Stoichiometry: Calculations with Chemical Formulas and Equations

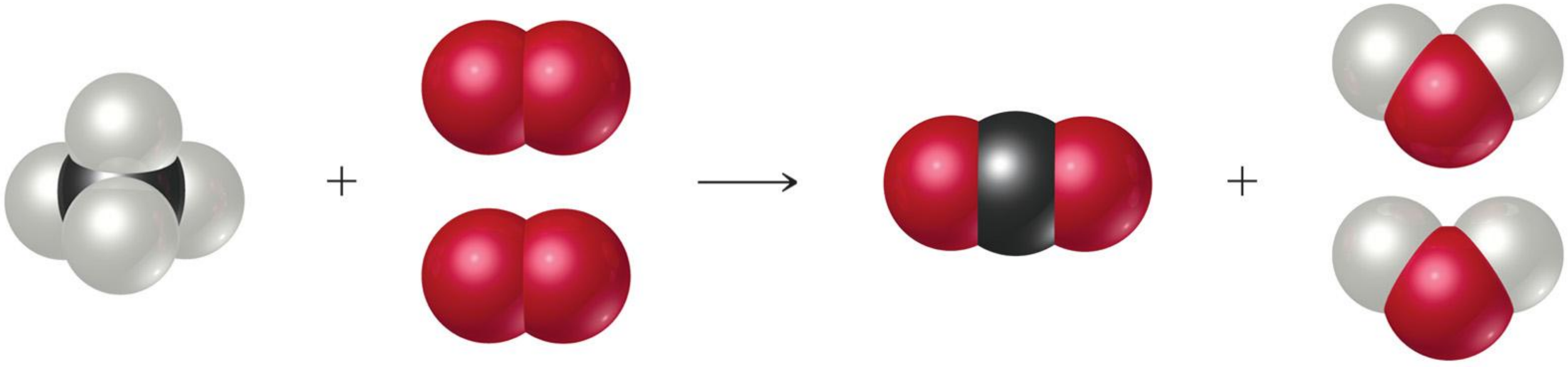
Law of Conservation of Mass

"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, 1789

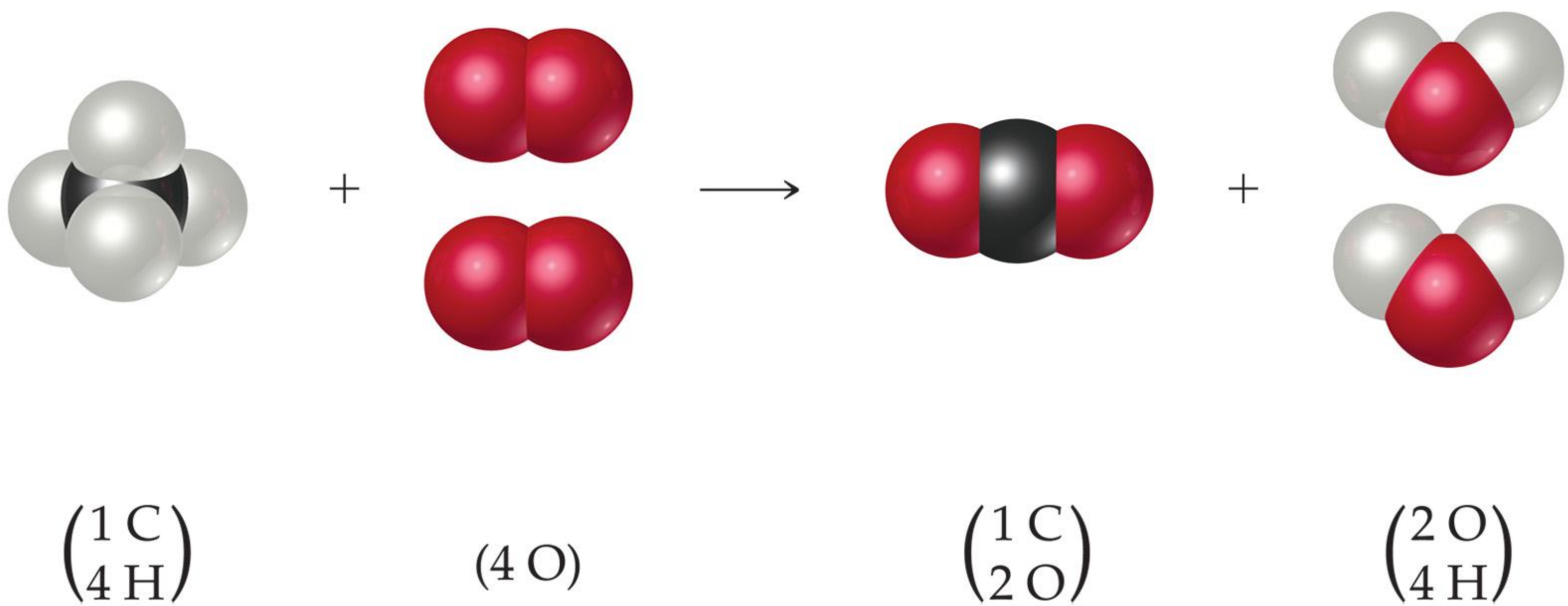
