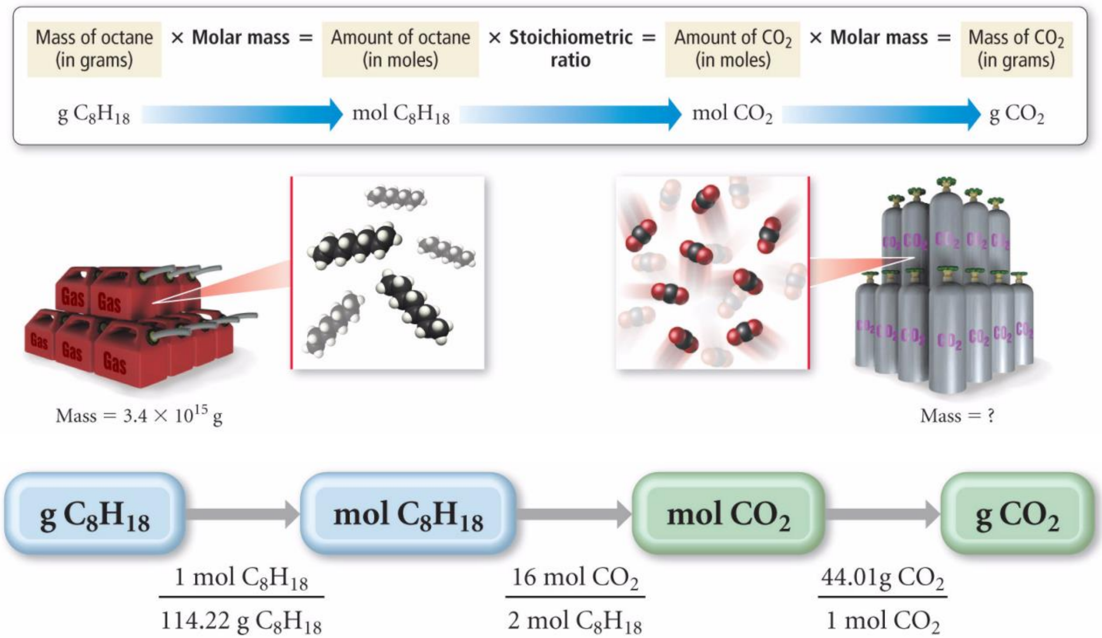
1d. How many moles of CO_2 can be produced from 3.5 mol O_2?

1e. How many grams of CO_2 are produced from 50.0 g of C_3H_8?

Examples: Reaction Stoichiometry

2. In 2004, the world burned 3.0×10^{10} barrels of petroleum, roughly equivalent to 3.4×10^{15} g of gasoline (C_8H_{18}). How much CO_2 is released into the atmosphere from the combustion of this much gasoline?

$$2C_8H_{18}(l) + 25O_2(g) \rightarrow 16CO_2(g) + 18H_2O(g)$$



Answer: 1.0×10^{16} g CO_2

Examples: Reaction Stoichiometry

3. Aqueous sodium hypochlorite (NaOCl), best known as household bleach, is prepared by reaction of sodium hydroxide with chlorine:

$$2NaOH(aq) + Cl_2(g) \rightarrow NaOCl(aq) + NaCl(aq) + H_2O$$

How many grams of NaOH are needed to react with 25.0 g of Cl_2?

Answer: 28.2 g NaOH

Examples: Molecule Stoichiometry

4. How many grams of Cl atoms are needed to combine with 24.4 g of Si atoms to make silicon tetrachloride, $SiCl_4$?

Answer: 123 g Cl

Examples: Reaction Stoichiometry

5. One of the most spectacular reactions of aluminum, the thermite reaction, is with iron(III) oxide, Fe_2O_3, by which metallic iron is made. So much heat is generated that the iron forms in the liquid state. The equation is

$$2Al(s) + Fe_2O_3(s) \rightarrow Al_2O_3(s) + 2Fe(l)$$

A certain welding operation, used over and over, requires that each time at least 86.0 g of Fe be produced. (*a*) What is the minimum mass in grams of Fe_2O_3 that must be used for each operation? (*b*) How many grams of aluminum are also needed?

Answer: (a) 123 g Fe_2O_3; (b) 41.5 g Al

Yields of Chemical Reactions

- In the examples we've seen, we have assumed that all of the reactions "go to completion" — that is, that *all* reactant molecules are converted into product molecules.
- In real life, some product is almost always lost due to:
  - small amounts of contamination in the glassware
  - impurities in the reactants
  - incomplete reactions
  - reactants evaporating into the air
  - *side reactions* that that form other products
  - too much heating
  - too little heating
  - klutzes
  - gremlins
  - evil spirits
  - evil co-workers
  - etc.

Yields of Chemical Reactions

- The **theoretical yield** is the amount that would be obtained if the reaction goes to completion (i.e., the *maximum amount* that could be made).
- The **actual yield** of a reaction is the amount that is actually obtained. (You could've guessed that.)
- The **percent yield** (**% yield**) is the actual yield expressed as a percentage of the theoretical yield:

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

Yields of Chemical Reactions

- Whenever there is a reaction between more than one reactant, we can run out of one reactant before we run out of the other one.
  - The reactant we run out of first, which limits the yield of the entire reaction, is the **limiting reactant** (or **limiting reagent**).
  - The **excess reactant** is any reactant that is present in a larger amount than what is required to react completely with the limiting reactant.

