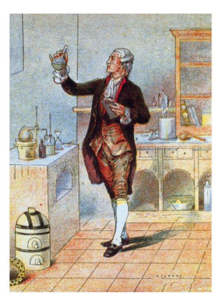
Chapter 3: Stoichiometry

Key Skills:

- ➢Balance chemical equations
- ➢Predict the products of simple combination, decomposition, and combustion reactions.
- ➢Calculate formula weights
- ➢Convert grams to moles and moles to grams using molar masses.
- ➢Convert number of molecules to moles and moles to number of molecules using Avogadro's number
- ➢Calculate the empirical and molecular formulas of a compound from percentage composition and molecular weight.
- ➢Identify limiting reactants and calculate amounts, in grams or moles, or reactants consumed and products formed for a reaction.
- ➢Calculate the percent yield of a reaction.

Stoichiometry is the study of the *quantitative* relationships in substances and their reactions

- –Chemical equations
- –The mole and molar mass
- –Chemical formulas
- –Mass relationships in equations
- –Limiting reactant



Definitions

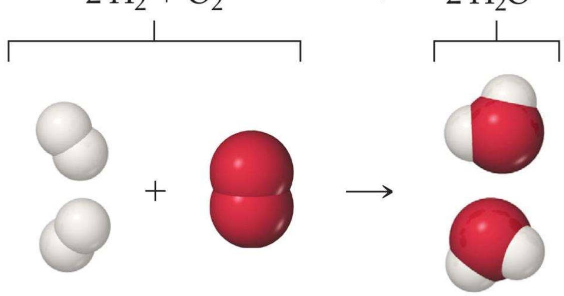
- **Reactants** are the substances consumed
- **Products** are the substances formed
- **Coefficients** are numbers before the formula of a substance in an equation
- A **balanced** equation has the same number of atoms of each element on both sides of the equation

Chemical Equations

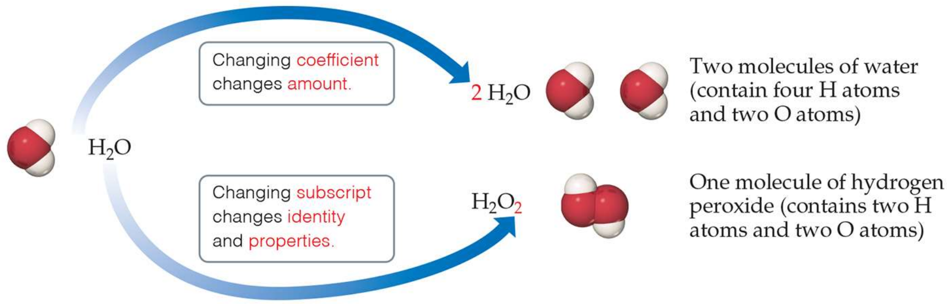
- A chemical equation is a shorthand notation to describe a chemical reaction
  - Just like a chemical formula, a chemical equation expresses quantitative relations
- Subscripts tell the number of atoms of each element in a molecule
- Coefficients tell the number of molecules