Chemical Equations

Concise representations of chemical reactions



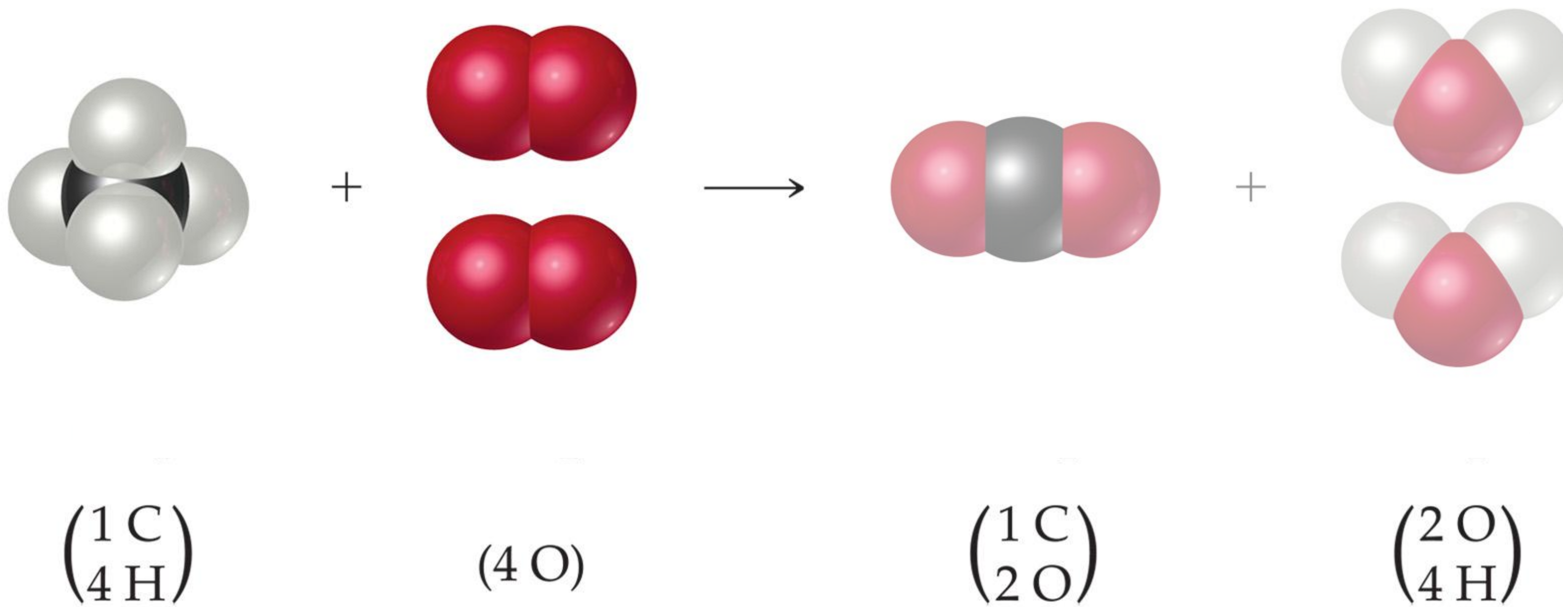
Anatomy of a Chemical Equation

$$CH_{4\,(g)} + 2\ O_{2\,(g)} \longrightarrow CO_{2\,(g)} + 2\ H_2O_{\,(g)}$$



