CHEM 103
CHEMISTRY I

CHAPTER 3
CHEMICAL REACTIONS AND REACTION STOICHIOMETRY

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Stoichiometry

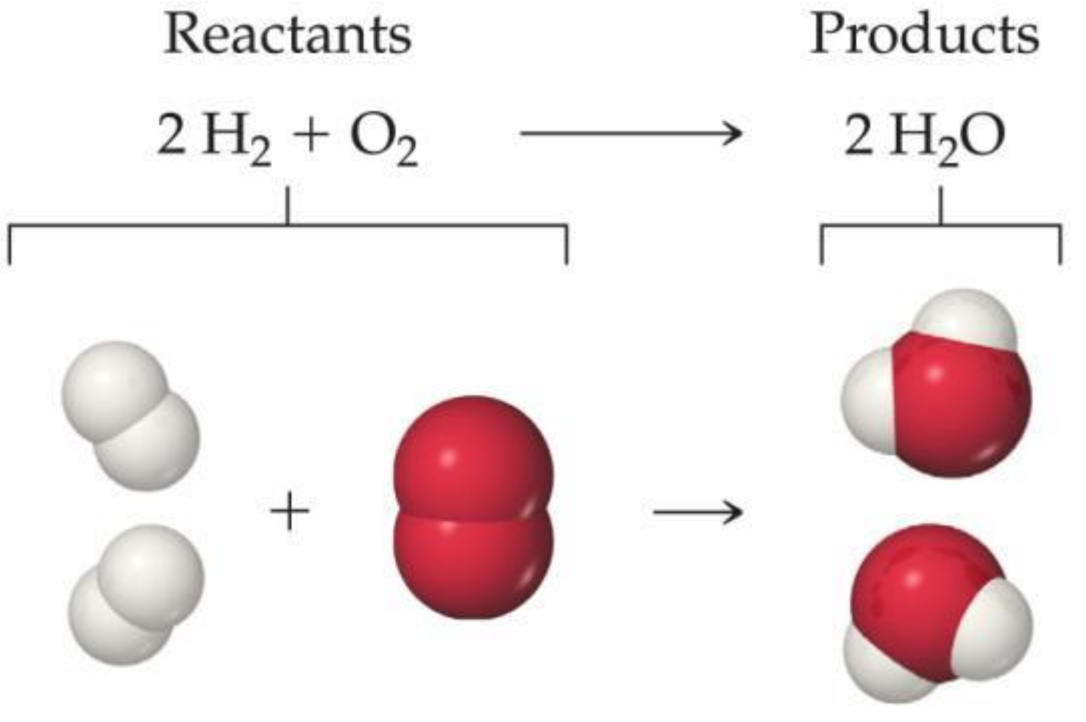
- The study of the mass relationships in chemistry
- Based on the Law of Conservation of Mass (Antoine Lavoisier, 1789)

"We may lay it down as an incontestable axiom that, in all the operations of art and nature, nothing is created; an equal amount of matter exists both before and after the experiment. Upon this principle, the whole art of performing chemical experiments depends."

—Antoine Lavoisier

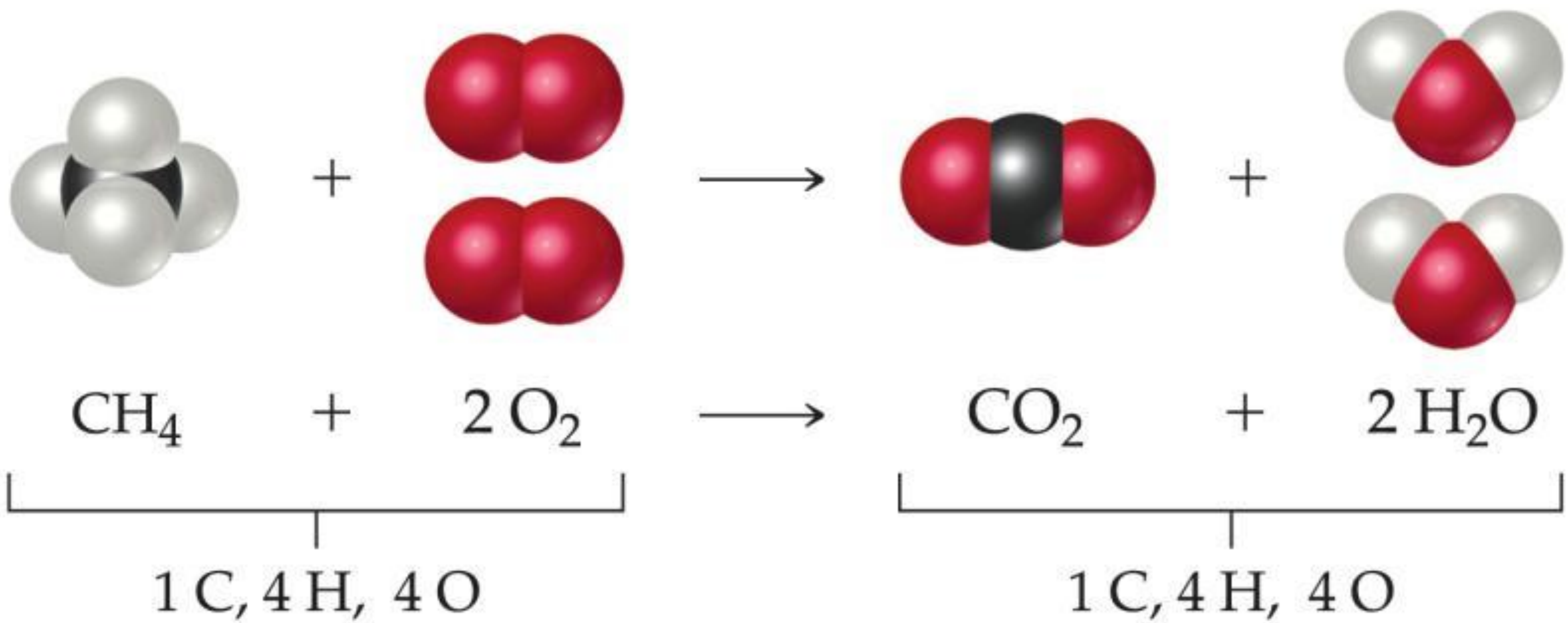
Chemical Equations

Chemical equations are concise representations of chemical reactions.



What Is in a Chemical Equation?