Examples: Percent Yield

6. Methyl *tert*-butyl ether (MTBE, $C_5H_{12}O$), a substance used as an octane booster in gasoline, can be made by reaction of isobutylene (C_4H_8), with methanol (CH_3OH). What is the percent yield of the reaction if 32.8 g of MTBE is obtained from reaction of 26.3 g of isobutylene with sufficient methanol?

$$C_4H_8(g) + CH_3OH(l) \rightarrow C_5H_{12}O(l)$$

Answer: 79.4%

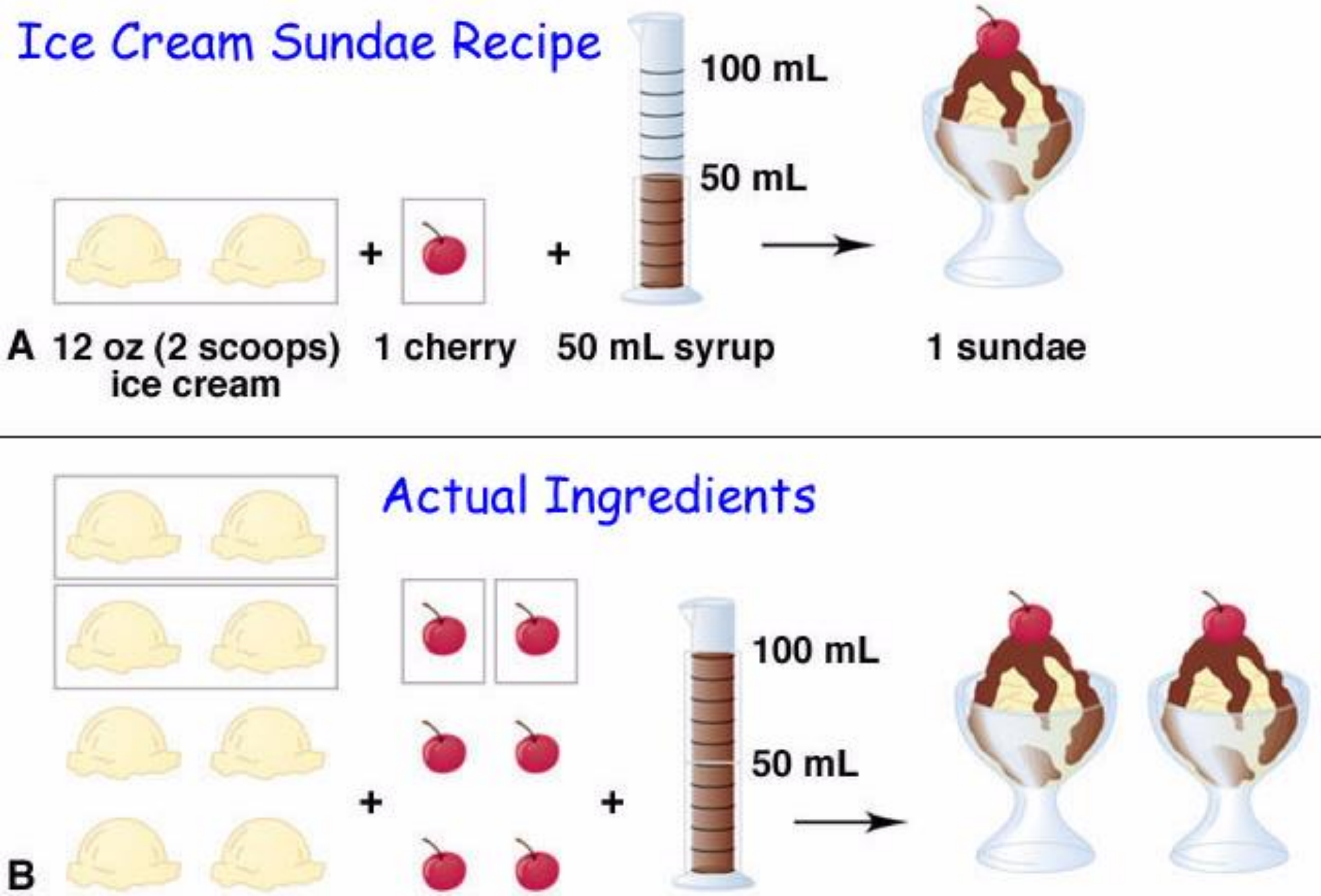
Limiting Reactants

Limiting Reactants

- When we are given a reaction between two or more reactants, one may be completely consumed before the other(s). *The reaction must* ***stop*** *at this point*, leaving us with the remaining reactants *in excess*.
- The amount of this reactant, then, determines the maximum amount of the product(s) that can form, and is known as the **limiting reactant**.
- For example, suppose we were making standard 4-door cars, and we had the following (incomplete) list of "ingredients." How many cars could we make?