Anatomy of a Chemical Equation

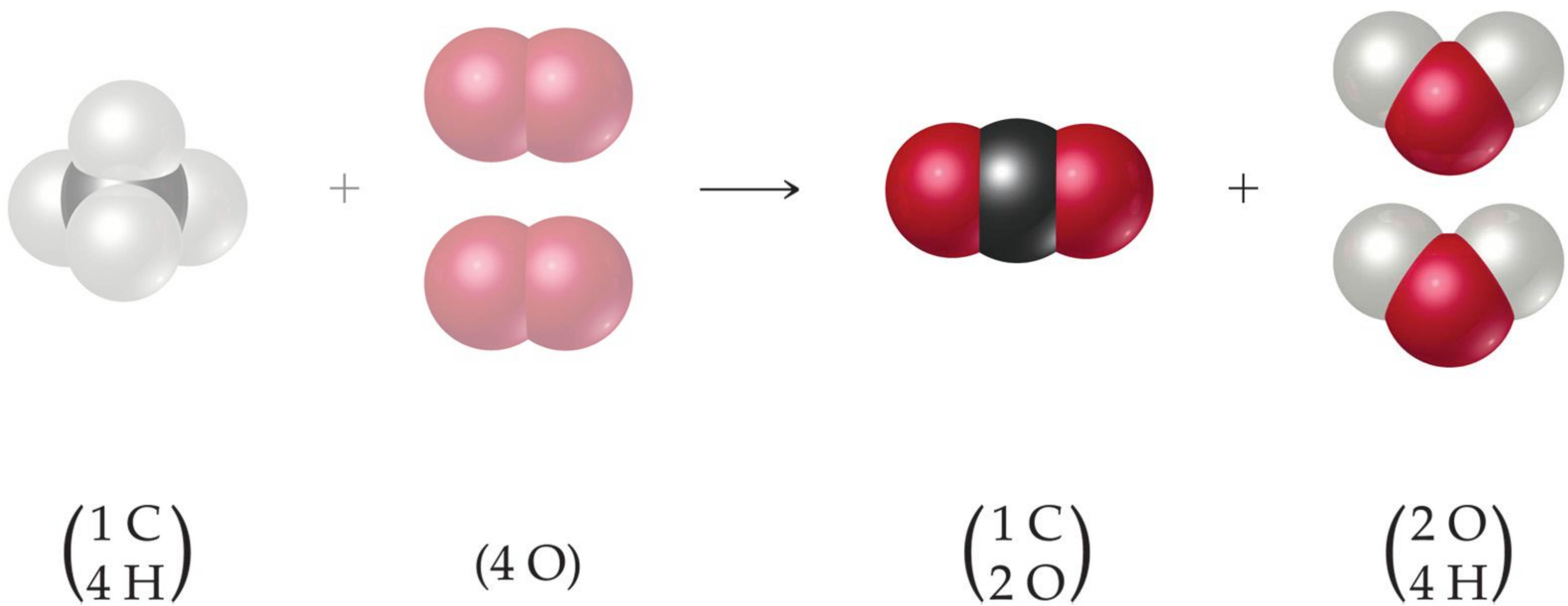
$$CH_{4\,(g)} + 2\ O_{2\,(g)} \longrightarrow CO_{2\,(g)} + 2\ H_2O_{\,(g)}$$



Reactants appear on the left side of the equation.