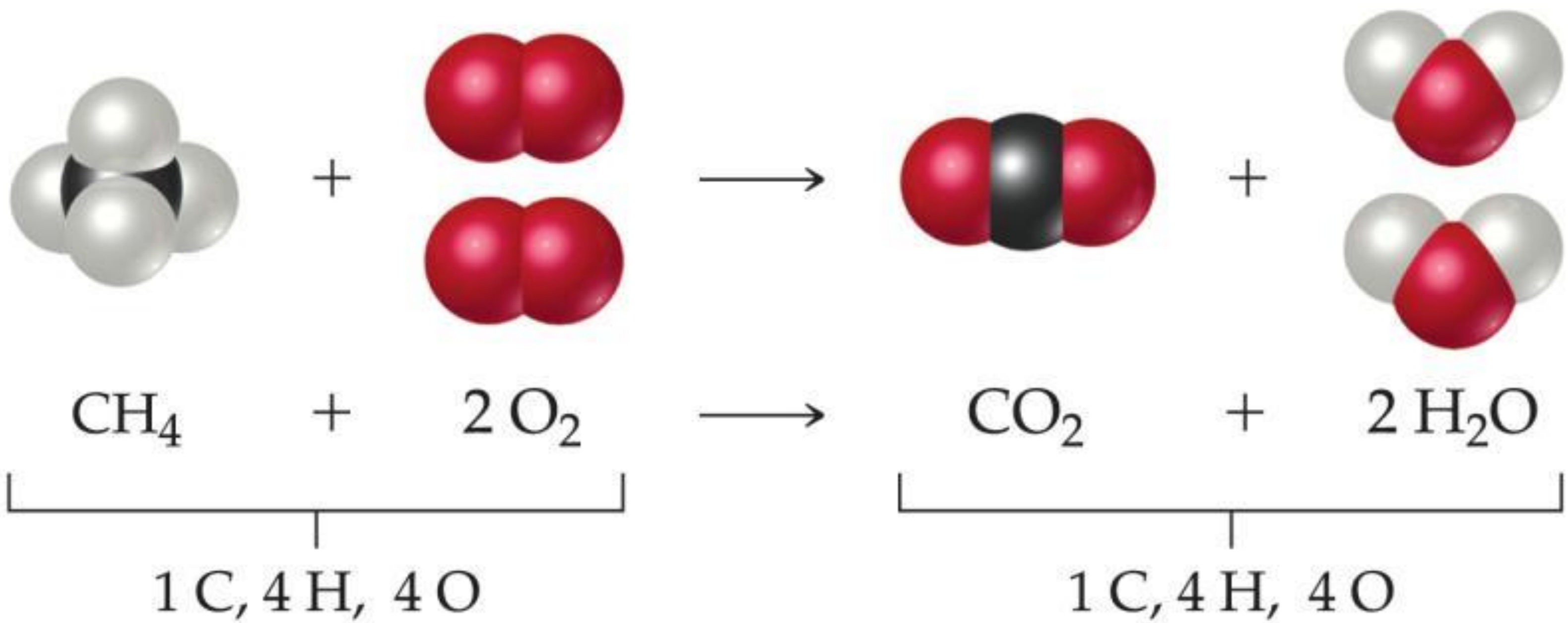
$$CH_4(g) + 2O_2(g) \longrightarrow CO_2(g) + 2H_2O(g)$$



Reactants appear on the left side of the equation.

What Is in a Chemical Equation?

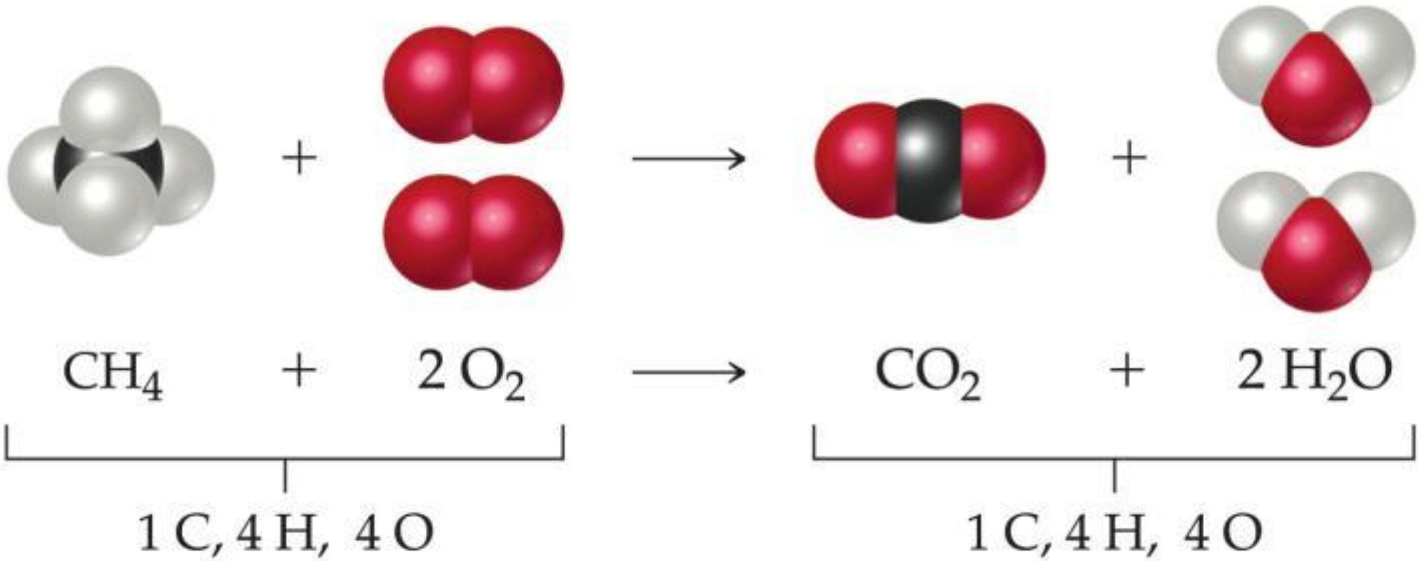
$$CH_4(g) + 2O_2(g) \longrightarrow CO_2(g) + 2H_2O(g)$$



Products appear on the right side of the equation.

