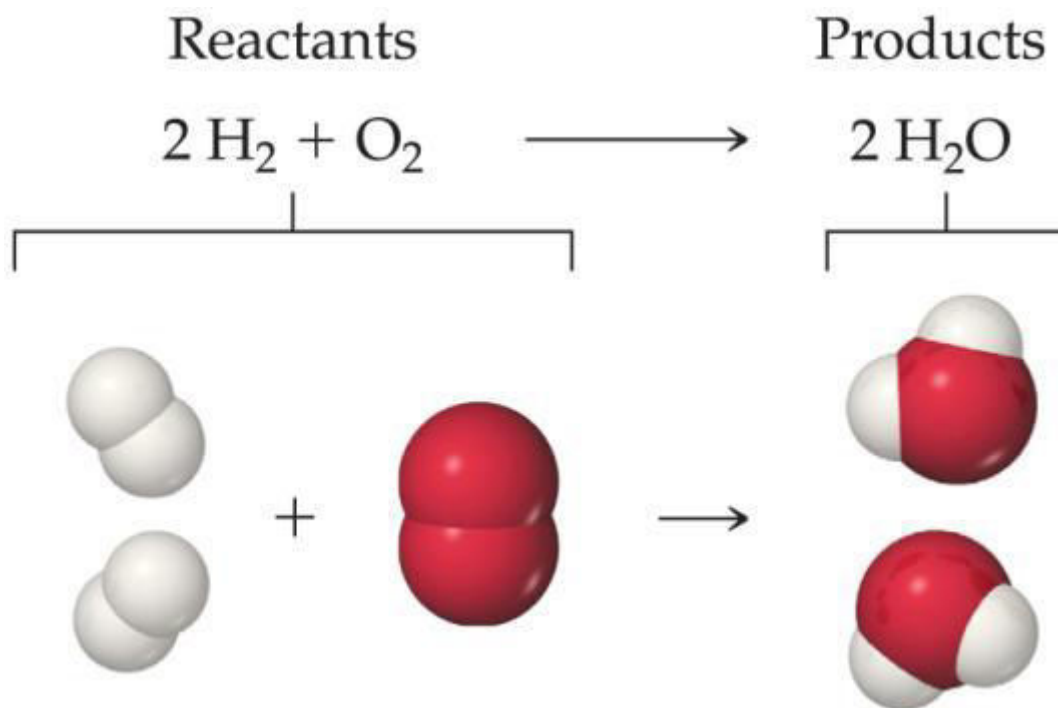


Stoichiometry: Calculations with Chemical Formulas and Equations

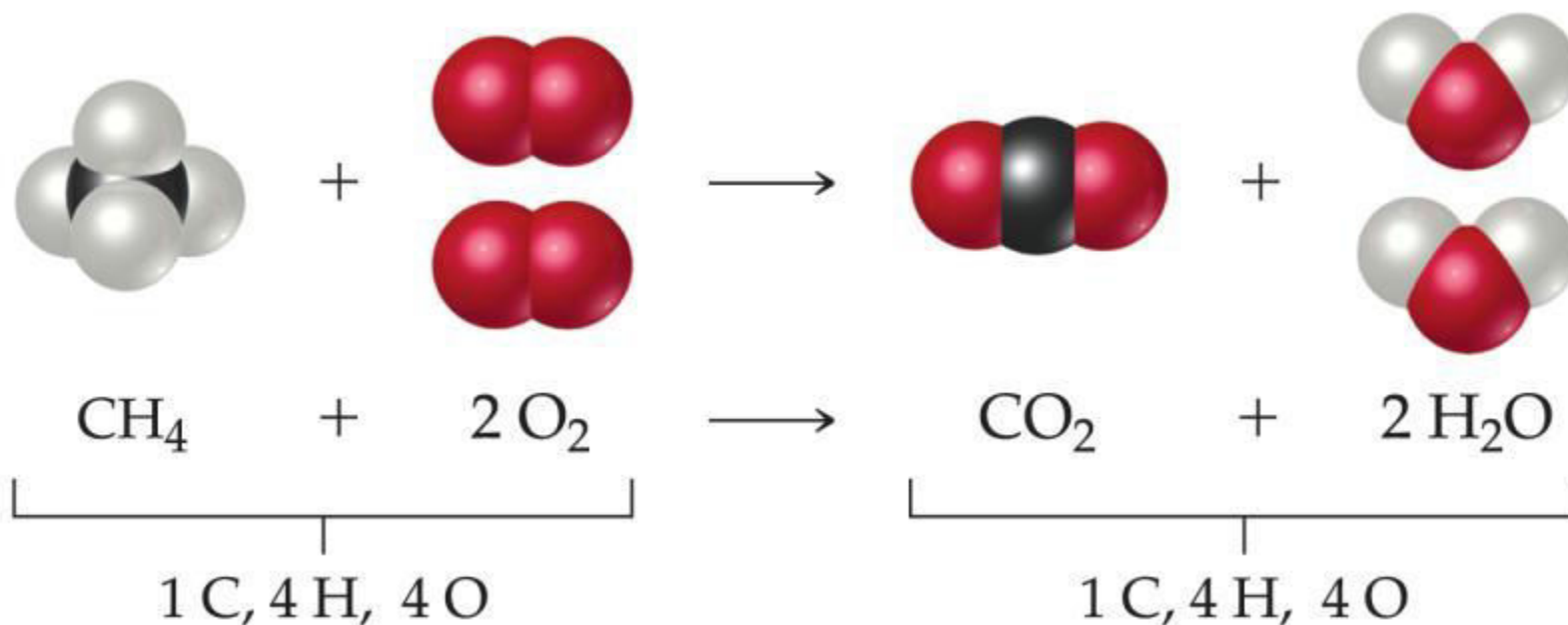
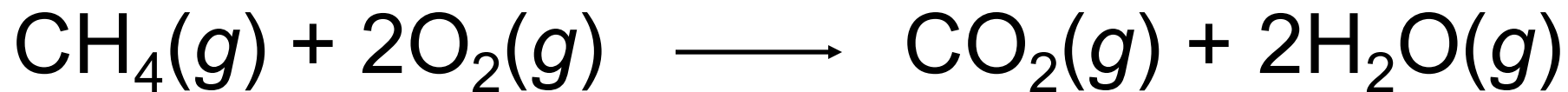
ARINDAM GOSWAMI
DELHI PUBLIC SCHOOL GHAZIABAD

Chemical Equations

Chemical equations are concise representations of chemical reactions.