Reactants → Products

$$2\,H_2 + O_2 \longrightarrow 2\,H_2O$$



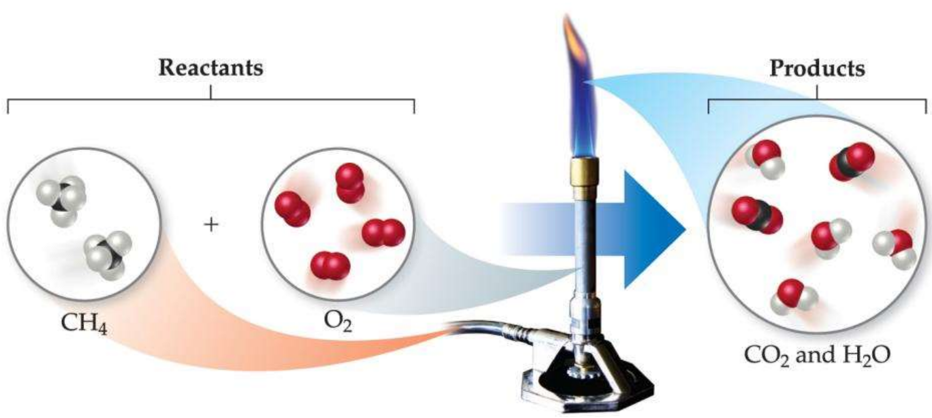
Coefficients vs. Subscripts



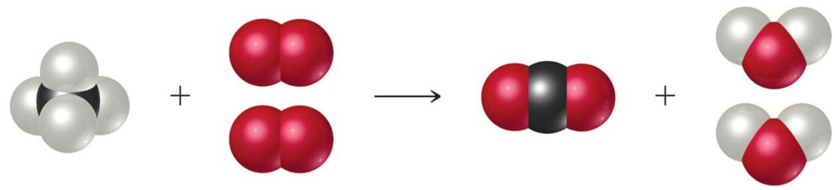
Hydrogen and oxygen can make water or hydrogen peroxide

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

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



Anatomy of a Chemical Equation



$$CH_4 + 2\,O_2 \longrightarrow CO_2 + 2\,H_2O$$

(1 C, 4 H, 4 O) (1 C, 4 H, 4 O)

Reactants appear on the left side of the equation.

Products appear on the right side of the equation.

The *states* of the reactants and products are written in parentheses to the right of each element symbol or formula.

Writing Balanced Equations

- Write the *correct formula* for each substance

  $H_2 + Cl_2 \rightarrow HCl$

- Add *coefficients* so the number of atoms of each element are the *same* on both sides of the equation

  $H_2 + Cl_2 \rightarrow 2HCl$

Balancing Chemical Equations

- Assume one molecule of the most complicated substance
  $C_5H_{12} + O_2 \rightarrow CO_2 + H_2O$
- Adjust the coefficient of CO_2 to balance C
  $C_5H_{12} + O_2 \rightarrow 5CO_2 + H_2O$
- Adjust the coefficient of H_2O to balance H
  $C_5H_{12} + O_2 \rightarrow 5CO_2 + 6H_2O$
- Adjust the coefficient of O_2 to balance O
  $C_5H_{12} + 8O_2 \rightarrow 5CO_2 + 6H_2O$
- Check the balance by counting the number of atoms of each element.

Balancing Equations

- Sometimes *fractional* coefficients are obtained

  $C_5H_{10} + O_2 \rightarrow CO_2 + H_2O$

  $C_5H_{10} + O_2 \rightarrow 5\ CO_2 + H_2O$

  $C_5H_{10} + O_2 \rightarrow 5\ CO_2 + 5\ H_2O$

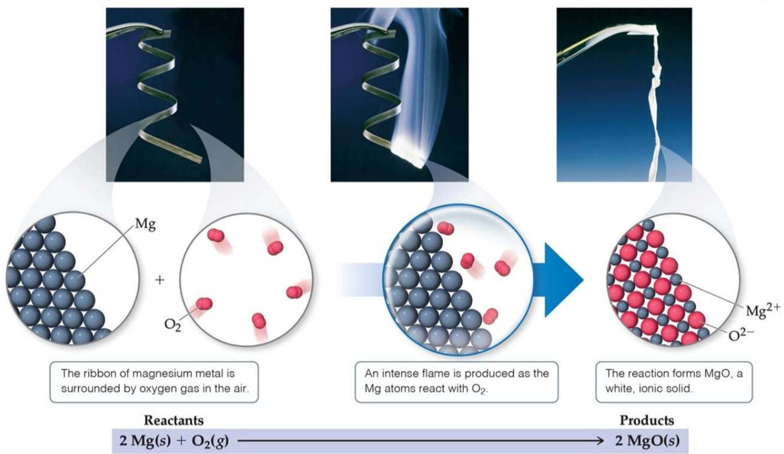
  $C_5H_{10} + (15/2)\ O_2 \rightarrow 5\ CO_2 + 5\ H_2O$
- Multiply <u>all</u> coefficients by the denominator

  $2\ C_5H_{10} + 15\ O_2 \rightarrow 10\ CO_2 + 10\ H_2O$

Combination

TABLE 3.1 Combination and Decomposition Reactions

Combination Reactions	
$A + B \longrightarrow C$	Two or more reactants combine to form a single product. Many elements react with one another in this fashion to form compounds.
$C(s) + O_2(g) \longrightarrow CO_2(g)$	
$N_2(g) + 3\,H_2(g) \longrightarrow 2\,NH_3(g)$	
$CaO(s) + H_2O(l) \longrightarrow Ca(OH)_2(aq)$	



Decomposition

One substance breaks down into two or more substances

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

TABLE 3.1 Combination and Decomposition Reactions

Decomposition Reactions	
$C \longrightarrow A + B$	A single reactant breaks apart to form two or more substances. Many compounds react this way when heated.
$2\,KClO_3(s) \longrightarrow 2\,KCl(s) + 3\,O_2(g)$	
$PbCO_3(s) \longrightarrow PbO(s) + CO_2(g)$	
$Cu(OH)_2(s) \longrightarrow CuO(s) + H_2O(g)$	

Combustion

Is the process of burning, the combination of an organic substance with oxygen to produce a flame.