What Is in a Chemical Equation?

$$CH_4(g) + 2O_2(g) \longrightarrow CO_2(g) + 2H_2O(g)$$



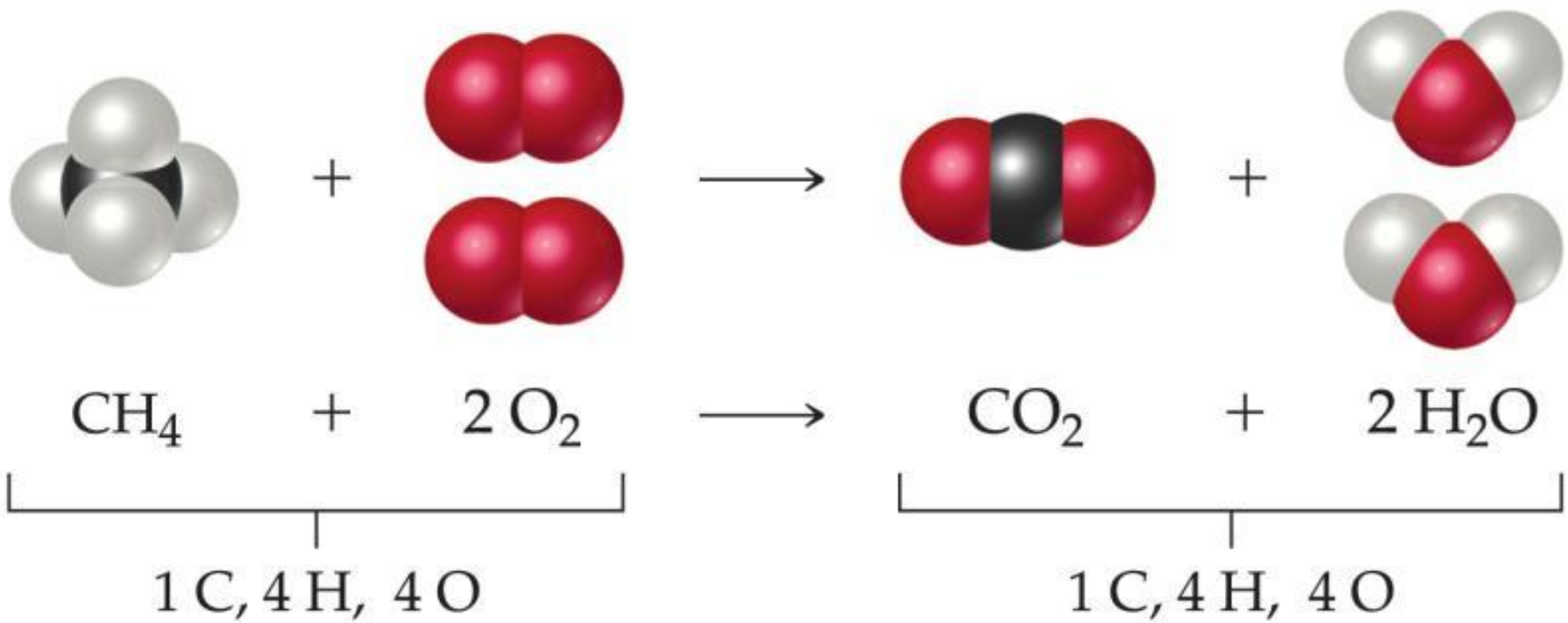
The **states** of the reactants and products are written in parentheses to the right of each compound.

(*g*) = gas; (*l*) = liquid; (*s*) = solid;

(*aq*) = in aqueous solution

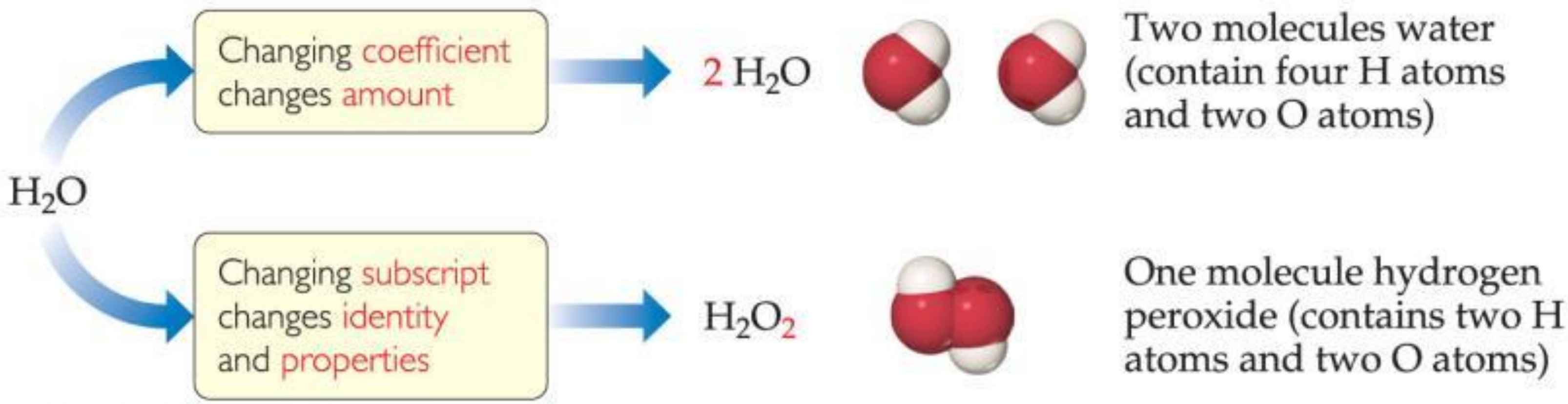
What Is in a Chemical Equation?

$$CH_4(g) + 2O_2(g) \longrightarrow CO_2(g) + 2H_2O(g)$$



Coefficients are inserted to balance the equation to follow the law of conservation of mass.

Why Do We Add Coefficients Instead of Changing Subscripts to Balance?



- Hydrogen and oxygen can make water OR hydrogen peroxide:

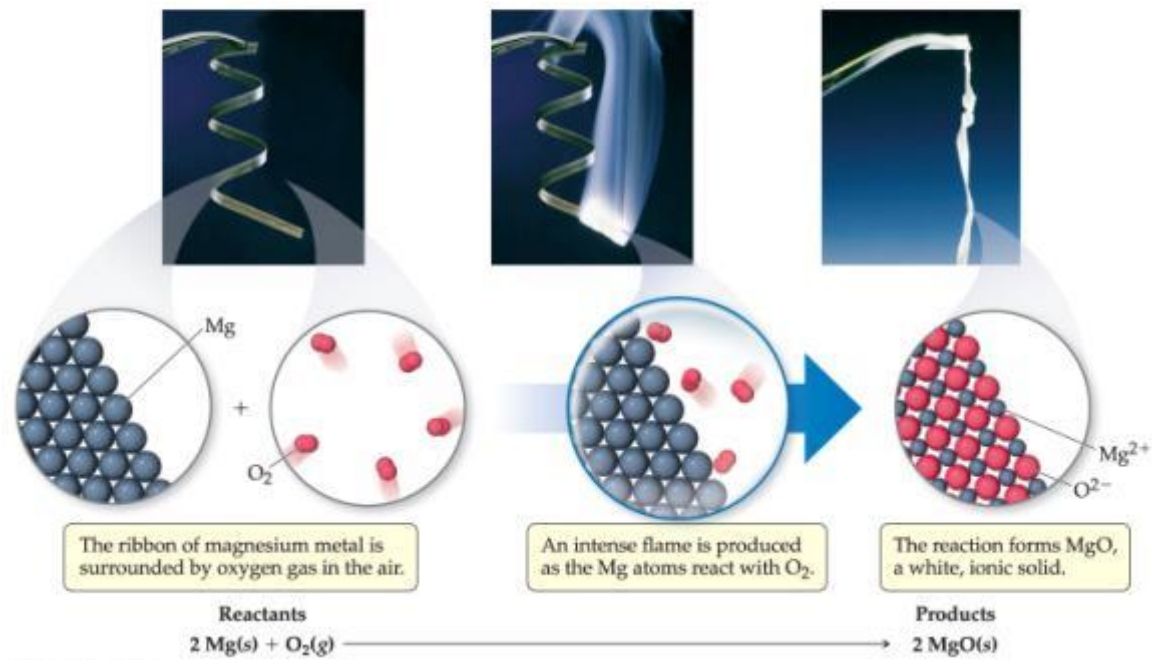
➢ $2\ H_2(g) + O_2(g) \rightarrow 2\ H_2O(l)$