4 engines	4 drivers' seats
4 steering wheels	4 rear-view mirrors
15 doors	8 windshield wipers
8 headlights	11 wheels

Limiting Reactants and Sundaes



Limiting Reactants and Pizza

Pizza recipe:

1 crust + 5 oz. tomato sauce + 2 cups cheese → 1 pizza

If we have 4 crusts, 10 cups of cheese, and 15 oz. of tomato sauce, how many pizzas can we make?

$$4\ \text{crusts} \times \frac{1\ \text{pizza}}{1\ \text{crust}} = 4\ \text{pizzas}$$

$$10\ \text{cups cheese} \times \frac{1\ \text{pizza}}{2\ \text{cups cheese}} = 5\ \text{pizzas}$$

$$15\ \text{ounces tomato sauce} \times \frac{1\ \text{pizza}}{5\ \text{ounces tomato sauce}} = 3\ \text{pizzas}$$

Tomato sauce is the **limiting reagent**, and the **theoretical yield** is 3 pizzas.

Limiting Reactants

$$N_2(g) + 3H_2(g) \rightarrow 2NH_3(g) \quad \text{[Haber process]}$$

- Suppose we mix 1.00 mol of N_2 and 5.00 mol of H_2. What is the maximum amount of NH_3 that can be produced? How much H_2 will be left over?
- Now suppose we mix 2.15 mol of N_2 and 6.15 mol of H_2. What is the theoretical yield of NH_3?

Assuming the N_2 reacts completely, how much NH_3 can be made?

$$2.15\,\text{mol N}_2 \times \frac{2\,\text{mol NH}_3}{1\,\text{mol N}_2} = 4.30\,\text{mol NH}_3$$

Assuming the H_2 reacts completely, how much NH_3 can be made?

$$6.15\,\text{mol H}_2 \times \frac{2\,\text{mol NH}_3}{3\,\text{mol H}_2} = 4.10\,\text{mol NH}_3$$

H_2 is the limiting reactant; the theoretical yield of NH_3 is 4.10 mol

Examples: Limiting Reactants

1. Butane, C_4H_{10}, undergoes combustion with oxygen, O_2, to form carbon dioxide and water:

$$\mathbf{2C_4H_{10}(g) + 13O_2(g) \rightarrow 8CO_2(g) + 10H_2O(g)}$$

58.12 g/mol *32.00 g/mol* *44.01 g/mol* *18.02 g/mol*

If 100. g of C_4H_{10} and 100. g of O_2 are mixed,

a. Which of the two reactants is the limiting reagent, and how many grams of CO_2 will be formed?

b. How many grams of H_2O will be formed?

c. How many grams of excess reagent are left over?

d. If the actual yield of CO_2 had been 75.0 g, what would be the percent yield of the reaction?

Answer: (a) O_2 limiting; 84.6 g CO_2; (b) 43.3 g H_2O; (c) 72 g C_4H_{10}; (d) 88.6%

Examples: Limiting Reactants

2. Ammonia, NH_3, can be synthesized by the following reaction:

$$2NO(g) + 5H_2(g) \rightarrow 2NH_3(g) + 2H_2O(g)$$

Starting with 86.3 g NO and 25.6 g H_2, find the theoretical yield of ammonia in grams.

Answer: NO limiting; 49.0 g NH_3

Examples: Limiting Reactants

3. In a synthesis of phosphorus trichloride, a chemist mixed 12.0 g P with 35.0 g Cl_2; she obtained 42.4 g of PCl_3. What is the % yield of PCl_3?

$$2P(s) + 3Cl_2(g) \rightarrow 2PCl_3(l)$$

Answer: 93.8%

Percent Composition and Empirical Formulas

Percent Composition and Mass Percentage

- The **percent composition** of a compound is a list of the elements present in a substance listed by *mass percent*. Knowing the percent composition is often a first step to determining the formula of an unknown compound.
- The **mass percentage** (**mass %**) of an element in the compound is the portion of the compound's mass contributed by that element, expressed as a percentage:

$$\text{Mass \% of element X} = \frac{\text{atoms of X in formula} \times \text{molar mass of X}}{\text{molar mass of compound}} \times 100$$

Percent Composition and Mass Percentage

- What is the mass percentage of Cl in the chlorofluorocarbon CCl_2F_2 (Freon-12)?

$$\text{Mass \% of Cl} = \frac{2 \times \text{atomic mass of Cl}}{\text{molar mass of } CCl_2F_2} \times 100$$

$$= \frac{2 \times 35.453 \text{ g/mol}}{120.91 \text{ g/mol}} \times 100$$

$$= 58.64\%$$

Examples: Mass Percentage

1. Glucose, or blood sugar, has the molecular formula $C_6H_{12}O_6$.

a. What is the percent composition of glucose?

b. How many grams of carbon are in 39.0 g of glucose (the amount of sugar in a typical soft drink)?

Answer: a) 40.00% C, 6.714% H, 53.29% O
b) 15.6 g C

Examples: Mass Percentage

2. The U.S. Food and Drug Administration (FDA) recommends that you consume less than 2.4 g of sodium per day. What mass of sodium chloride in grams can you consume and still be within the FDA guidelines?