- When an organic compound burns in oxygen, the carbon reacts with oxygen to form CO_2, and the hydrogen forms water, H_2O.

Balance the following combustion reactions:

$$C_3H_8 + O_2 \rightarrow CO_2 + H_2O$$

$$(C_2H_5)_2O + O_2 \rightarrow CO_2 + H_2O$$

Formula Weight (FW)

- Sum of the atomic weights for the atoms in a chemical formula
- The formula weight of calcium chloride, $CaCl_2$, would be

  Ca: 1(40.08 amu)
  + Cl: 2(35.45 amu)
  110.98 amu

- Formula weights are generally reported for *ionic* compounds

Molecular Weight (MW)

- Sum of the atomic weights of the atoms in a molecule
- For the molecule ethane, C_2H_6, the molecular weight would be

$$\begin{array}{rl} \text{C:} & 2(12.01\ \text{amu}) \\ +\ \text{H:} & 6(1.008\ \text{amu}) \\ \hline & 30.07\ \text{amu} \end{array}$$

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 by mass of carbon in ethane (C_2H_6) is…

$$\%C = \frac{(2)(12.01\ \text{amu})}{(30.068\ \text{amu})} \times 100$$

$$= \frac{24.02\ \text{amu}}{30.068\ \text{amu}} \times 100$$

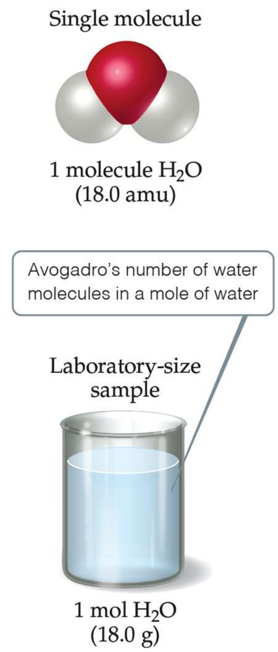
$$= 79.89\%$$

The Mole

- One **mole** is the amount of substance that contains as many entities as the number of atoms in exactly 12 grams of the ^{12}C isotope of carbon.
- **Avogadro's number** is the *experimentally determined* number of atoms in 12 g of isotopically pure ^{12}C, and is equal to 6.022×10^{23}
- One mole of anything contains 6.022×10^{23} entities
  - 1 mol H = 6.022×10^{23} atoms of H
  - 1 mol H_2 = 6.022×10^{23} molecules of H_2
  - 1 mol CH_4 = 6.022×10^{23} molecules of CH_4
  - 1 mol $CaCl_2$ = 6.022×10^{23} formula units of $CaCl_2$

Moles to Number of Entities

Moles of substance $\xrightarrow{\text{Avogadro's number}}$ **Number of atoms or molecules**



Example Calculations

- How many Na atoms are present in 0.35 mol of Na?
- How many moles of C_2H_6 are present in 3.00×10^{21} molecules of C_2H_6?

TABLE 3.2 Mole Relationships

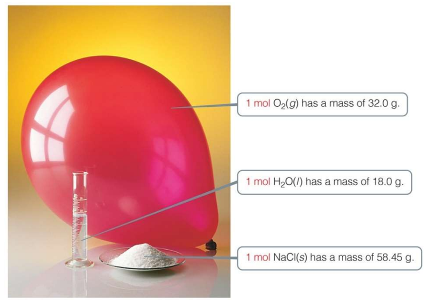
Name of Substance	Formula	Formula Weight (amu)	Molar Mass (g/mol)	Number and Kind of Particles in One Mole
Atomic nitrogen	N	14.0	14.0	6.02×10^{23} N atoms
Molecular nitrogen or “dinitrogen”	N_2	28.0	28.0	6.02×10^{23} N_2 molecules $2(6.02 \times 10^{23})$ N atoms
Silver	Ag	107.9	107.9	6.02×10^{23} Ag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

[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.