➢ $H_2(g) + O_2(g) \rightarrow H_2O_2(l)$

Three Types of Reactions

- Combination reactions
- Decomposition reactions
- Combustion reactions

Combination Reactions



In **combination reactions** two or more substances react to form one product.

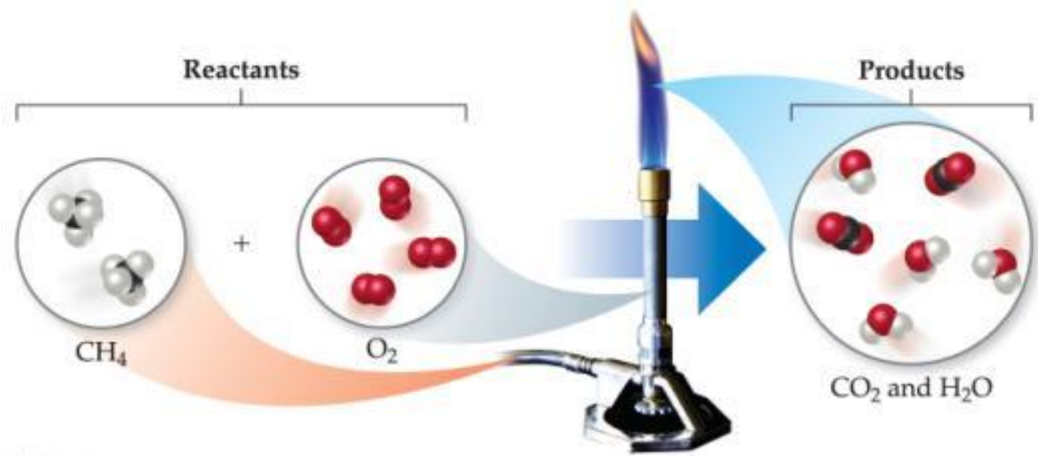
- Examples:
  - $2\,Mg(s) + O_2(g) \longrightarrow 2\,MgO(s)$
  - $N_2(g) + 3\,H_2(g) \longrightarrow 2\,NH_3(g)$
  - $C_3H_6(g) + Br_2(l) \longrightarrow C_3H_6Br_2(l)$

Decomposition Reactions

In a **decomposition reaction** one substance breaks down into two or more substances.

- Examples:
  - $CaCO_3(s) \longrightarrow CaO(s) + CO_2(g)$
  - $2\ KClO_3(s) \longrightarrow 2\ KCl(s) + O_2(g)$
  - $2\ NaN_3(s) \longrightarrow 2\ Na(s) + 3\ N_2(g)$

Combustion Reactions



- **Combustion reactions** are generally rapid reactions that produce a flame.
- **Combustion reactions** most often involve oxygen in the air as a reactant.

- Examples:
  - $CH_4(g) + 2\ O_2(g) \longrightarrow CO_2(g) + 2\ H_2O(g)$
  - $C_3H_8(g) + 5\ O_2(g) \longrightarrow 3\ CO_2(g) + 4\ H_2O(g)$

Formula Weight (FW)

- A **formula weight** is the sum of the atomic weights for the atoms in a chemical formula.
- This is the quantitative significance of a formula.
- The formula weight of calcium chloride, $CaCl_2$, would be

$$\begin{array}{r} \text{Ca: } 1(40.08 \text{ amu}) \\ \underline{+ \text{ Cl: } 2(35.453 \text{ amu})} \\ 110.99 \text{ amu} \end{array}$$

Molecular Weight (MW)

- A **molecular weight** is the sum of the atomic weights of the atoms in a molecule.
- For the molecule ethane, C_2H_6, the molecular weight would be

$$\begin{array}{rl} \text{C:} & 2(12.011\ \text{amu}) \\ +\ \text{H:} & 6(1.00794\ \text{amu}) \\ \hline & 30.070\ \text{amu} \end{array}$$

Ionic Compounds and Formulas

- Remember, ionic compounds exist with a three-dimensional order of ions. There is no simple group of atoms to call a molecule.
- As such, ionic compounds use empirical formulas and formula weights (not molecular weights).

Percent Composition

One can find the percentage of the mass of a compound that comes from each of the elements in the compound by using this equation:

$$\% \text{ Element} = \frac{(\text{number of atoms})(\text{atomic weight})}{(\text{FW of the compound})} \times 100$$

Percent Composition

So the percentage of carbon in ethane is

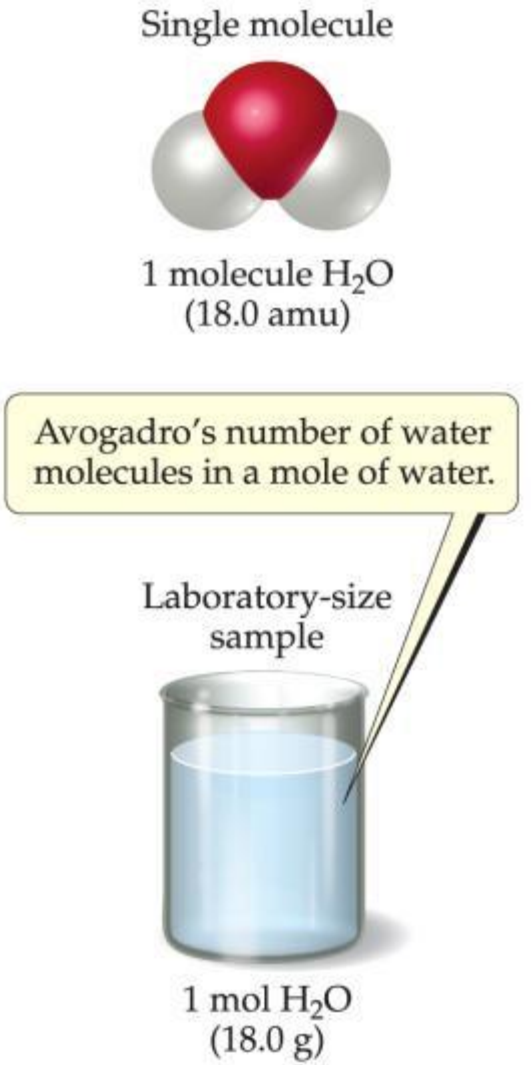
$$\%C = \frac{(2)(12.011\text{ amu})}{(30.070\text{ amu})}$$