Anatomy of a Chemical Equation

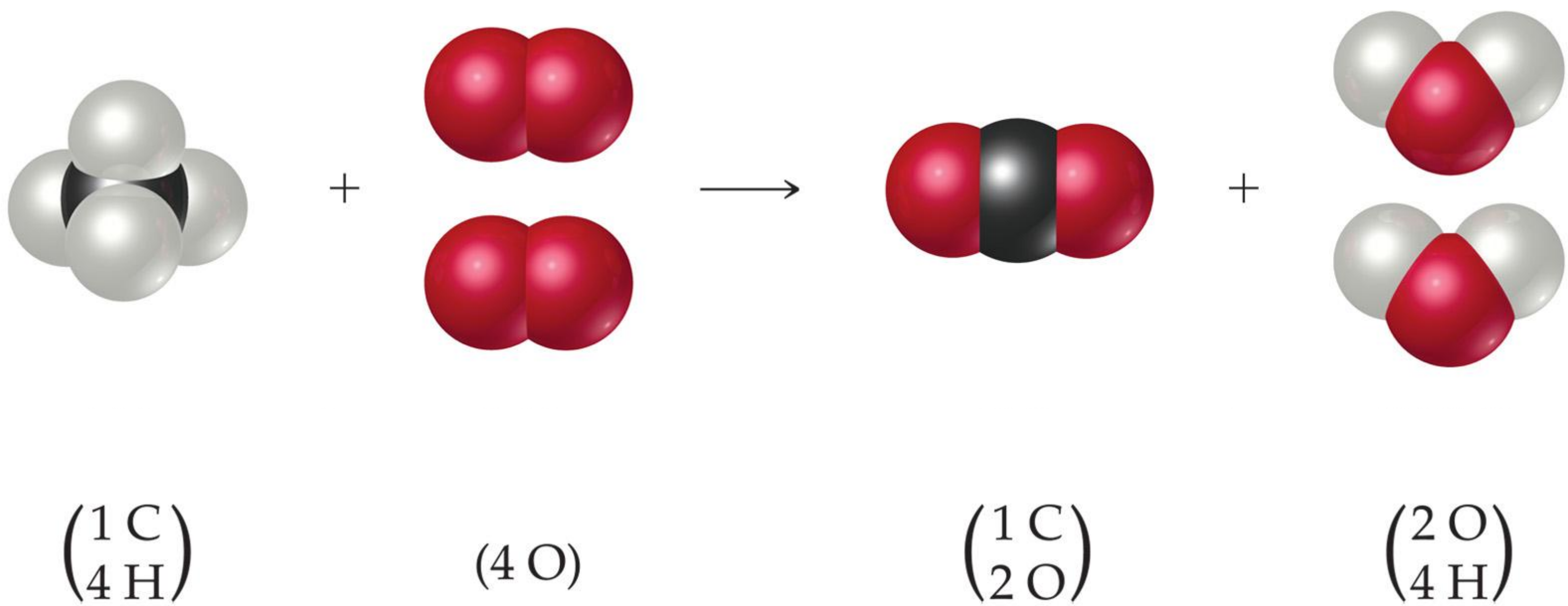
$$CH_{4\,(g)} + 2\ O_{2\,(g)} \longrightarrow CO_{2\,(g)} + 2\ H_2O_{\,(g)}$$



Products appear on the right side of the equation.

Anatomy of a Chemical Equation

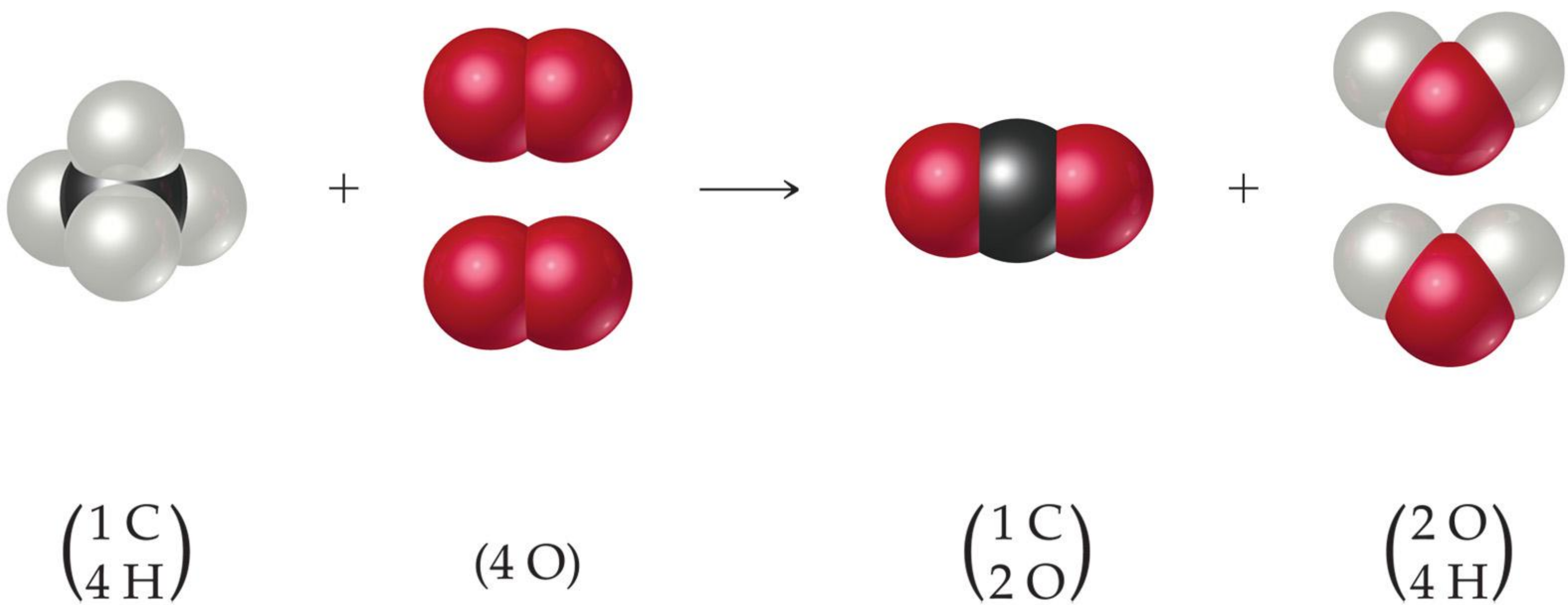
$$CH_{4\,(g)} + 2\,O_{2\,(g)} \longrightarrow CO_{2\,(g)} + 2\,H_2O_{\,(g)}$$