Answer: 6.1 g NaCl

Empirical Formula from Mass Percentage

- We can use the percent composition of a substance to find its *empirical* and *molecular formula*.
- If by some process we determine the percent composition of an unknown compound, we can convert this into a gram ratio by assuming that we have 100 g of the compound, and then to a mole ratio by using the atomic weights:

Sample: 84.1% C, 15.9% H

Assume 100 g of sample:

$$84.1\,\mathrm{g\,C} \times \frac{1\,\mathrm{mol\,C}}{12.01115\,\mathrm{g\,C}} = 7.00\,\mathrm{mol\,C}$$

$$15.9\,\mathrm{g\,H} \times \frac{1\,\mathrm{mol\,H}}{1.00797\,\mathrm{g\,H}} = 15.8\,\mathrm{mol\,H}$$

Empirical Formula from Mass Percentage

- Since atoms combine in the same ratio that moles do, we divide all of the numbers of moles by the smallest number to put everything into lowest terms:

$$C_{7.00}H_{15.8} \xrightarrow{\text{divide by smallest number}} C_{\frac{7.00}{7.00}}H_{\frac{15.8}{7.00}} \rightarrow C_{1.00}H_{2.26}$$

- If the mole ratio is not all whole numbers, we multiply through by the smallest integer which will turn all of the numbers into integers. These numbers are the subscripts of the elements in the **empirical formula**.

$$\left(C_{1.00}H_{2.26}\right)_4 \rightarrow C_{4.00}H_{9.04} \rightarrow C_4H_9 \ \text{(empirical formula)}$$

Molecular Formula from Empirical Formula

- If we know the molar mass of the compound, we can obtain the **molecular formula** by dividing the weight of the empirical formula into the molar mass; this will determine the number of empirical formula units in the molecule.

Suppose the molar mass of the substance is found to be 228.48 g/mol. What is its molecular formula?

$$\frac{\text{molecular weight}}{\text{empirical formula weight}} \rightarrow \frac{228.48\ \text{g/mol}}{57.12\ \text{g/mol}} = 4.000$$

$$\left(C_4H_9\right)_4 \rightarrow C_{16}H_{36}\ \text{(molecular formula)}$$

Examples: Empirical & Molecular Formulas

3. Vitamin C (ascorbic acid) contains 40.92% C, 4.58% H, and 54.50% O by mass. What is the empirical formula of ascorbic acid?

Answer: $C_3H_4O_3$

Examples: Empirical & Molecular Formulas

4. Black iron oxide is an ore containing iron and oxygen that occurs in magnetite. A 2.4480 g sample of the ore is found to contain 1.7714 g of iron. Calculate the empirical formula of black iron oxide.

Answer: Fe_3O_4

Examples: Empirical & Molecular Formulas

5. Styrofoam is a polymer made from the monomer styrene. Elemental analysis of styrene shows its percent composition to be 92.26 % C and 7.75% H. Its molecular mass is found to be 104.15 g/mol. What are the empirical and molecular formulas of styrene?

Answer: empirical = CH, molecular = C_8H_8

Examples: Empirical & Molecular Formulas

6. Butanedione is a main component in the smell and taste of butter and cheese. The empirical formula of butanedione is C_2H_3O and its molar mass is 86.09 g/mol. What is its molecular formula?

Answer: $\mathbf{C_4H_6O_2}$

Elemental / Combustion Analysis

- One common way of obtaining a chemical formula is by performing a **combustion analysis** (a specific type of *elemental analysis*).
- In this technique, an unknown sample is burned in pure O_2 (a combustion reaction), which converts all of the carbon atoms in the sample into CO_2 and all of the hydrogen atoms into H_2O.