$$= \frac{24.022\text{ amu}}{30.070\text{ amu}} \times 100$$

$$= 79.887\%$$

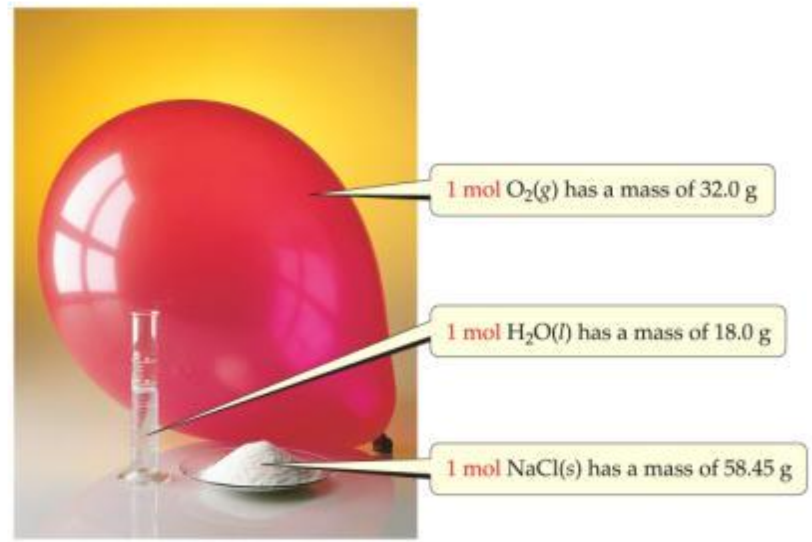
Avogadro's Number

- In a lab, we cannot work with individual molecules. They are too small.
- 6.02×10^{23} atoms or molecules is an amount that brings us to lab size. It is ONE MOLE.
- One mole of ^{12}C has a mass of 12.000 g.



Molar Mass

- A **molar mass** is the mass of 1 mol of a substance (i.e., g/mol).
- The molar mass of an element is the atomic weight for the element from the periodic table. If it is diatomic, it is twice that atomic weight.
- The formula weight (in amu's) will be the same number as the molar mass (in g/mol).



Using Moles

Moles provide a bridge from the molecular scale to the real-world scale.

Mole Relationships

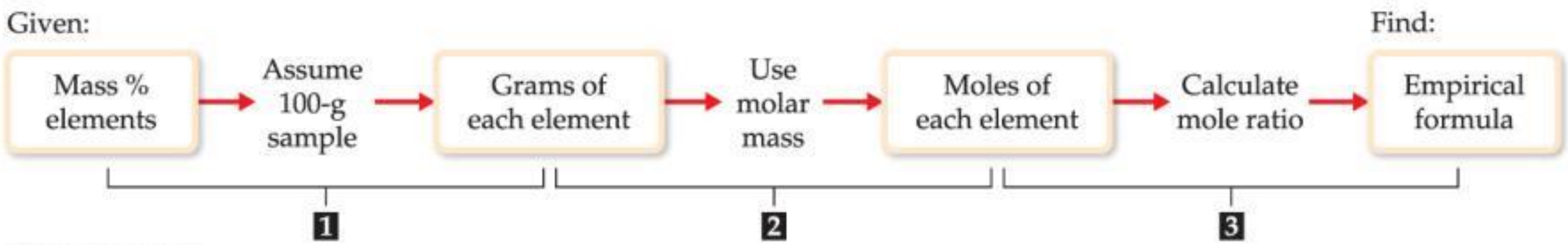
Table 3.2 Mole Relationships

Name of Substance	Formula	Formula Weight (amu)	Molar Mass (g/mol)	Number and Kind of Particles in One Mole
Atomic nitrogen	N	14.0	14.0	6.02×10^{23} N atoms
Molecular nitrogen	N_2	28.0	28.0	$\begin{cases} 6.02 \times 10^{23}\ N_2 \text{ molecules} \\ 2(6.02 \times 10^{23})\ N \text{ atoms} \end{cases}$
Silver	Ag	107.9	107.9	6.02×10^{23} Ag atoms
Silver ions	Ag^+	107.9[a]	107.9	$6.02 \times 10^{23}\ Ag^+$ ions
Barium chloride	$BaCl_2$	208.2	208.2	$\begin{cases} 6.02 \times 10^{23}\ BaCl_2 \text{ formula units} \\ 6.02 \times 10^{23}\ Ba^{2+} \text{ ions} \\ 2(6.02 \times 10^{23})\ Cl^- \text{ ions} \end{cases}$

[a]Recall that the mass of an electron is more than 1800 times smaller than the masses of the proton and the neutron; thus, ions and atoms have essentially the same mass.

- One mole of atoms, ions, or molecules contains Avogadro's number of those particles.
- One mole of molecules or formula units contains Avogadro's number times the number of atoms or ions of each element in the compound.

Determining Empirical Formulas



One can determine the empirical formula from the percent composition by following these three steps.

Determining Empirical Formulas—an Example

The compound *para*-aminobenzoic acid (you may have seen it listed as PABA on your bottle of sunscreen) is composed of carbon (61.31%), hydrogen (5.14%), nitrogen (10.21%), and oxygen (23.33%). Find the empirical formula of PABA.

Determining Empirical Formulas—an Example

Assuming 100.00 g of *para*-aminobenzoic acid,

$$\text{C:}\quad 61.31\text{ g} \times \frac{1\text{ mol}}{12.01\text{ g}} = 5.105\text{ mol C}$$

$$\text{H:}\quad 5.14\text{ g} \times \frac{1\text{ mol}}{1.01\text{ g}} = 5.09\text{ mol H}$$

$$\text{N:}\quad 10.21\text{ g} \times \frac{1\text{ mol}}{14.01\text{ g}} = 0.7288\text{ mol N}$$

$$\text{O:}\quad 23.33\text{ g} \times \frac{1\text{ mol}}{16.00\text{ g}} = 1.456\text{ mol O}$$

Determining Empirical Formulas—an Example

Calculate the mole ratio by dividing by the smallest number of moles:

$$C: \quad \frac{5.105 \text{ mol}}{0.7288 \text{ mol}} = 7.005 \approx 7$$

$$H: \quad \frac{5.09 \text{ mol}}{0.7288 \text{ mol}} = 6.984 \approx 7$$

$$N: \quad \frac{0.7288 \text{ mol}}{0.7288 \text{ mol}} = 1.000$$

$$O: \quad \frac{1.458 \text{ mol}}{0.7288 \text{ mol}} = 2.001 \approx 2$$

Determining Empirical Formulas—an Example

These are the subscripts for the empirical formula:

$C_7H_7NO_2$

Determining a Molecular Formula

- Remember, the number of atoms in a molecular formula is a multiple of the number of atoms in an empirical formula.
- If we find the empirical formula and know a molar mass (molecular weight) for the compound, we can find the molecular formula.