Molar Mass

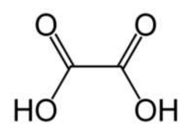
The **molar mass** ($\mathcal{M}$) of any atom, molecule or compound is the mass (in grams) of one mole of that substance.

The molar mass *in grams* is numerically equal to the atomic mass or molecular mass expressed *in u (or amu)*.



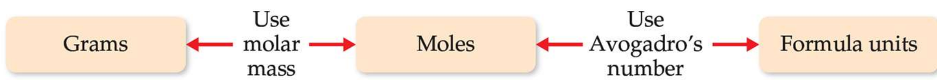
	Atomic Scale		Lab Scale
Substance	**Name**	**Mass**	**Molar Mass**
Ar	atomic mass	39.95 u	39.95 g/mol
C_2H_6	molecular mass	30.07 u	30.07 g/mol
NaF	formula mass	41.99 u	41.99 g/mol

What mass of compound must be weighed out, to have a 0.0223 mol sample of $H_2C_2O_4$ ($\mathcal{M}$ = 90.04 g/mol)?



Oxalic acid

Interconverting masses and number of formula units

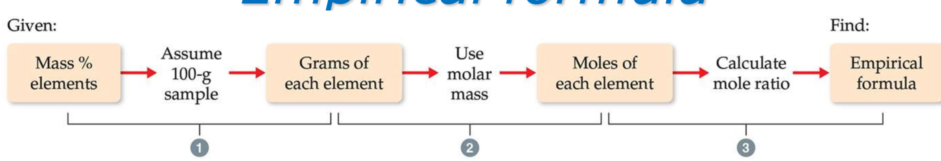


Example Calculation

What is the mass of 0.25 moles of CH_4?

$$0.25\ \cancel{\text{mol CH}_4}\left(\frac{16.0\text{ g CH}_4}{1\ \cancel{\text{mol CH}_4}}\right) = 4.0\text{ g CH}_4$$

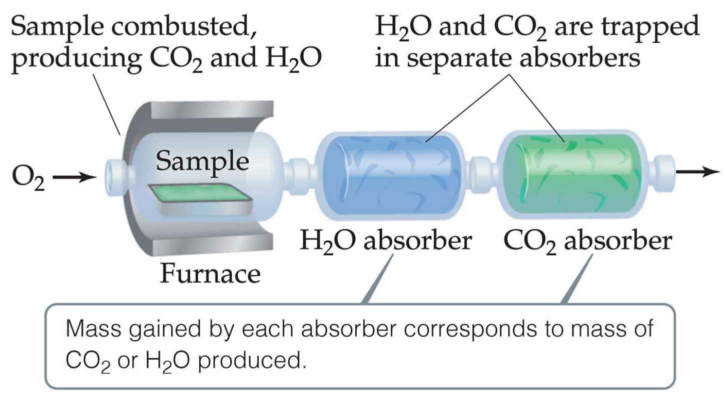
Empirical formula



Example 1: What is the empirical formula of a compound that contains 0.799 g C and 0.201 g H in a 1.000 g sample?

Example 2: What is the empirical formula of a chromium oxide that is 68.4% Cr by mass?

Combustion Analysis



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

Finding C and H content

- A weighed sample of compound is burned, and the masses of H_2O and CO_2 formed is measured.

Mass CO_2 produced $\xrightarrow{\text{Molar mass } CO_2 \text{ 44.0 g/mol}}$ Moles CO_2 produced $\xrightarrow{\text{1 C atom per } CO_2 \text{ molecule}}$ Moles of C original sample $\xrightarrow{\text{Molar mass C 12.0 g/mol}}$ Mass C in original sample

Mass H_2O produced $\xrightarrow{\text{Molar mass } H_2O \text{ 18.0 g/mol}}$ Moles H_2O produced $\xrightarrow{\text{2 H atoms per } H_2O \text{ molecule}}$ Moles H in original sample $\xrightarrow{\text{Molar mass H 1.01 g/mol}}$ Mass H in original sample

Calculating Empirical Formulas

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.