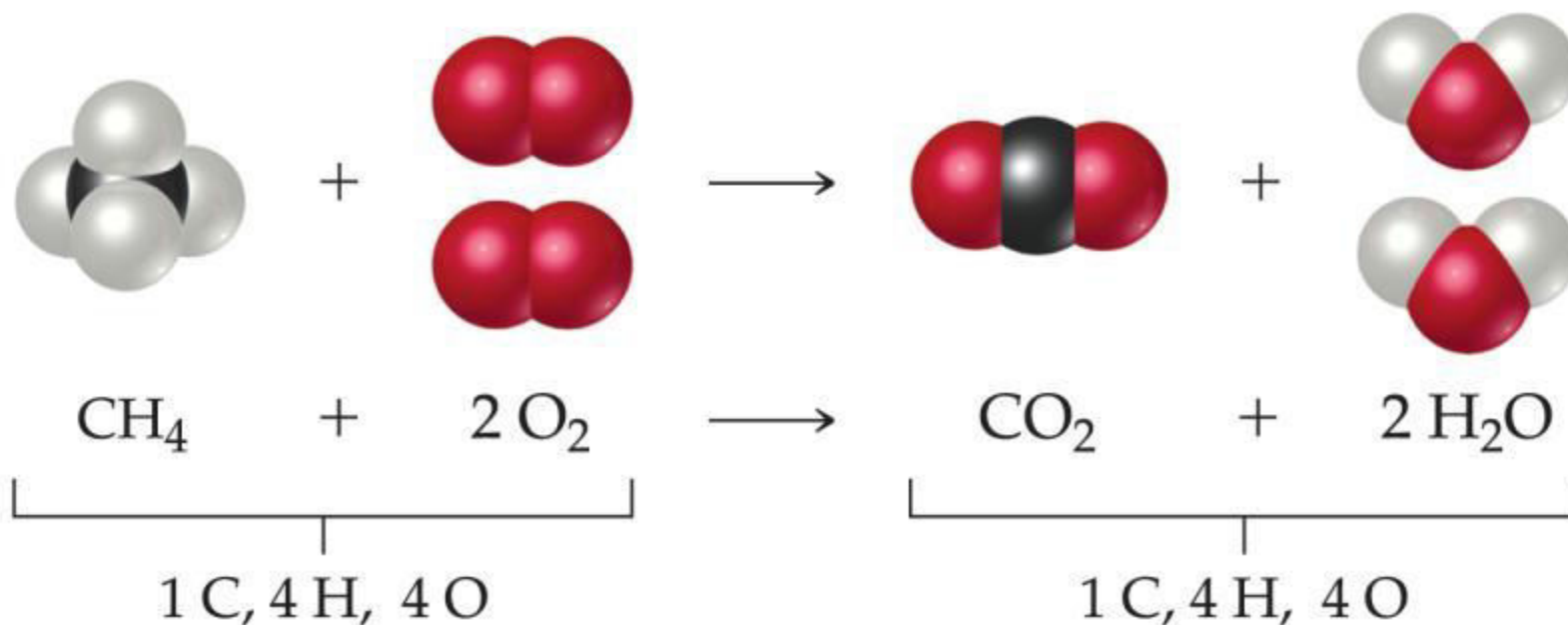
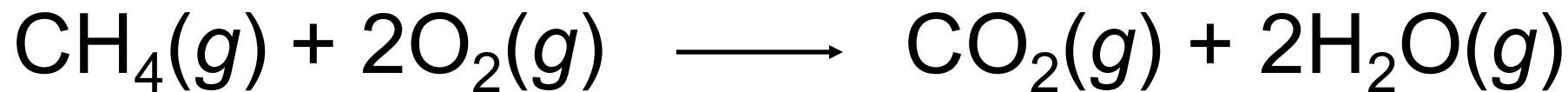


What Is in a Chemical Equation?



Reactants appear on the left side of the equation.

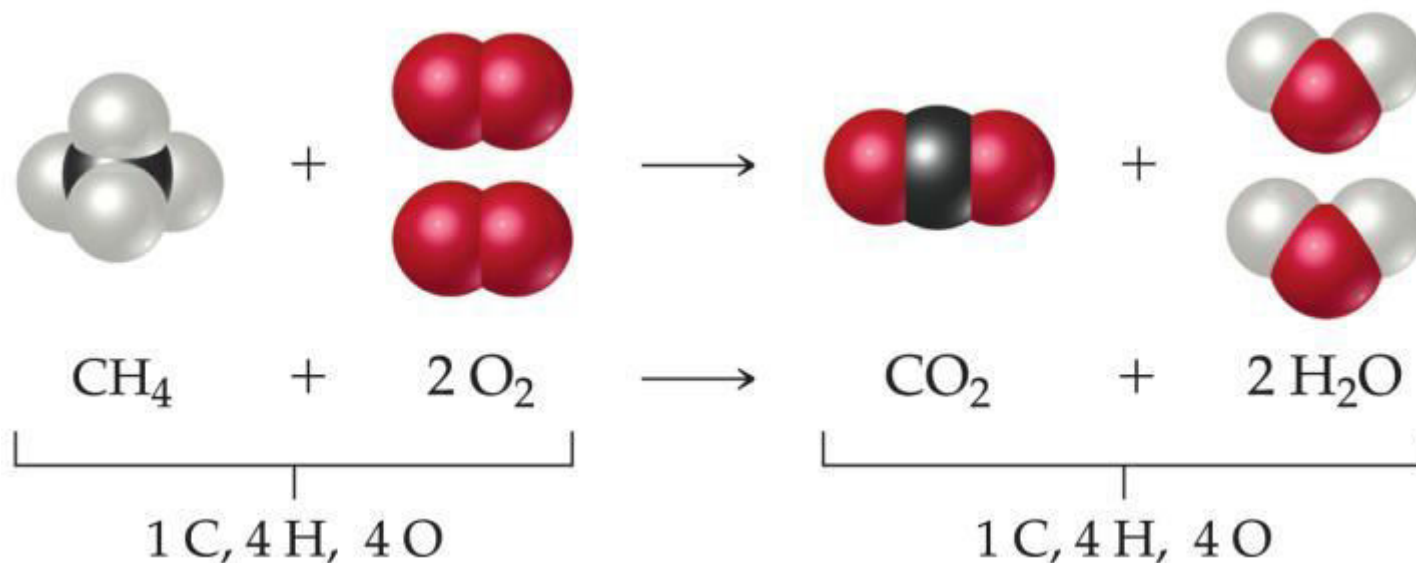
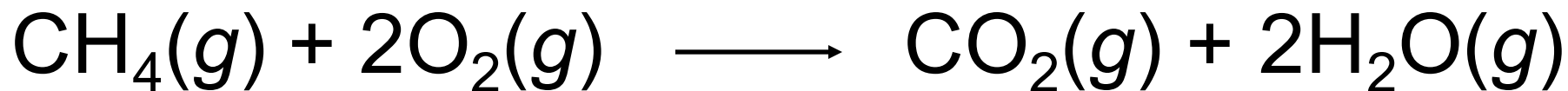
What Is in a Chemical Equation?



Products appear on the right side of the equation.



What Is in a Chemical Equation?

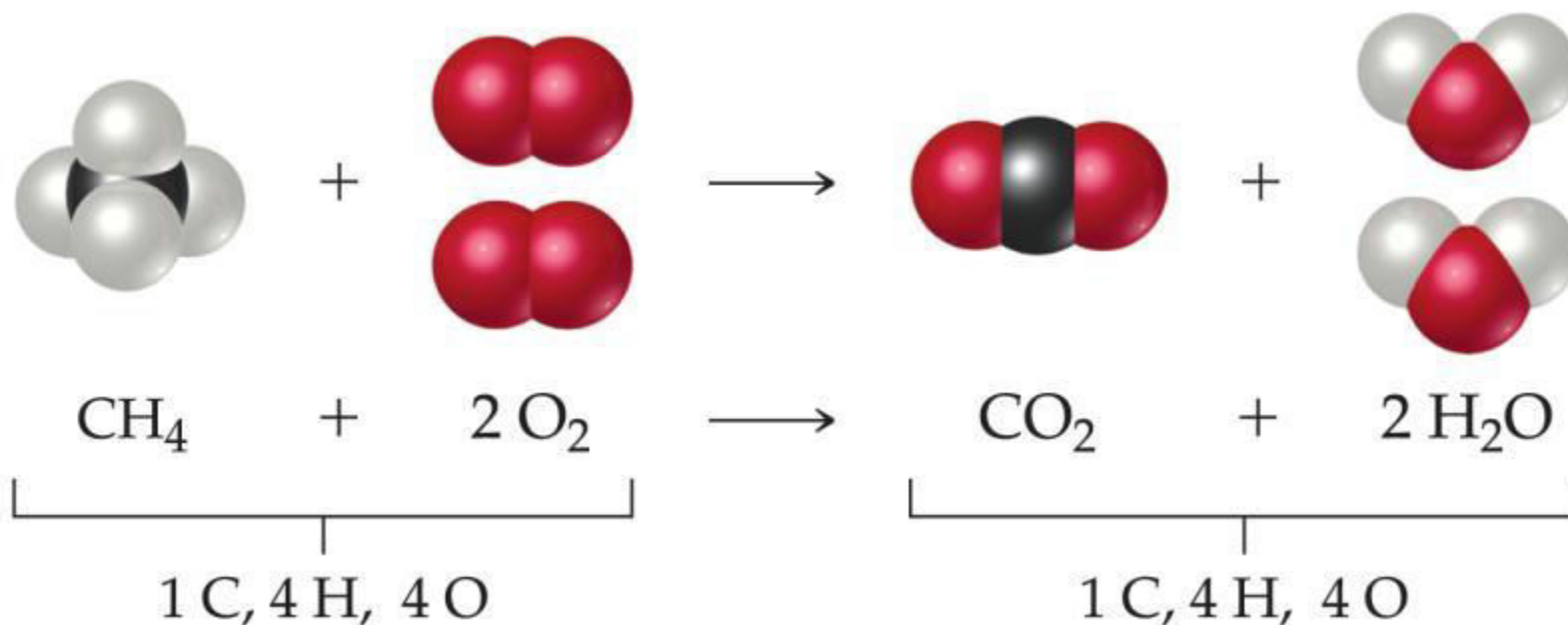
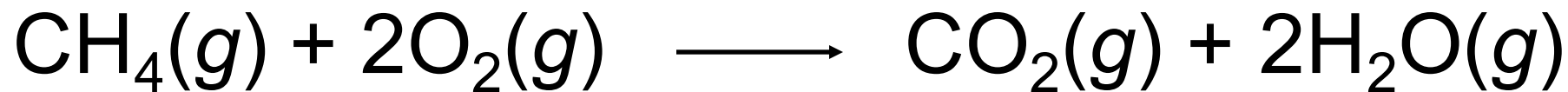