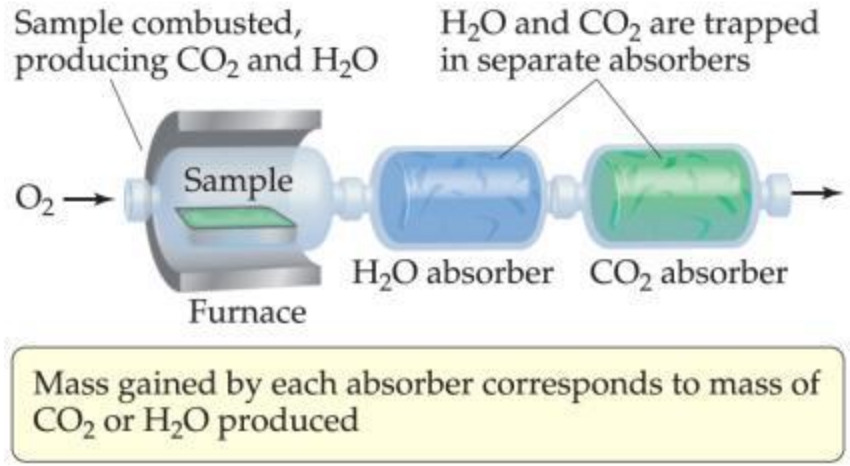
Determining a Molecular Formula—an Example

- The empirical formula of a compound was found to be CH. It has a molar mass of 78 g/mol. What is its molecular formula?
- Solution:

Whole-number multiple = 78/13 = 6

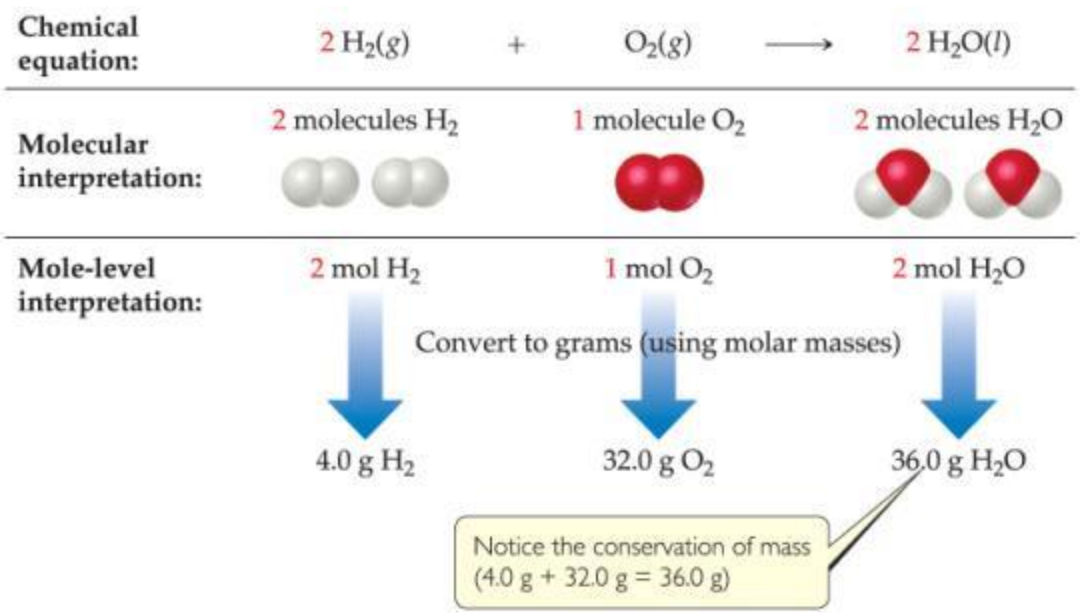
The molecular formula is C_6H_6.

Combustion Analysis



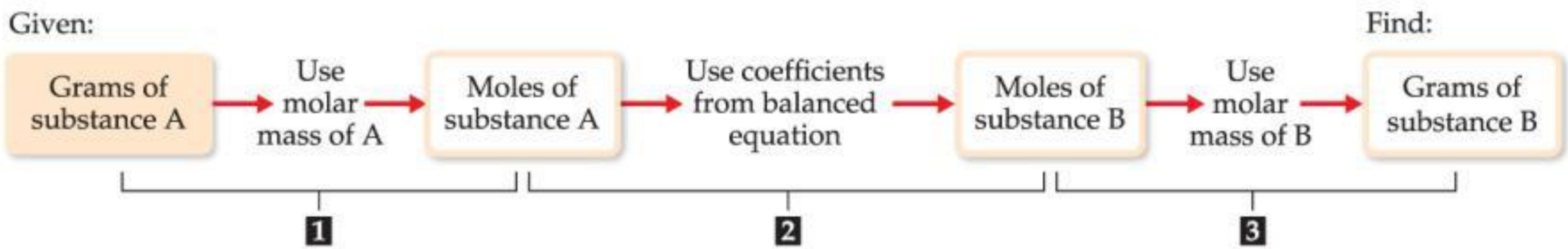
- Compounds containing C, H, and O are routinely analyzed through combustion in a chamber like the one shown in Figure 3.14.
  - C is determined from the mass of CO_2 produced.
  - H is determined from the mass of H_2O produced.
  - O is determined by the difference after C and H have been determined.

Quantitative Relationships



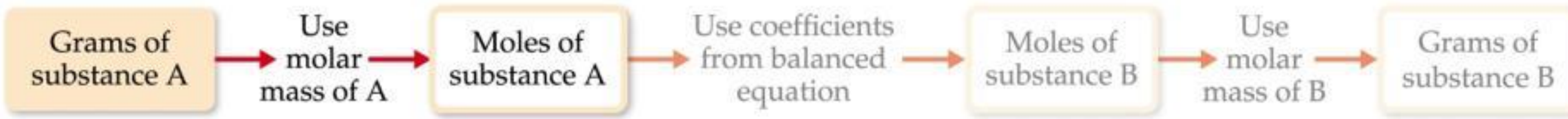
- The coefficients in the balanced equation show
  - relative numbers of *molecules* of reactants and products.
  - relative numbers of *moles* of reactants and products, which can be converted to *mass*.