Assuming 100.00 g of *para*-aminobenzoic acid,

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

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

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

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

Calculating Empirical Formulas

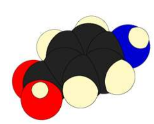
Calculate the mole ratio by dividing by the smallest number of moles:

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

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

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

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

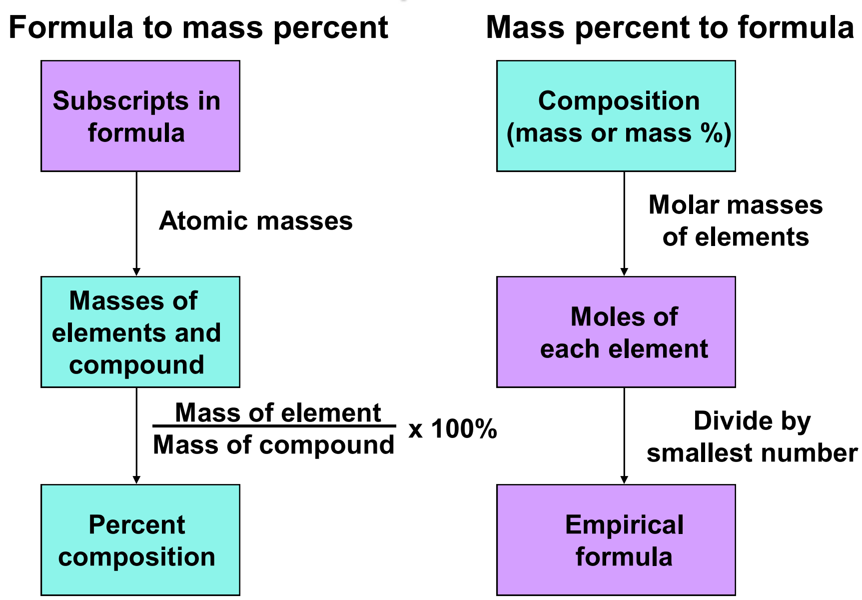


$C_7H_7NO_2$

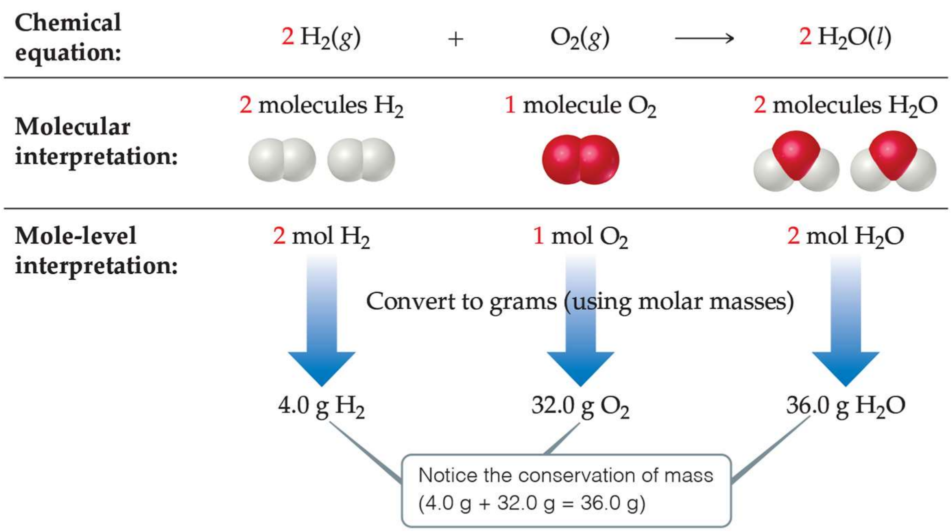
Example Calculation

A compound contains only C, H, and O. A 0.1000 g-sample burns completely in oxygen to form 0.0930 g water and 0.2271 g CO_2. Calculate the mass of each element in this sample. What is the empirical formula of the compound?

Comparison

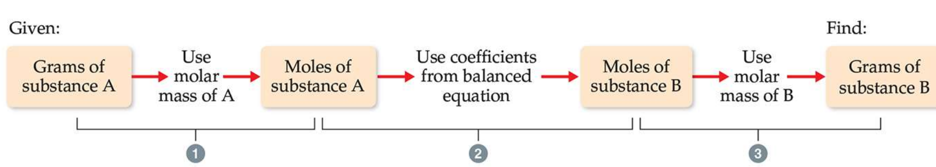


Mole Relationships in Equations



Guidelines for Reaction Stoichiometry

- Write the balanced equation.
- Calculate the number of moles of the species for which the mass is given.
- Use the coefficients in the equation to convert the moles of the given substance into moles of the substance desired.
- Calculate the mass of the desired species.