$$C, H, O + O_2 \rightarrow CO_2 + H_2O$$

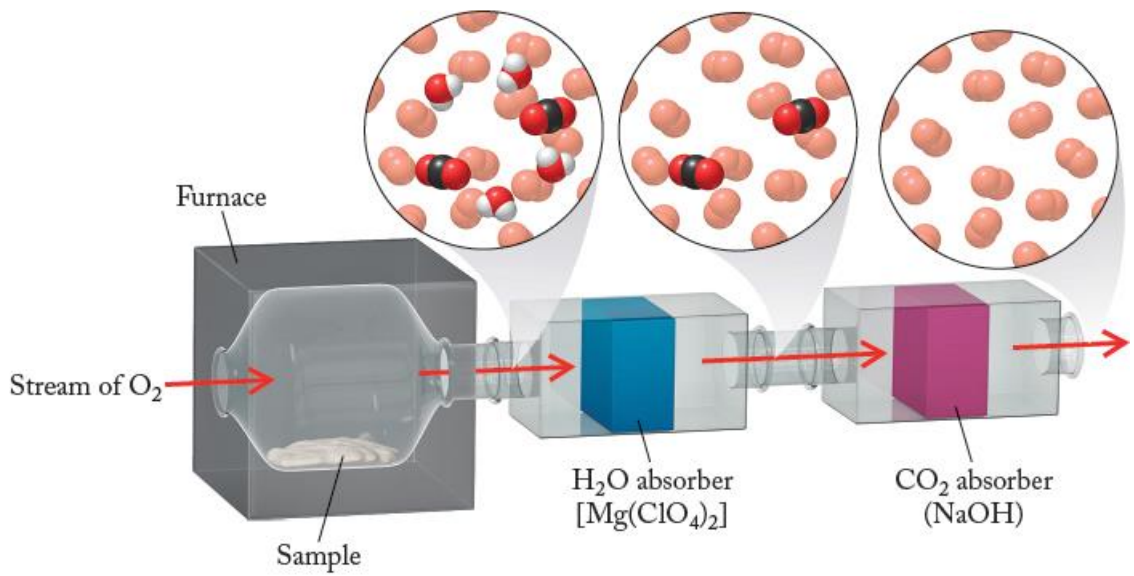


Figure 3.33

Elemental / Combustion Analysis

- The masses of CO_2 and H_2O are measured after the process is complete, and from this data, the amount of carbon and hydrogen in the original sample can be determined.
- Elements besides C and H must be determined by other methods; O is usually found by difference.

$$\text{g } CO_2 \rightarrow \text{mol } CO_2 \rightarrow \text{mol C} \rightarrow \text{g C in sample} \rightarrow \text{\% C}$$

$$\text{g } H_2O \rightarrow \text{mol } H_2O \rightarrow \text{mol H} \rightarrow \text{g H in sample} \rightarrow \text{\% H}$$

$$\text{\% O} = 100\% - (\text{\% C} + \text{\% H})$$

Examples: Combustion Analysis

7. A sample of an unknown compound with a mass of 0.5438 g is burned in a combustion analysis. The mass of CO_2 produced was 1.039 g and the mass of H_2O was 0.6369 g. What is the empirical formula of the compound?

Answer: C_2H_6O

Molecules and Isomers

- Even knowing the empirical or molecular formulas of a compound does not necessarily tell us what that compound actually *is*.
- We've already seen that the empirical formula only tells us about the *relative* numbers of atoms present within the formula unit or molecule.
- Many different compounds can have the same empirical formula. For instance, there are dozens of different compounds that have the empirical formula CH_2O.
  - Notice that in on the following slide, there is no relationship between the structure and how many 'CH_2O' units the molecule contains.

Some Compounds with Empirical Formula CH_2O

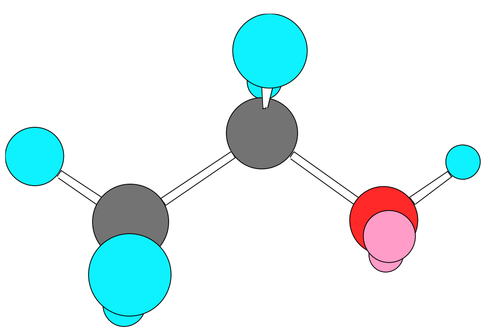
- Composition by mass 40.0% C, 6.71% H, 53.3% O

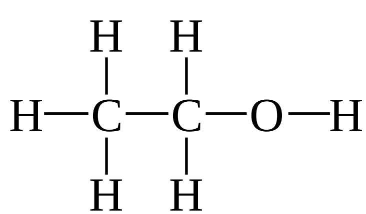
Name	Molecular Formula	No. of 'CH_2O' Units	Molar Mass (g/mol)	Function
Formaldehyde	CH_2O	1	30.03	Disinfectant; biological preservative
Acetic acid	$C_2H_4O_2$	2	60.05	Vinegar (5% solution); acetate polymers
Lactic acid	$C_3H_6O_3$	3	90.08	Found in sour milk and sourdough bread; forms in muscles during exercise
Erythrose	$C_4H_8O_4$	4	120.10	Forms during sugar metabolism
Ribose	$C_5H_{10}O_5$	5	150.13	Component of ribonucleic acid (RNA); found in vitamin B_2
Glucose	$C_6H_{12}O_6$	6	180.16	Major nutrient for energy in cells

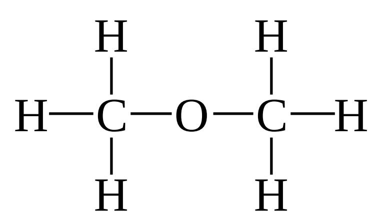
Structural Isomers

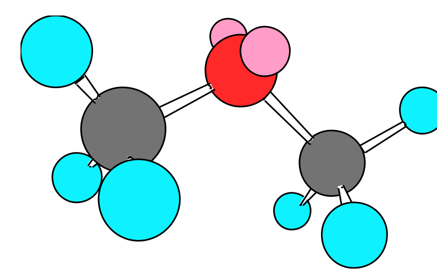
- Even compounds that have the *same* molecular formula can have the atoms connected in a *different order* — these are **structural isomers**.