The **states** of the reactants and products are written in parentheses to the right of each compound.

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

(*aq*) = in aqueous solution

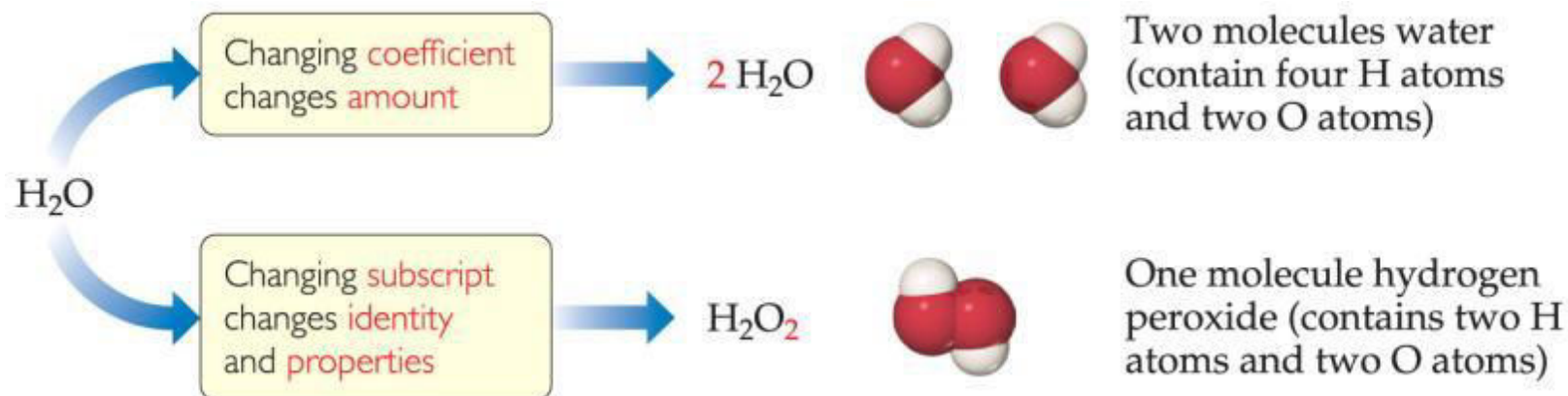
What Is in a Chemical Equation?



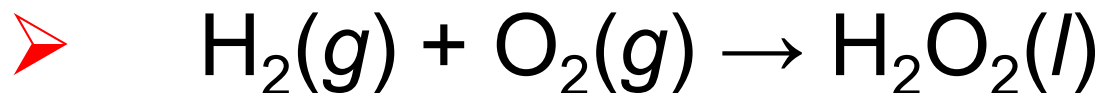
Coefficients are inserted to balance the equation to follow the law of conservation of mass.



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



- Hydrogen and oxygen can make water
OR hydrogen peroxide:



Balancing Chemical Equation

Exercise 1:

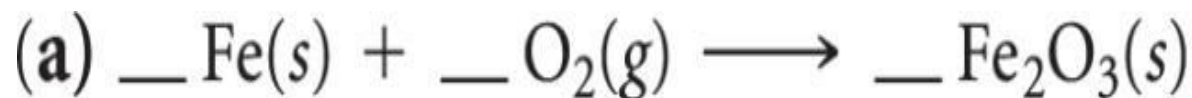
Balance following equations:



Balancing Chemical Equations

Exercise 2

Balance these equations by providing the missing coefficients:

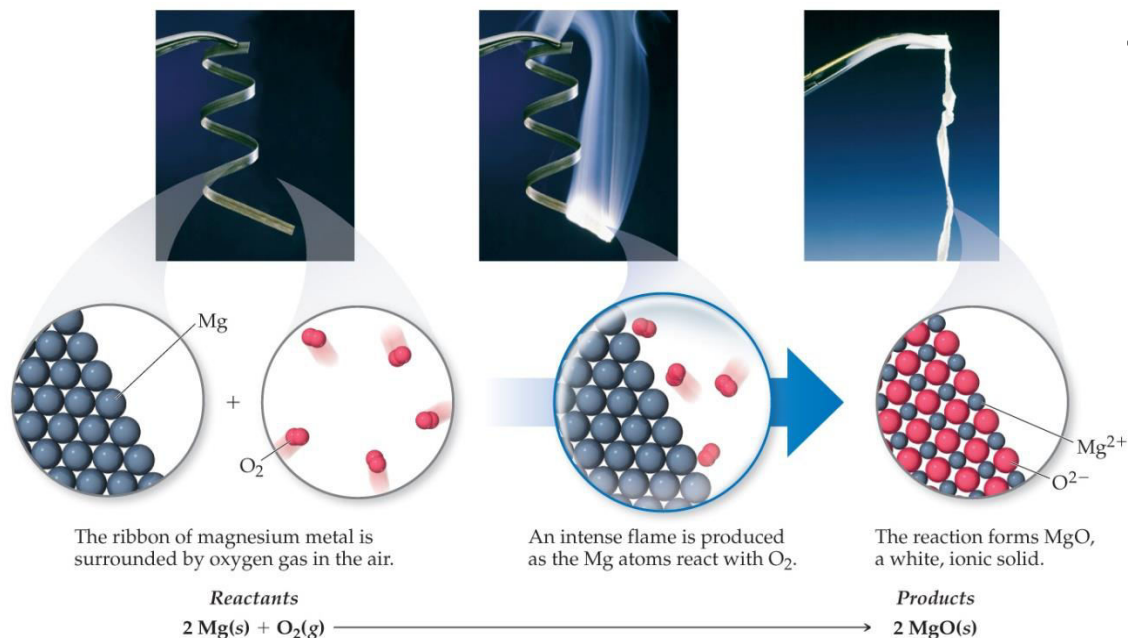


Three Types of Reactions

- Combination reactions
- Decomposition reactions
- Combustion reactions

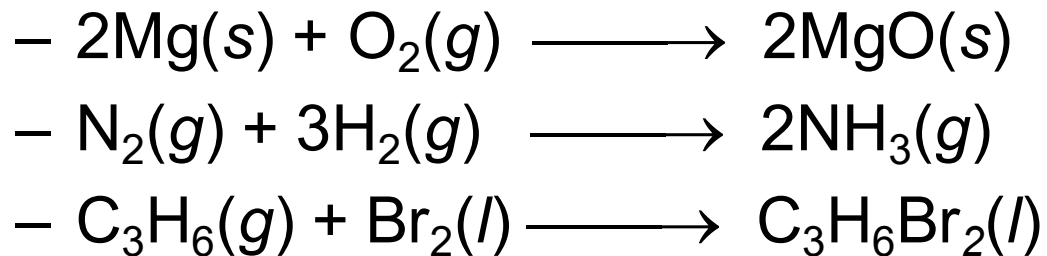


Combination Reactions



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

- **Examples:**

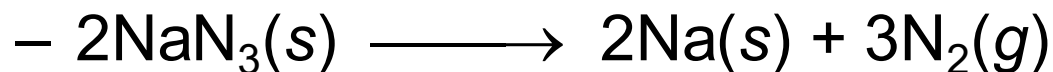
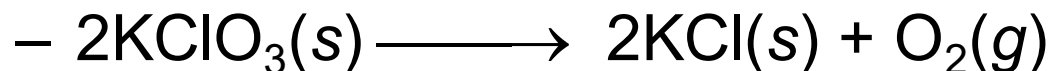
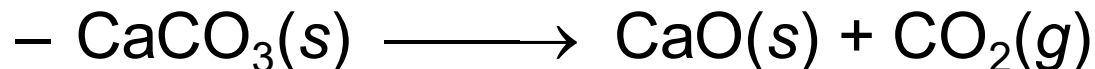


Decomposition Reactions



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

- Examples:



Sodium azide is used in air-bags of cars.

Exercise 3

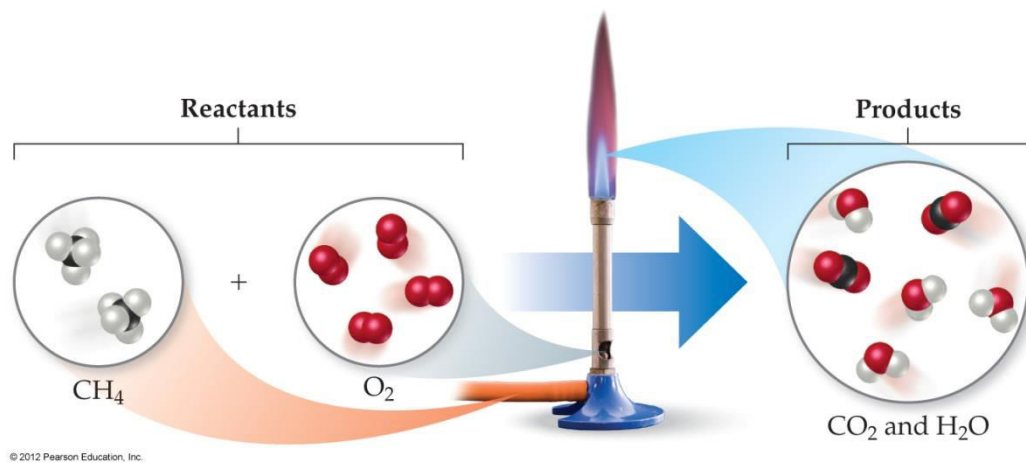
Write a balanced equation for **(a)** the combination reaction between lithium metal and fluorine gas and **(b)** the decomposition reaction that occurs when solid barium carbonate is heated (two products form, a solid and a gas).

Solution

Exercise 4

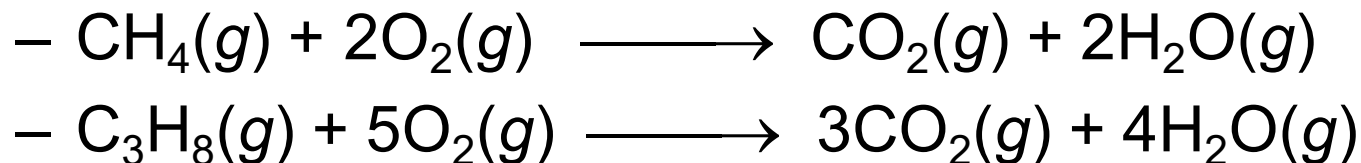
Write a balanced equation for **(a)** solid mercury(II) sulfide decomposing into its component elements when heated and **(b)** aluminum metal combining with oxygen in the air.

Combustion Reactions



- **Combustion reactions** are generally rapid reactions that produce a flame.
- **Combustion reactions** most often involve hydrocarbons reacting with oxygen in the air.

- **Examples:**



Exercise 5: Writing Balanced Equations for Combustion Reactions

Write the balanced equation for the reaction that occurs when methanol, $\text{CH}_3\text{OH}(l)$, is burned in air.

Exercise 6

Write the balanced equation for the reaction that occurs when ethanol, $\text{C}_2\text{H}_5\text{OH}(l)$, burns in air.

Formula Weights

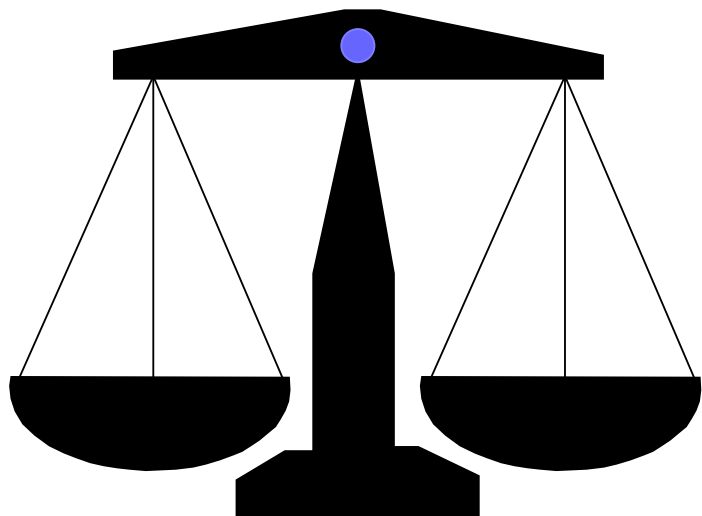


Micro World
atoms & molecules



Macro World
grams

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



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

On this scale

$^1\text{H} = 1.008 \text{ amu}$

$^{16}\text{O} = 16.00 \text{ amu}$

Formula Weight (FW)

- A **formula weight** is the sum of the atomic weights for the atoms in a chemical formula.
- So, the formula weight of calcium chloride, CaCl_2 , would be

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

- Formula weights are generally reported for ionic compounds.

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

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

Exercise 7: Calculating Formula Weights

Calculate the formula weight of **(a)** sucrose, $\text{C}_{12}\text{H}_{22}\text{O}_{11}$ (table sugar), and **(b)** calcium nitrate, $\text{Ca}(\text{NO}_3)_2$.

Exercise 8

Calculate the formula weight of **(a)** $\text{Al}(\text{OH})_3$ and **(b)** CH_3OH .

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:

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



Percent Composition

So the percentage of carbon in ethane is

$$\begin{aligned}\%C &= \frac{(2)(12.011 \text{ amu})}{(30.070 \text{ amu})} \\ &= \frac{24.022 \text{ amu}}{30.070 \text{ amu}} \times 100 \\ &= 79.887\%\end{aligned}$$



Exercise 9: Calculating Percentage Composition

Calculate the percentage of carbon, hydrogen, and oxygen (by mass) in $\text{C}_{12}\text{H}_{22}\text{O}_{11}$.

$$\% \text{C} = \frac{(12)(12.0 \text{ amu})}{342.0 \text{ amu}} \times 100\% = 42.1\%$$

$$\% \text{H} = \frac{(22)(1.0 \text{ amu})}{342.0 \text{ amu}} \times 100\% = 6.4\%$$

$$\% \text{O} = \frac{(11)(16.0 \text{ amu})}{342.0 \text{ amu}} \times 100\% = 51.5\%$$

Avogadro's Number and Moles



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.