Example Calculation

Given the reaction

$$4FeS_2 + 11\ O_2 \rightarrow 2Fe_2O_3 + 8SO_2$$

What mass of SO_2 is produced from reaction of 3.8 g of FeS_2 and excess O_2?

Example Calculation

What mass of SO_3 forms from the reaction of 4.1 g of SO_2 with an excess of O_2?

Reaction Yields

Actual yield is found by measuring the quantity of product formed in the experiment.

Theoretical yield is calculated from reaction stoichiometry.

$$\%\ \text{yield} = \frac{\text{Actual yield}}{\text{Theoretical yield}} \times 100\%$$

Example: Calculating Percent Yield

A 10.0 g-sample of potassium bromide is treated with perchloric acid solution. The reaction mixture is cooled and solid $KClO_4$ is removed by filtering, then it is dried and weighed.

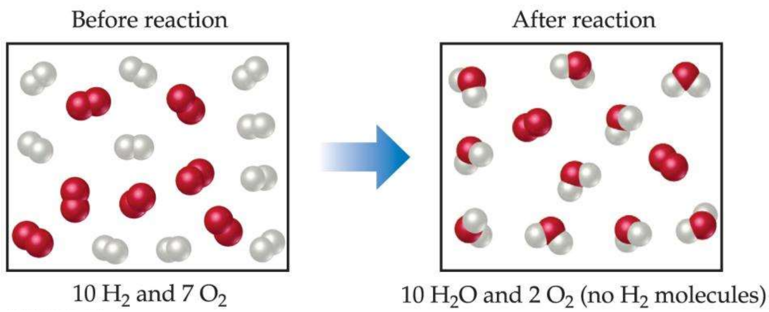
$$KBr\ (aq) + HClO_4\ (aq) \rightarrow KClO_4\ (s) + HBr\ (aq)$$

The product weighed 8.8 g. What was the percent yield?

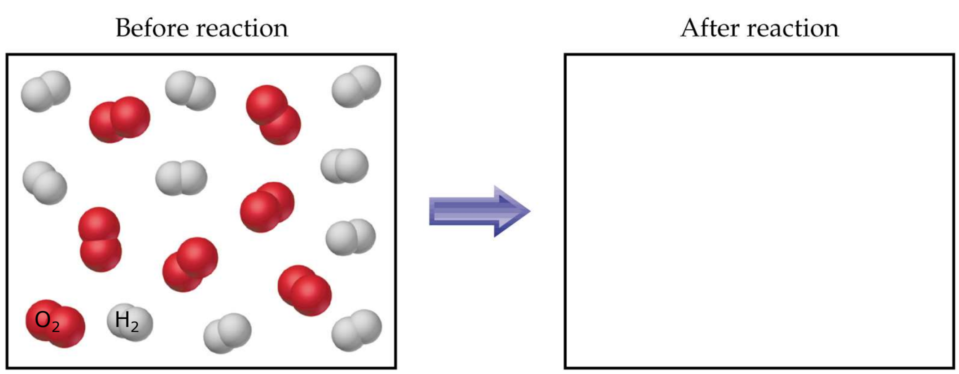
Limiting Reactant

Limiting reactant : the reactant that is completely consumed in a reaction. When it is used up, the reaction stops, thus limiting the quantities of products formed.

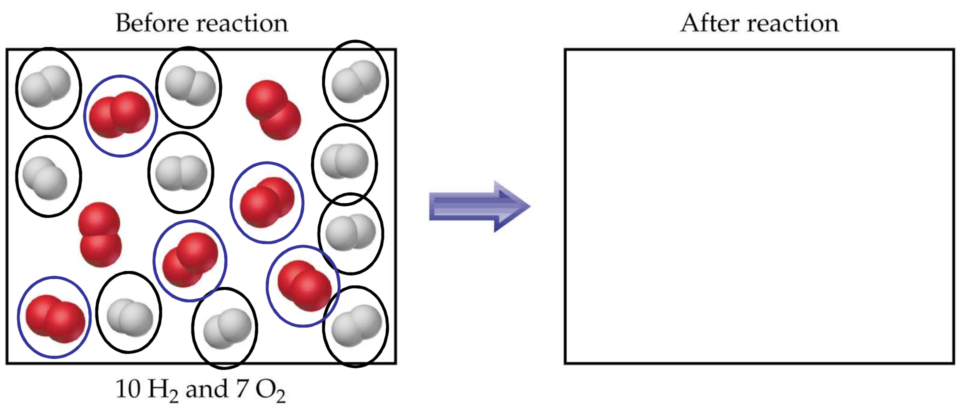
Excess reactant : the other reactants present, not completely consumed