	Ethanol	Dimethyl ether
Molecular Formula	C_2H_6O	C_2H_6O
Molar Mass (g/mol)	46.07	46.07
Appearance	Colorless liquid	Colorless gas
Melting point	-117°C	-139°C
Boiling point	78.5°C	-25°C
Density (at 20°C)	0.789 g/mL	0.00195 g/mL
Function	Intoxicant	Refrigerant









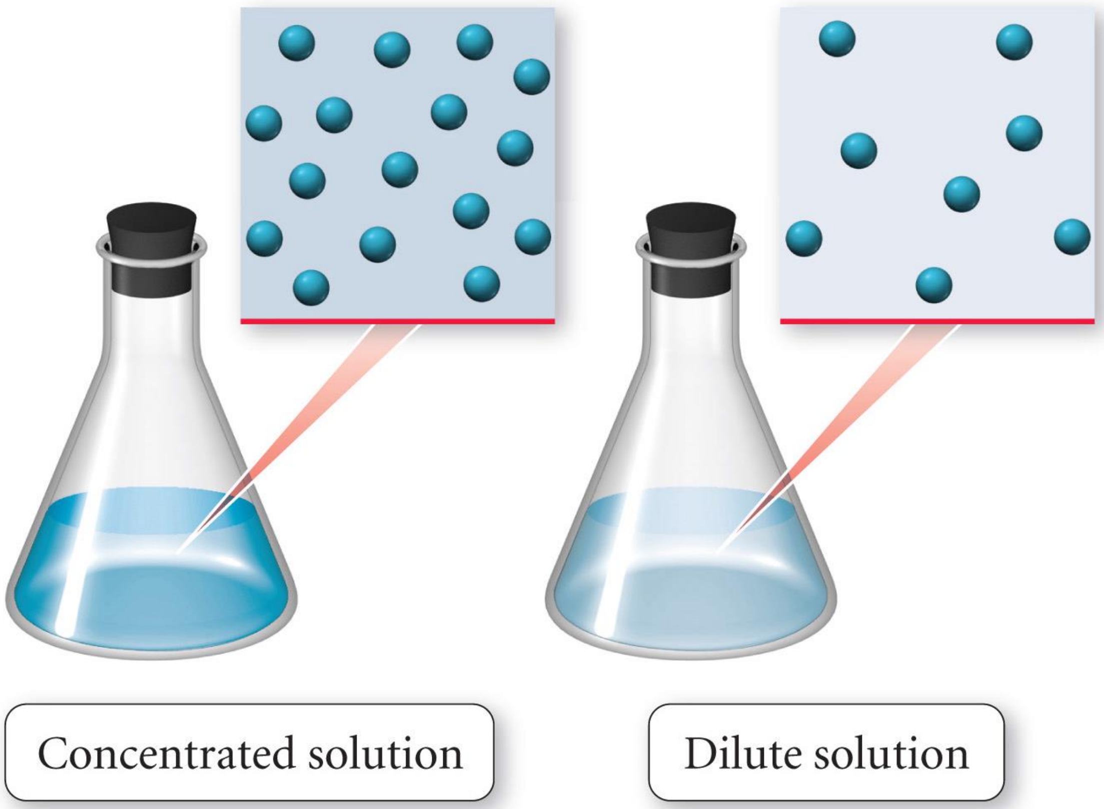
Solution Stoichiometry

Solutions

- For a chemical reaction to occur, the reacting species have to come in close contact with each other. Most chemical reactions are performed in a *solution* (or in the gas phase) rather than in the solid state.
- A **solution** consists of a smaller amount of one substance, the **solute** (usually a liquid or solid), dissolved in a larger amount of another substance, the **solvent** (usually a liquid).
  - Other kinds of solutions, such as of two or more solids (e.g., metal alloys), or gases dissolved in solids, or gases dissolved in other gases (e.g., the atmosphere), are also possible.
- Solutions in which water is the solvent are known as **aqueous solutions**.

Dilute and Concentrated Solutions

- A solution that contains a small amount of solute relative to the solvent is a **dilute solution**.
- A solution that contains a large amount of solute relative to the solvent is a **concentrated solution**.

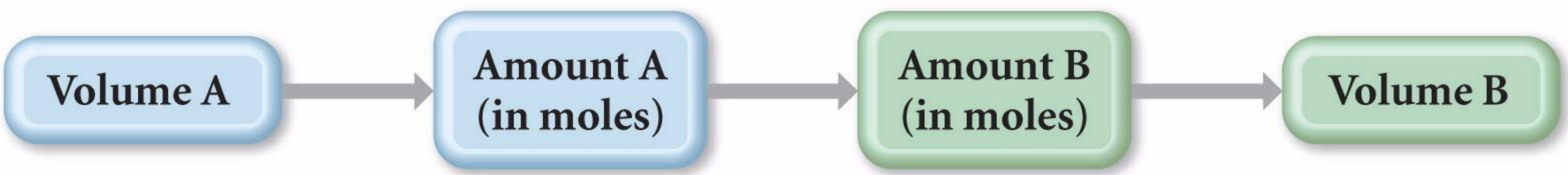


Solution Concentration — Molarity

- We must know the amount of material present in a certain volume of solution — the **concentration** — in order to perform measurements and calculations.
- A common unit of concentration is **molarity** (*M*), defined as the number of *moles of solute* per *liter of solution* (that's solution, <u>not</u> solvent!):