Stoichiometric Calculations



We have already seen in this chapter how to convert from grams to moles or moles to grams. The NEW calculation is how to compare two DIFFERENT materials, using the MOLE RATIO from the balanced equation!

An Example of a Stoichiometric Calculation



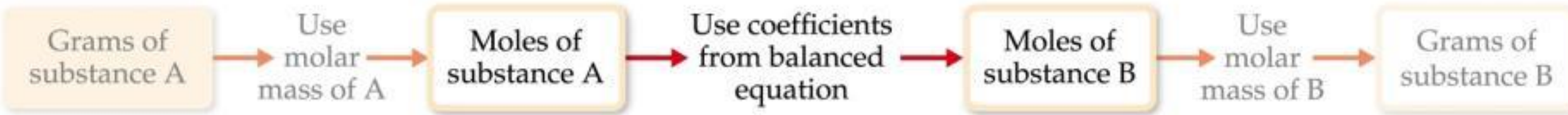
$$\text{Moles } C_6H_{12}O_6 = (1.00\ \cancel{g\ C_6H_{12}O_6})\left(\frac{1\ \text{mol } C_6H_{12}O_6}{180.0\ \cancel{g\ C_6H_{12}O_6}}\right)$$

- How many grams of water can be produced from 1.00 g of glucose?

$C_6H_{12}O_6(s) + 6\ O_2(g) \rightarrow 6\ CO_2(g) + 6\ H_2O(l)$

- There is 1.00 g of glucose to start.
- The first step is to convert it to moles.

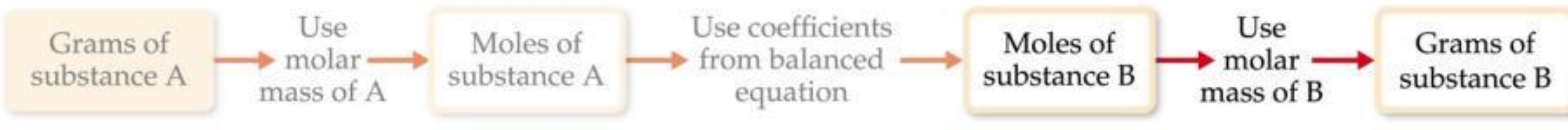
An Example of a Stoichiometric Calculation



$$\text{Moles } H_2O = (1.00\ \cancel{g\ C_6H_{12}O_6})\left(\frac{1\ \cancel{mol\ C_6H_{12}O_6}}{180.0\ \cancel{g\ C_6H_{12}O_6}}\right)\left(\frac{6\ mol\ H_2O}{1\ \cancel{mol\ C_6H_{12}O_6}}\right)$$

- The NEW calculation is to convert moles of one substance in the equation to moles of another substance.
- The MOLE RATIO comes from the balanced equation.

An Example of a Stoichiometric Calculation



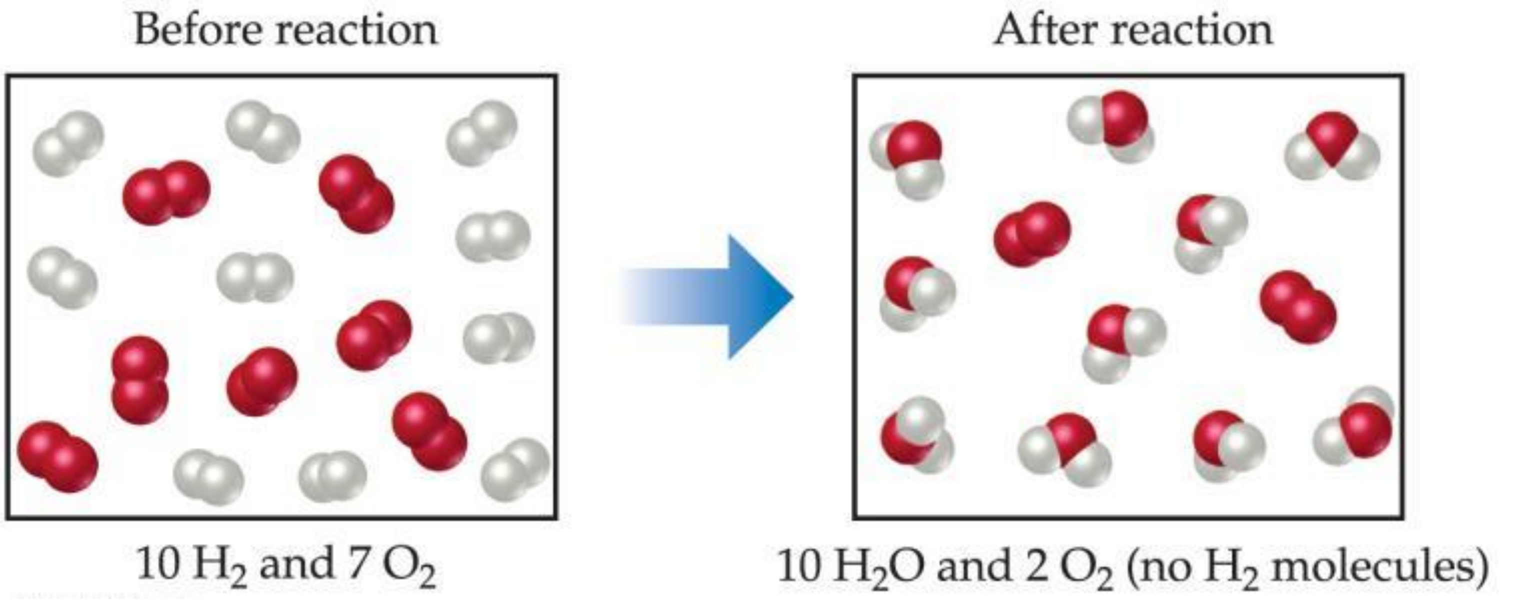
$$\text{Grams } H_2O = (1.00 \text{ g } \cancel{C_6H_{12}O_6})\left(\frac{1 \text{ } \cancel{\text{mol } C_6H_{12}O_6}}{180.0 \text{ g } \cancel{C_6H_{12}O_6}}\right)\left(\frac{6 \text{ } \cancel{\text{mol } H_2O}}{1 \text{ } \cancel{\text{mol } C_6H_{12}O_6}}\right)\left(\frac{18.0 \text{ g } H_2O}{1 \text{ } \cancel{\text{mol } H_2O}}\right)$$

$$= 0.600 \text{ g } H_2O$$

- There is 1.00 g of glucose to start.
- The first step is to convert it to moles.