Single molecule



1 molecule H_2O
(18.0 amu)

Avogadro's number of water molecules in a mole of water.

Laboratory-size sample



1 mol H_2O
(18.0 g)

Avogadro's Number

6.02×10^{23} particles

1 mole

or

1 mole

6.02×10^{23} particles

Molar Mass

- By definition, a **molar mass** is the mass of 1 mol of a substance (i.e., g/mol).
 - The molar mass of an element is the mass number for the element that we find on the periodic table.
 - The formula weight (in amu's) will be the same number as the molar mass (in g/mol).



A Moles of Particles

Contains **6.02×10^{23}** particles

1 mole C = **6.02×10^{23}** C atoms

1 mole H₂O = **6.02×10^{23}** H₂O molecules

1 mole NaCl = **6.02×10^{23}** Na⁺ ions and
 6.02×10^{23} Cl⁻ ions

Examples of Moles

Moles of elements

1 mole Mg = 6.02×10^{23} Mg atoms

1 mole Au = 6.02×10^{23} Au atoms

Moles of compounds

1 mole NH_3 = 6.02×10^{23} NH_3 molecules

1 mole $\text{C}_9\text{H}_8\text{O}_4$ = 6.02×10^{23} aspirin molecules

Exercise 10: How many atoms are in 0.551 g of potassium (K) ?

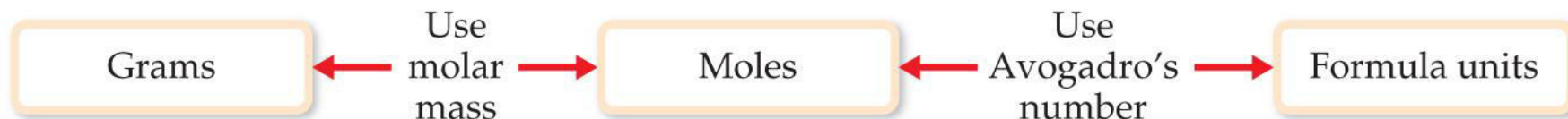
$$1 \text{ mol K} = 39.10 \text{ g K}$$

$$1 \text{ mol K} = 6.022 \times 10^{23} \text{ atoms K}$$

$$0.551 \text{ g K} \times \frac{1 \text{ mol K}}{39.10 \text{ g K}} \times \frac{6.022 \times 10^{23} \text{ atoms K}}{1 \text{ mol K}} =$$

$$8.49 \times 10^{21} \text{ atoms K}$$

Using Moles



© 2012 Pearson Education, Inc.

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	$\left\{ \begin{array}{l} 6.02 \times 10^{23} \text{ N}_2 \text{ molecules} \\ 2(6.02 \times 10^{23}) \text{ N atoms} \end{array} \right.$
Silver	Ag	107.9	107.9	6.02×10^{23} Ag atoms
Silver ions	Ag ⁺	107.9*	107.9	6.02×10^{23} Ag ⁺ ions
Barium chloride	BaCl ₂	208.2	208.2	$\left\{ \begin{array}{l} 6.02 \times 10^{23} \text{ BaCl}_2 \text{ formula units} \\ 6.02 \times 10^{23} \text{ Ba}^{2+} \text{ ions} \\ 2(6.02 \times 10^{23}) \text{ Cl}^- \text{ ions} \end{array} \right.$

*Recall that the electron has negligible mass; thus, ions and atoms have essentially the same mass.

© 2012 Pearson Education, Inc.

- 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.



Exercise 11: Converting Grams to Moles

Calculate the number of moles of glucose ($\text{C}_6\text{H}_{12}\text{O}_6$) in 5.380 g of $\text{C}_6\text{H}_{12}\text{O}_6$.

$$\text{Moles } \text{C}_6\text{H}_{12}\text{O}_6 = (5.380 \text{ g } \text{C}_6\text{H}_{12}\text{O}_6) \left(\frac{1 \text{ mol } \text{C}_6\text{H}_{12}\text{O}_6}{180.0 \text{ g } \text{C}_6\text{H}_{12}\text{O}_6} \right) = 0.02989 \text{ mol } \text{C}_6\text{H}_{12}\text{O}_6$$

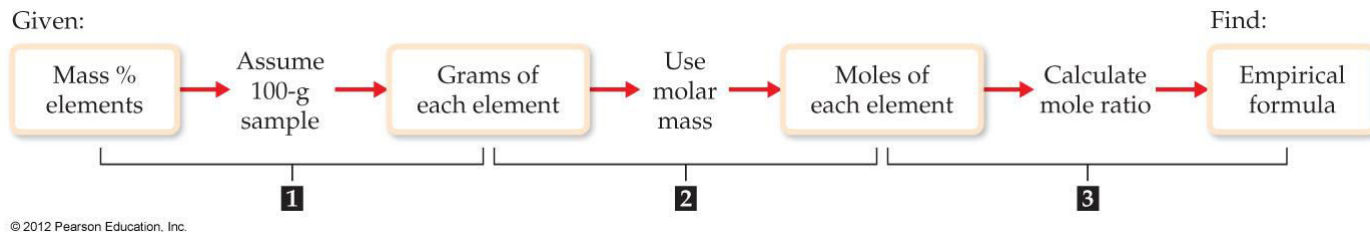
Exercise 12

How many moles of sodium bicarbonate (NaHCO_3) are in 508 g of NaHCO_3 ?

Finding Empirical Formulas



Calculating Empirical Formulas



One can calculate the empirical formula from the percent composition.

Calculating Empirical Formulas

Example 13: 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.



Calculating Empirical Formulas

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:

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

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

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

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

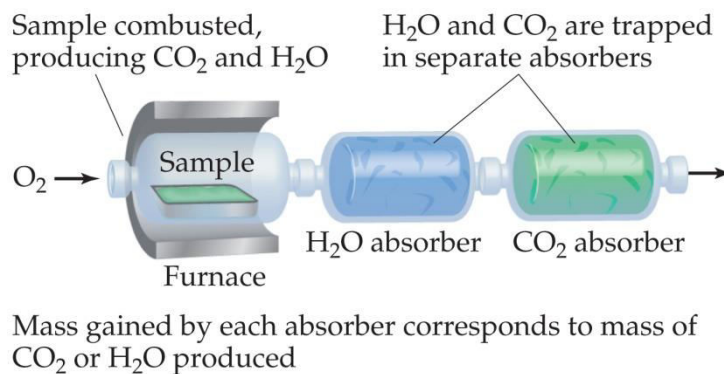


Calculating Empirical Formulas

These are the subscripts for the empirical formula:

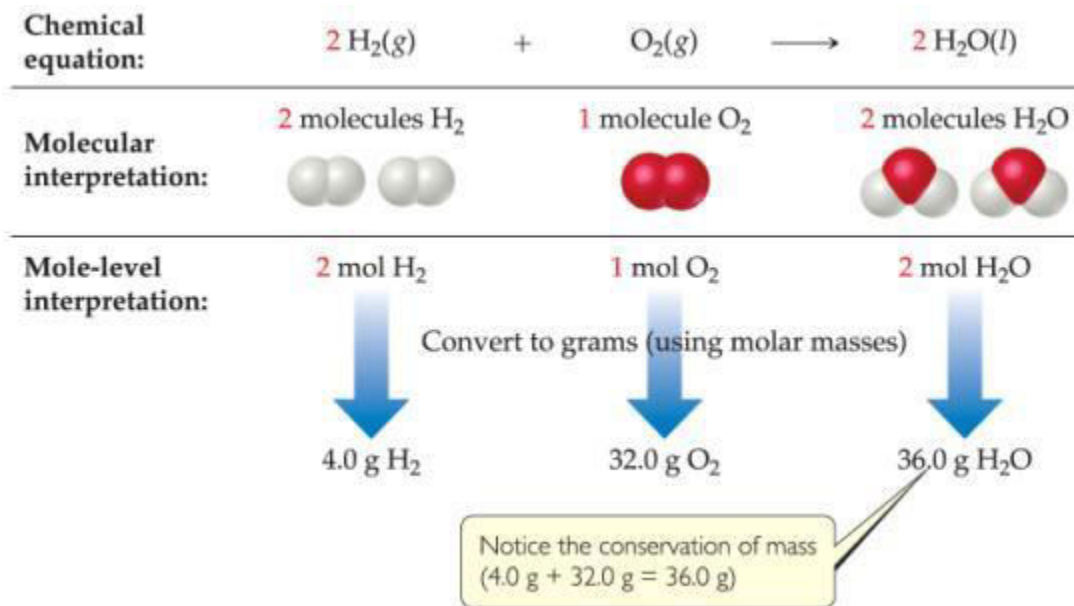


Combustion Analysis



- 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 difference after the 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



2 atoms of sodium combines with one molecule of chlorine to produce two molecules of sodium chloride.

In terms of mole, 2 moles of sodium combines with one mole of chlorine to produce two mole of sodium chloride.

In grams, 2 moles Na = $2 \times 23 = 46 \text{ g}$

1 mole of $\text{Cl}_2 = 2 \times 35.45 = 70.9 \text{ g}$

2 moles of NaCl = $2(23 + 35.45) = 116.9 \text{ g}$

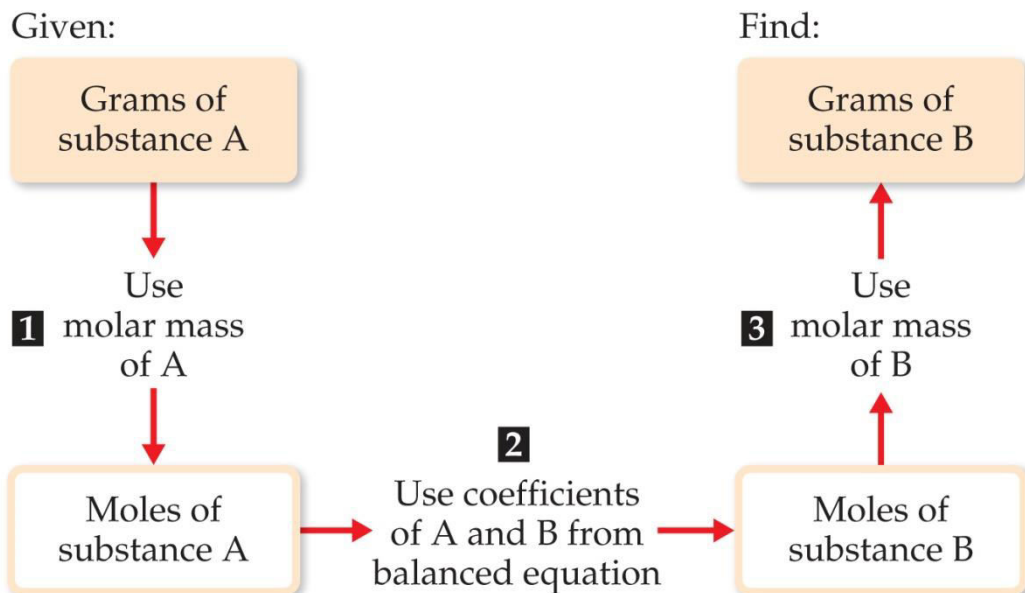
(Note: Law of Conservation of Mass holds here)

The coefficients in the balanced equation give the ratio of *moles* of reactants and products.



Stoichiometric Calculations

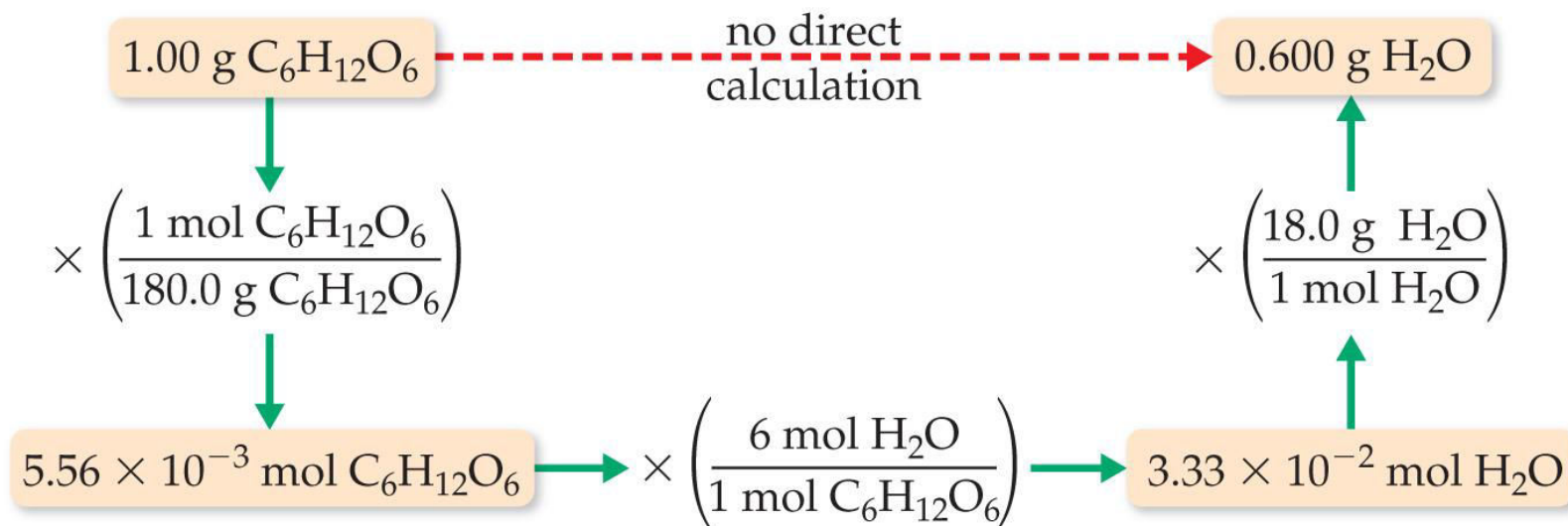
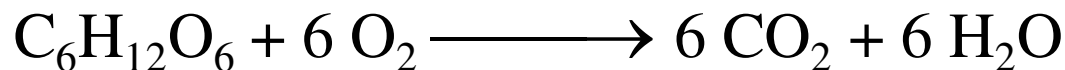
Starting with the mass of Substance A, you can use the ratio of the coefficients of A and B to calculate the mass of Substance B formed (if it's a product) or used (if it's a reactant).



© 2012 Pearson Education, Inc.



Stoichiometric Calculations



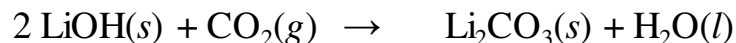
© 2012 Pearson Education, Inc.

Starting with 1.00 g of $\text{C}_6\text{H}_{12}\text{O}_6$...
we calculate the moles of $\text{C}_6\text{H}_{12}\text{O}_6$...
use the coefficients to find the moles of H_2O ...
and then turn the moles of water to grams.