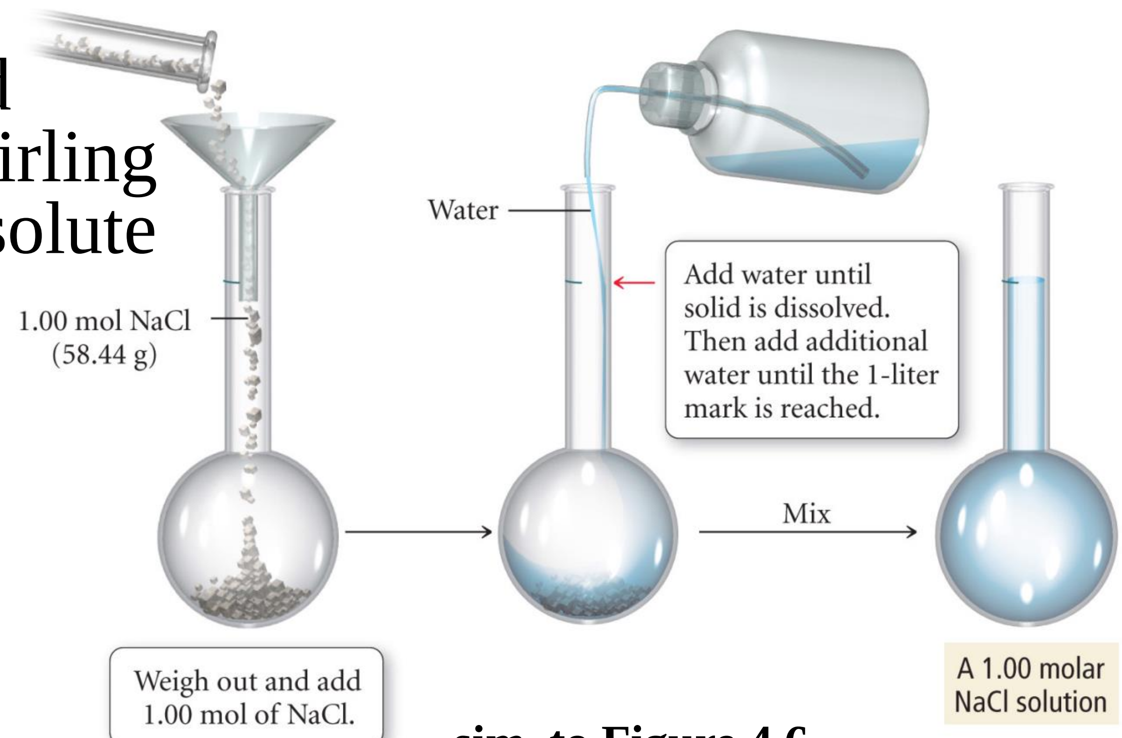
$$\text{Molarity } (M) = \frac{\text{moles of solute}}{\text{liters of solution}} = \text{mol / L} = \text{mol L}^{-1}$$

- The molarity of a solution can be used as a conversion factor to relate the solution volume to the number of moles of solute present.



Making Solutions of a Desired Molarity

- Because the volume of a solution comes from the solute *and the* solvent, a 1 molar solution cannot be made by adding one mole of solute to 1 L of solvent.
- Solutions of a desired molarity are usually prepared by placing the appropriate amount of solute in a *volumetric flask*, and adding solvent until a calibrated final volume is reached (with frequent swirling to make sure the solute dissolves).



sim. to Figure 4.6

Other Concentration Units

- **Mass percentage** — ratio of the solute's mass to the mass of the solution:

$$\text{mass percentage} = \frac{\text{mass of solute}}{\text{mass of solution}} \times 100\%$$

  - also known as *percent mass*, *percent weight*, *weight/weight percent*; abbreviated as (w/w)%

- **Volume percentage** — ratio of the solute's volume to the volume of the solution:

$$\text{volume percentage} = \frac{\text{volume of solute}}{\text{volume of solution}} \times 100\%$$

  - commonly used when one liquid is dissolved in another; abbreviated as %vol or (v/v)%

- **Mass-volume percentage** — sometimes used when a solid is dissolved in a liquid (e.g., 0.9 (m/v)% saline is 0.9 g of NaCl per 100 mL of solution).

Other Concentration Units

- Small concentrations may be expressed as **parts per million** (**ppm**) or **parts per billion** (**ppb**):

$$\text{ppm} = \frac{\text{mass of solute}}{\text{mass of solution}} \times 10^6$$

$$\text{ppb} = \frac{\text{mass of solute}}{\text{mass of solution}} \times 10^9$$

  – a solution of 1 ppm is equivalent to a mass of 1 mg of solute in 1 kg of solution