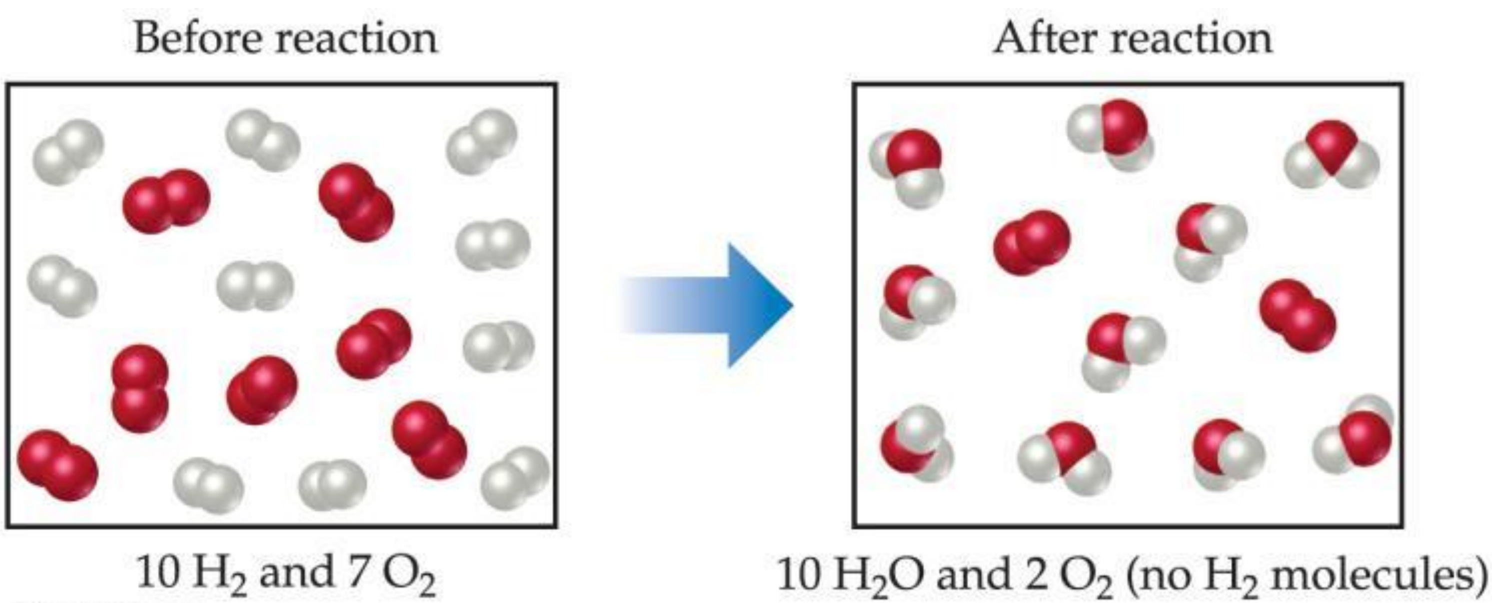
Limiting Reactants

- The **limiting reactant** is the reactant present in the smallest stoichiometric amount.
  - In other words, it's the reactant you'll run out of first (in this case, the H_2).



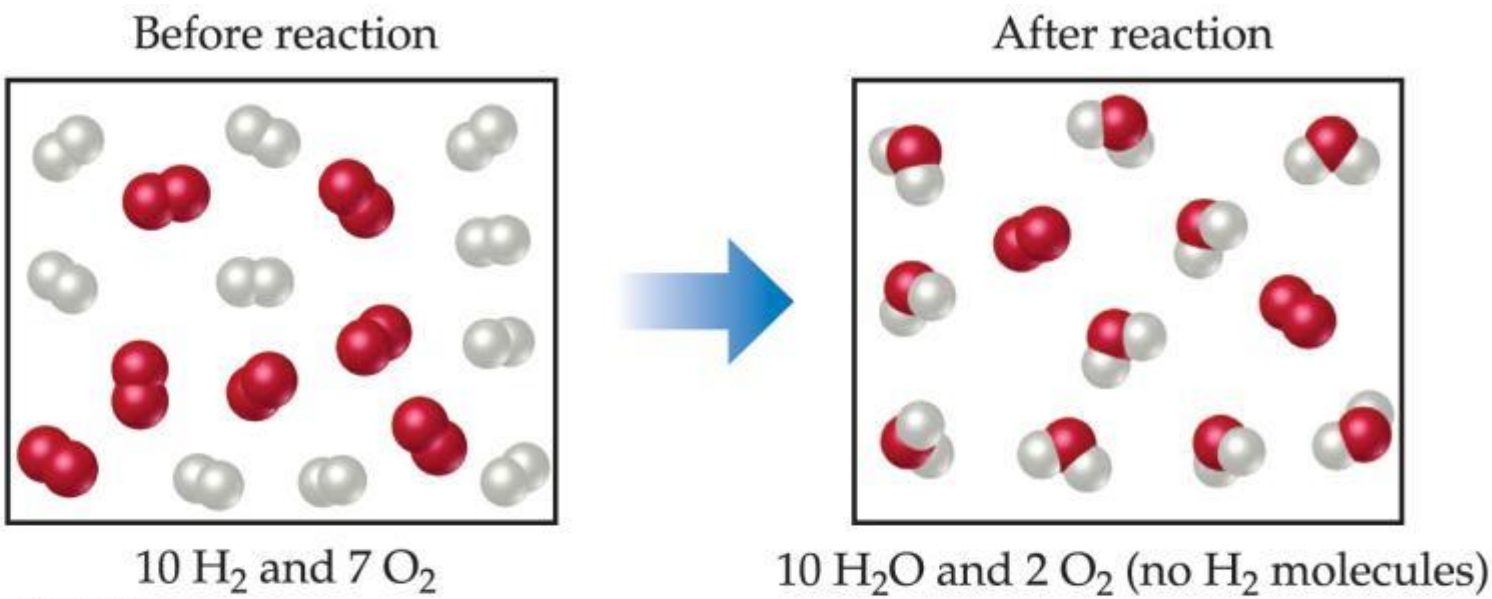
Limiting Reactants

In the example below, the O_2 would be the **excess reagent**.



Limiting Reactants

- The **limiting reactant** is used in all stoichiometry calculations to determine amounts of products and amounts of any other reactant(s) used in a reaction.



Theoretical Yield

- The **theoretical yield** is the maximum amount of product that can be made.
  - In other words, it's the amount of product possible as calculated through the stoichiometry problem.
- This is different from the **actual yield**, which is the amount one actually produces and measures.

Percent Yield

One finds the **percent yield** by comparing the amount actually obtained (actual yield) to the amount it was possible to make (theoretical yield):

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