Exercise 14 Calculating Amounts of Reactants and Products

Solid lithium hydroxide is used in space vehicles to remove the carbon dioxide gas exhaled by astronauts. The hydroxide reacts with the carbon dioxide to form solid lithium carbonate and liquid water. How many grams of carbon dioxide can be absorbed by 1.00 g of lithium hydroxide?

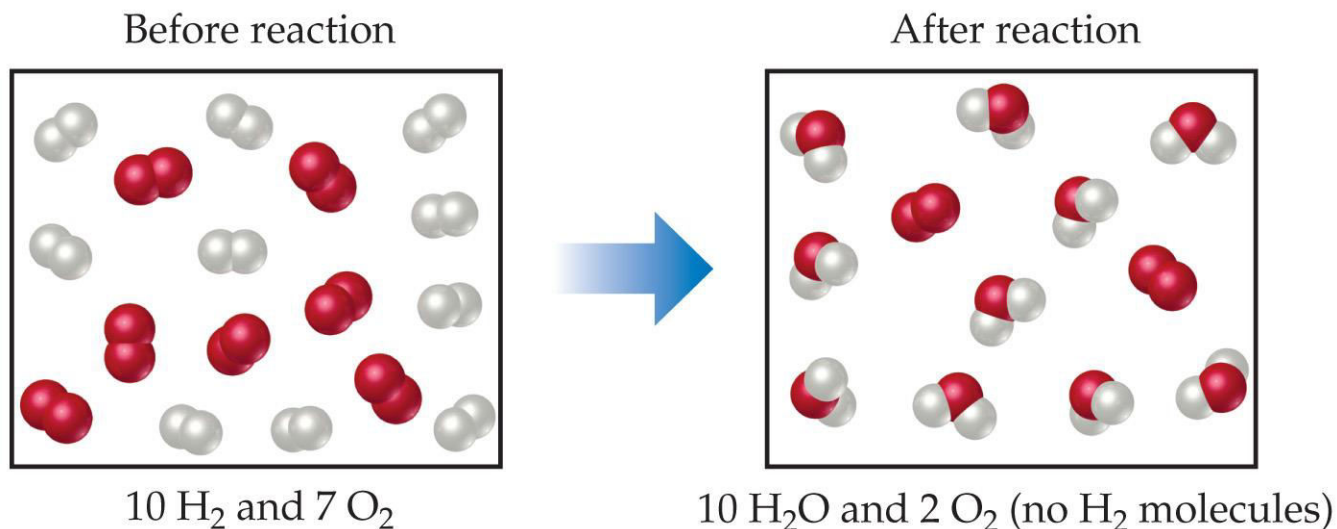


Limiting Reactants



Limiting Reactants

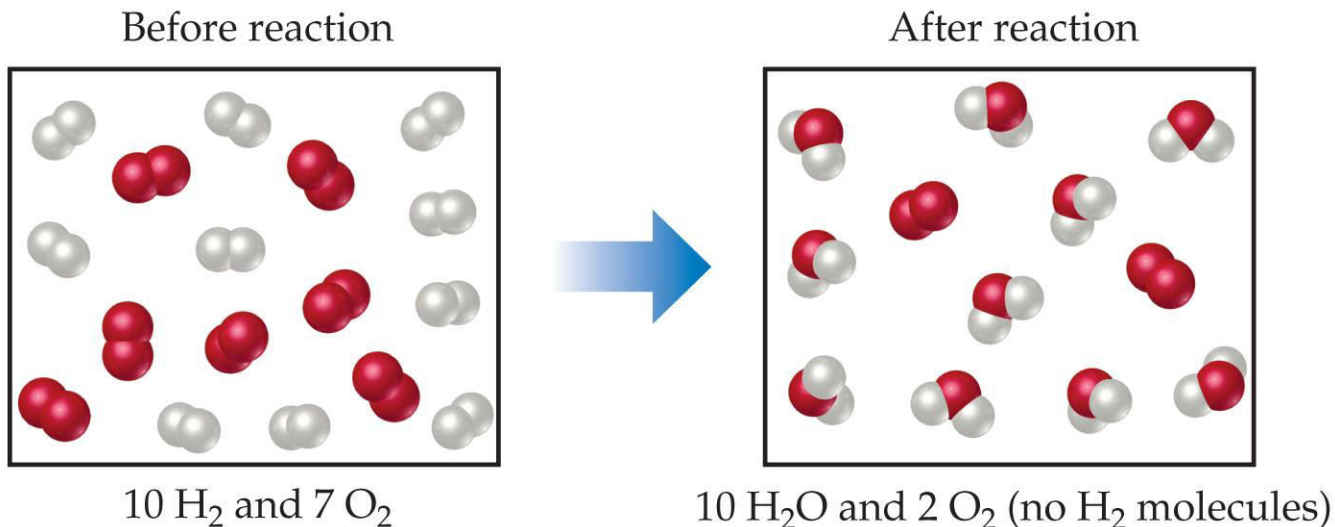
- The **limiting reactant** is the reactant present in the smallest stoichiometric amount.
 - In other words, it's the reactant you'll run out of first (in this case, the H_2).



© 2012 Pearson Education, Inc.

Limiting Reactants

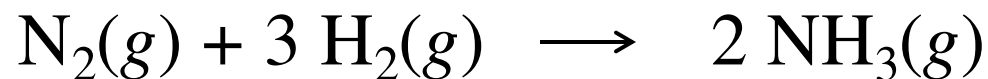
In the example below, the O_2 would be the **excess reagent**.



© 2012 Pearson Education, Inc.

Exercise 15 Calculating the Amount of Product Formed from a Limiting Reactant

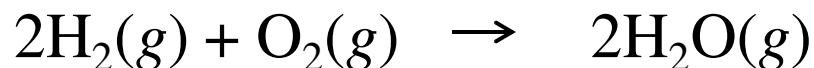
The most important commercial process for converting N_2 from the air into nitrogen-containing compounds is based on the reaction of N_2 and H_2 to form ammonia (NH_3):



How many moles of NH_3 can be formed from 3.0 mol of N_2 and 6.0 mol of H_2 ?

Exercise 16 Calculating the Amount of Product Formed from a Limiting Reactant

The reaction



is used to produce electricity in a hydrogen fuel cell. Suppose a fuel cell contains 150 g of $\text{H}_2(\text{g})$ and 1500 g of $\text{O}_2(\text{g})$ (each measured to two significant figures). How many grams of water can form?



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

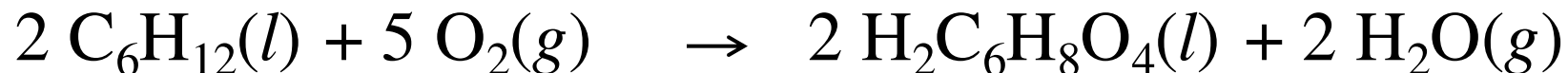
One finds the **percent yield** by comparing the amount actually obtained (actual yield) to the amount it was possible to make (theoretical yield):

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



Exercise 17: Calculating Theoretical Yield and Percent Yield

Adipic acid, $\text{H}_2\text{C}_6\text{H}_8\text{O}_4$, used to produce nylon, is made commercially by a reaction between cyclohexane (C_6H_{12}) and O_2 :



(a) Assume that you carry out this reaction with 25.0 g of cyclohexane and that cyclohexane is the limiting reactant. What is the theoretical yield of adipic acid? **(b)** If you obtain 33.5 g of adipic acid, what is the percent yield for the reaction?