Solution Dilution

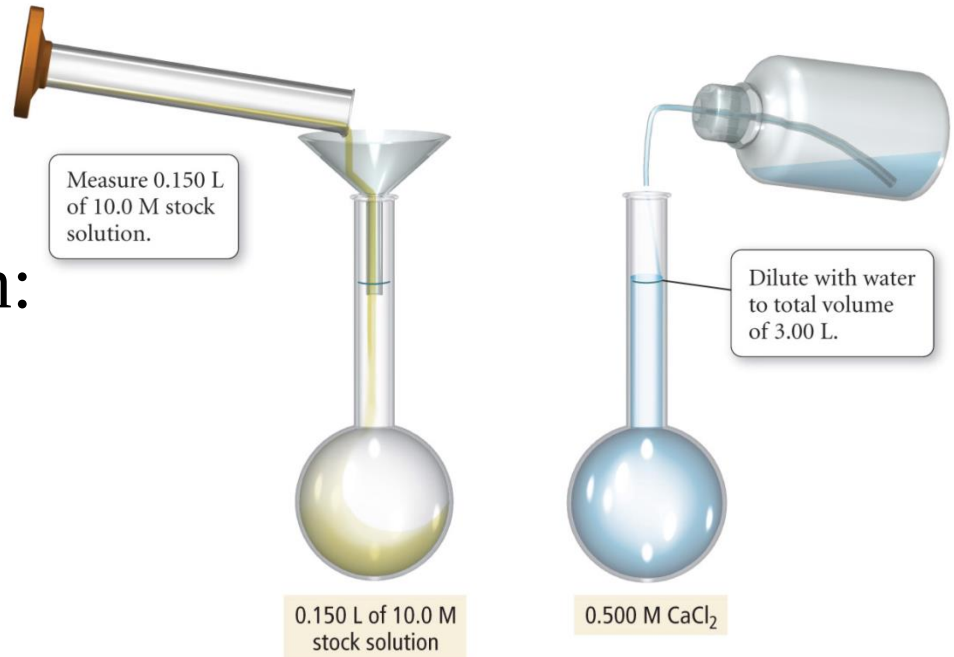
- Solutions can also be prepared by **diluting** a more concentrated stock solution.

Concentrated solution + Solvent → Dilute solution

- The initial molarity (M_1) and volume (V_1) of a concentrated solution are related to the final molarity (M_2) and volume (V_2) of a dilute solution by the equation:

$$M_1 V_1 = M_2 V_2$$

Note that the units for volume and concentration don't actually matter in this equation.



$$M_1V_1 = M_2V_2$$

$$\frac{10.0\text{ mol}}{\cancel{L}} \times 0.150\,\cancel{L} = \frac{0.500\text{ mol}}{\cancel{L}} \times 3.00\,\cancel{L}$$

$$1.50\text{ mol} = 1.50\text{ mol}$$

Examples: Molarity

1. What is the molarity of a solution made by dissolving 2.355 g of sulfuric acid in water and diluting to a final volume of 50.00 mL?

Answer: 0.4802 M H_2SO_4

Examples: Molarity

2. How many grams of solute are in 1.75 L of 0.460 M sodium monohydrogen phosphate?

Answer: 114 g

Examples: Molarity

3. How many liters of a 0.125 M NaOH solution contains 0.255 mol of NaOH?

Answer: 2.04 L soln.

Examples: Solution by Dilution

4. Isotonic saline is a 0.150 M aqueous solution of NaCl that simulates the total concentration of ions found in many cellular fluids. Its uses range from a cleansing rinse for contact lenses to a washing medium for red blood cells. How would you prepare 800. mL of isotonic saline from a 6.00 M stock solution?

Answer: Dilute **20.0 mL** of stock solution to 800. mL

Examples: Solution by Dilution

5. To what volume should you dilute 0.200 L of a 15.0 M NaOH solution to obtain a 3.00 M NaOH solution?

Answer: 1.00 L

Examples: Stoichiometry of Reactions in Soln

6. Stomach acid, a dilute solution of HCl in water, can be neutralized by reaction with sodium bicarbonate according to the equation

$$HCl(aq) + NaHCO_3(aq) \rightarrow NaCl(aq) + H_2O(l) + CO_2(g)$$

How many mL of 0.125 M $NaHCO_3$ solution are needed to neutralize 18.0 mL of 0.100 M HCl?

Answer: 14.4 mL

Examples: Stoichiometry of Reactions in Soln

7. The reaction of acid rain with limestone/marble (calcium carbonate) can be represented by the equation

$$2HCl(aq) + CaCO_3(aq) \rightarrow CaCl_2(aq) + H_2O(l) + CO_2(g)$$

How many mL of concentrated hydrochloric acid (12.0 M) would it take to dissolve 5.00 g of calcium carbonate?

Answer: 8.33 mL

Examples: Stoichiometry of Reactions in Soln

8. A 0.4550-g solid mixture containing $MgSO_4$ is dissolved in water and treated with an excess of $Ba(NO_3)_2$, resulting in the precipitation of 0.6168 g of $BaSO_4$.

$$MgSO_4(aq) + Ba(NO_3)_2(aq) \longrightarrow BaSO_4(s) + Mg(NO_3)_2(aq)$$

What is the concentration of $MgSO_4$ in the mixture, expressed as a mass percentage?

[This is an example of **gravimetric analysis**, in which a sample mixture is treated in a way that causes a change in the physical state of the analyte, which allows it to be separated from the other components of the sample. The concentration of the analyte is determined from a careful measurement of its mass, and the stoichiometry of the compounds involved.

Answer: 69.91%

The End