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



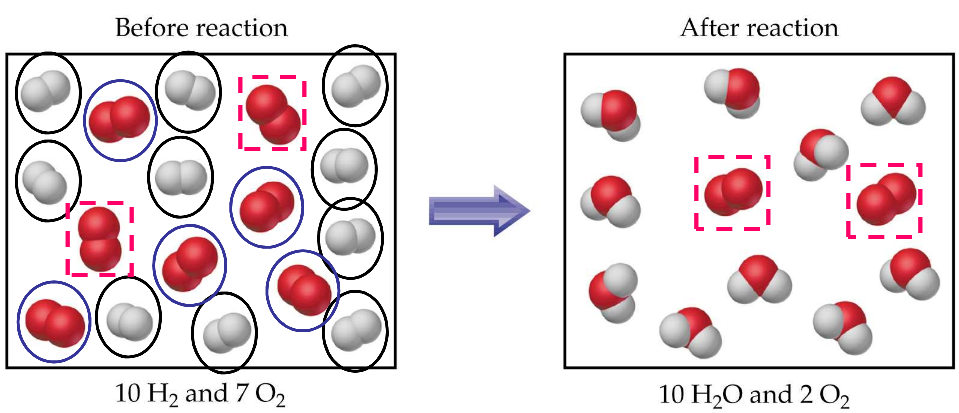
$2H_2(g) + O_2(g) \rightarrow 2H_2O(g)$



$5[2H_2(g) + O_2(g) \rightarrow 2H_2O(g)]$

$10H_2(g) + 5O_2(g) \rightarrow 10H_2O(g)$

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

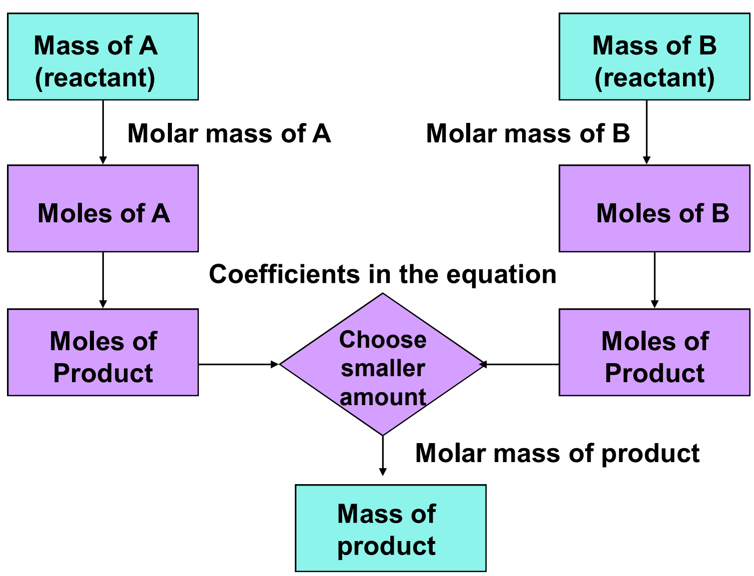


$5[2H_2(g) + O_2(g) \rightarrow 2H_2O(g)]$

$10H_2(g) + 5O_2(g) \rightarrow 10H_2O(g)$

	$2\,H_2(g)$	+	$O_2(g)$	$\longrightarrow$	$2\,H_2O(g)$
Before reaction:	10 mol		7 mol		0 mol
Change (reaction):	−10 mol		−5 mol		+10 mol
After reaction:	0 mol		2 mol		10 mol

Strategy for Limiting Reactant



Example Calculation

Calculate the theoretical yield (g) when 7.0 g of N_2 reacts with 2.0 g of H_2, forming NH_3.

Example Calculation

One reaction step in the conversion of ammonia to nitric acid involves converting NH_3 to NO by the following reaction:

$$4\ NH_3(g) + 5\ O_2(g) \rightarrow 4\ NO(g) + 6\ H_2O(g)$$

If 1.50 g of NH_3 reacts with 2.75 g O_2, then:

1. Which is the limiting reactant?

2. How many grams of NO and H_2O form?

3. How many grams of the excess reactant remain after the limiting reactant is completely consumed?

4. Is the law of conservation of mass obeyed?