Exercise 17

Continued

$$\begin{aligned}\text{Grams H}_2\text{C}_6\text{H}_8\text{O}_4 &= (25.0 \text{ g C}_6\text{H}_{12}) \left(\frac{1 \text{ mol C}_6\text{H}_{12}}{84.0 \text{ g C}_6\text{H}_{12}} \right) \left(\frac{2 \text{ mol H}_2\text{C}_6\text{H}_8\text{O}_4}{2 \text{ mol C}_6\text{H}_{12}} \right) \left(\frac{146.0 \text{ g H}_2\text{C}_6\text{H}_8\text{O}_4}{1 \text{ mol H}_2\text{C}_6\text{H}_8\text{O}_4} \right) \\ &= 43.5 \text{ g H}_2\text{C}_6\text{H}_8\text{O}_4\end{aligned}$$

$$\text{(b) Percent yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100\% = \frac{33.5 \text{ g}}{43.5 \text{ g}} \times 100\% = 77.0\%$$



Calculate the formula weight of the following compounds from their formulas. Report your answers to three significant figures.

calcium hydroxide, $\text{Ca}(\text{OH})_2$

methylamine, CH_3NH_2



1 Ca	1(40.08) =	40.08 amu
2 O	2(16.00) =	32.00 amu
2 H	2(1.008) =	<u>2.016 amu</u>

Total	74.096	2 decimal places
		74.10 amu



1 C	1(12.01) =	12.01 amu
1 N	1(14.01) =	14.01 amu
5 H	5(1.008) =	<u>5.040 amu</u>

Total	31.060	2 significant figures
		31.06 amu



What is the mass in grams of the nitric acid molecule, HNO_3 ?

First, find the molar mass of HNO_3 :

$$1 \text{ H} \quad 1(1.008) = \quad 1.008$$

$$1 \text{ N} \quad 1(14.01) = \quad 14.01$$

$$3 \text{ O} \quad 3(16.00) = \quad 48.00$$

$$\hline 63.018$$

(2 decimal places)

63.02 g/mol



A sample of nitric acid, HNO_3 , contains 0.253 mol HNO_3 . How many grams is this?

First, find the molar mass of HNO_3 :

1 H	$1(1.008) =$	1.008
1 N	$1(14.01) =$	14.01
3 O	$3(16.00) =$	48.00
		63.018

(2 decimal places)

63.02 g/mol

Note:

We need one digit more in the molar mass than in the measured quantity.

Next, using the molar mass, find the mass of 0.253 mole:

$$0.253 \text{ mole} \times \frac{63.02 \text{ g}}{1 \text{ mole}} \\ = 15.94406 \text{ g}$$

$$= 15.9 \text{ g}$$

(3 significant figures)



Calcite is a mineral composed of calcium carbonate, CaCO_3 . A sample of calcite composed of pure calcium carbonate weighs 23.6 g. How many moles of calcium carbonate is this?

First, find the molar mass of CaCO_3 :

1 Ca	1(40.08) =	40.08
1 C	1(12.01) =	12.01
3 O	3(16.00) =	48.00
		100.09

2 decimal places

100.09 g/mol

Next, find the number of moles in 23.6 g:

$$\begin{aligned} & 23.6 \text{ g} \times \frac{1 \text{ mole}}{100.09 \text{ g}} \\ &= 2.35787791 \times 10^{-1} \text{ g} \\ &= 2.36 \times 10^{-1} \text{ g or } 0.236 \text{ g} \\ & \quad (3 \text{ significant figures}) \end{aligned}$$



The average daily requirement of the essential amino acid leucine, $\text{C}_6\text{H}_{14}\text{O}_2\text{N}$, is 2.2 g for an adult. What is the average daily requirement of leucine in moles?

First, find the molar mass of leucine:

6 C	$6(12.01) =$	72.06
2 O	$2(16.00) =$	32.00
1 N	$1(14.01) =$	14.01
14 H	$14(1.008) =$	14.112
		132.182

2 decimal places

132.18 g/mol

Next, find the number of moles in 2.2 g:

$$2.2 \text{ g} \times \frac{1 \text{ mole}}{132.18 \text{ g}}$$

$$= 1.6643 \times 10^{-2} \text{ mol}$$

$$= 1.7 \times 10^{-2} \text{ mol} \quad \text{or} \quad 0.017 \text{ mol}$$

(2 significant figures)



The daily requirement of chromium in the human diet is 1.0×10^{-6} g. How many atoms of chromium does this represent?



First, find the molar mass of Cr:

$$1 \text{ Cr } 1(51.996) = 51.996$$

Now, convert 1.0×10^{-6} grams to moles:

$$1.0 \times 10^{-6} \text{ g} \times \frac{1 \text{ mol}}{51.996 \text{ g}} \times \frac{6.022 \times 10^{23} \text{ atoms}}{1 \text{ mol}}$$

$$= 1.158166 \times 10^{16} \text{ atoms}$$

$$\boxed{1.2 \times 10^{16} \text{ atoms}}$$

(2 significant figures)



Lead(II) chromate, PbCrO_4 , is used as a paint pigment (chrome yellow). What is the percentage composition of lead(II) chromate?

First, find the molar mass of PbCrO_4 :

$$\begin{array}{rcl} 1 \text{ Pb} & 1(207.2) = & 207.2 \\ 1 \text{ Cr} & 1(51.996) = & 51.996 \\ 4 \text{ O} & 4(16.00) = & 64.00 \\ & & \hline & & 323.196 \end{array}$$

(1 decimal place)

323.2 g/mol

Now, convert each to percent composition:

$$\text{Pb : } \frac{207.2 \text{ g}}{323.20 \text{ g}} \times 100\% = 64.11\%$$

$$\text{Cr : } \frac{51.996 \text{ g}}{323.20 \text{ g}} \times 100\% = 16.09\%$$

$$\text{O : } \frac{64.00 \text{ g}}{323.20 \text{ g}} \times 100\% = 19.80\%$$

Check:

$$64.11 + 16.09 + 19.80 = 100.00$$



The chemical name of table sugar is sucrose, $\text{C}_{12}\text{H}_{22}\text{O}_{11}$. How many grams of carbon are in 68.1 g of sucrose?

First, find the molar mass of $\text{C}_{12}\text{H}_{22}\text{O}_{11}$:

$$12 \text{ C } 12(12.01) = 144.12$$

$$11 \text{ O } 11(16.00) = 176.00$$

$$22 \text{ H } 22(1.008) = \underline{22.176}$$

$$342.296$$

(2 decimal places)

342.30 g/mol

Now, find the mass of carbon in 68.1 g sucrose:

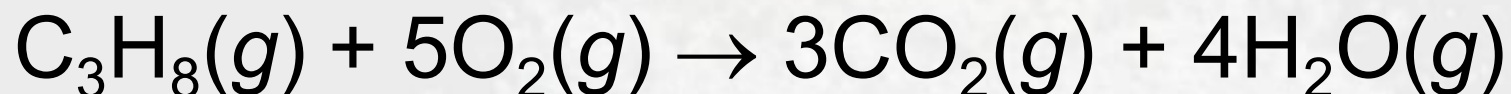
$$68.1 \text{ g sucrose} \times \frac{144.12 \text{ g carbon}}{342.30 \text{ g sucrose}}$$

$$= 28.7 \text{ g carbon}$$

(3 significant figures)



Propane, C_3H_8 , is normally a gas, but it is sold as a fuel compressed as a liquid in steel cylinders. The gas burns according to the following equation:



How many grams of O_2 are required to burn 20.0 g of propane?

Molar masses:

$$\text{O}_2 \quad 2(16.00) = 32.00 \text{ g}$$

$$\text{C}_3\text{H}_8 \quad 3(12.01) + 8(1.008) = 44.094 \text{ g}$$

$$20.0 \text{ g C}_3\text{H}_8 \frac{1 \text{ mol C}_3\text{H}_8}{44.094 \text{ g C}_3\text{H}_8} \frac{5 \text{ mol O}_2}{1 \text{ mol C}_3\text{H}_8} \frac{32.00 \text{ g O}_2}{1 \text{ mol O}_2}$$
$$= 72.57223205 \text{ g O}_2$$

$$72.6 \text{ g O}_2$$

(3 significant figures)