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

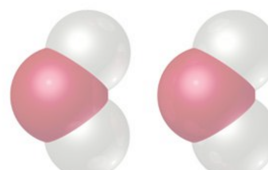
Anatomy of a Chemical Equation

$$CH_{4\,(g)} + 2\ O_{2\,(g)} \longrightarrow CO_{2\,(g)} + 2\ H_2O_{\,(g)}$$



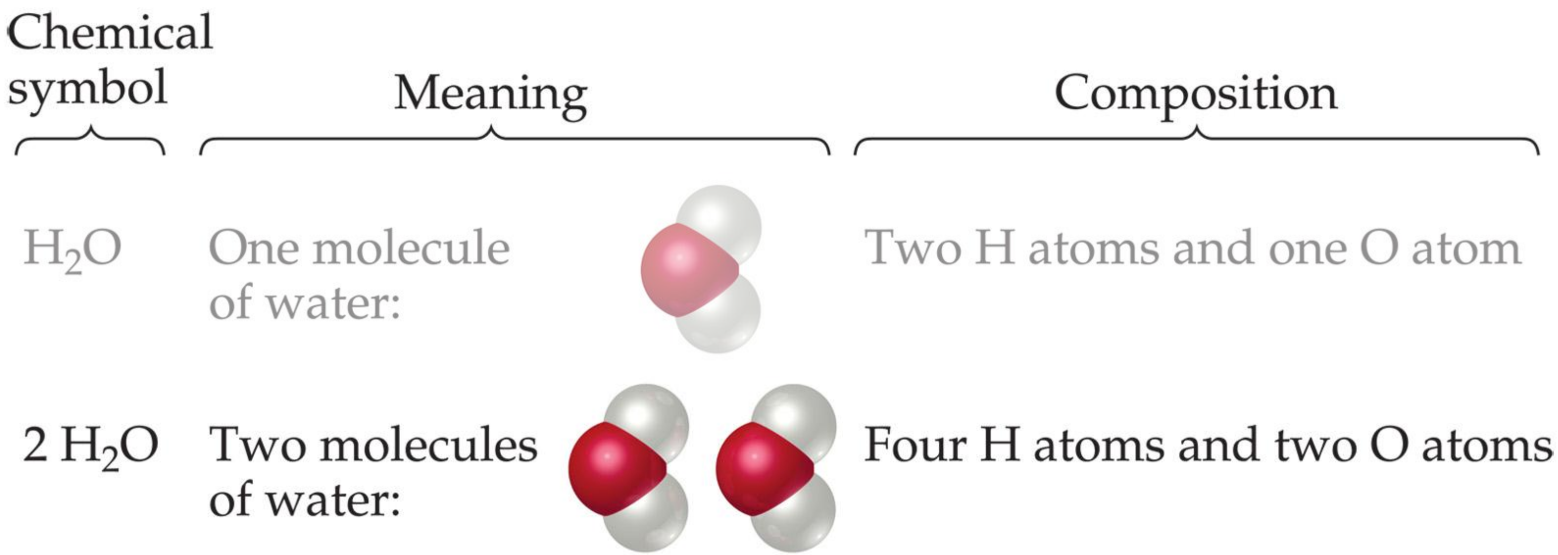
Coefficients are inserted to balance the equation.

Subscripts and Coefficients Give Different Information

Chemical symbol	Meaning		Composition
H_2O	One molecule of water:		Two H atoms and one O atom
$2\,H_2O$	Two molecules of water:		Four H atoms and two O atoms

- Subscripts tell the number of atoms of each element in a molecule

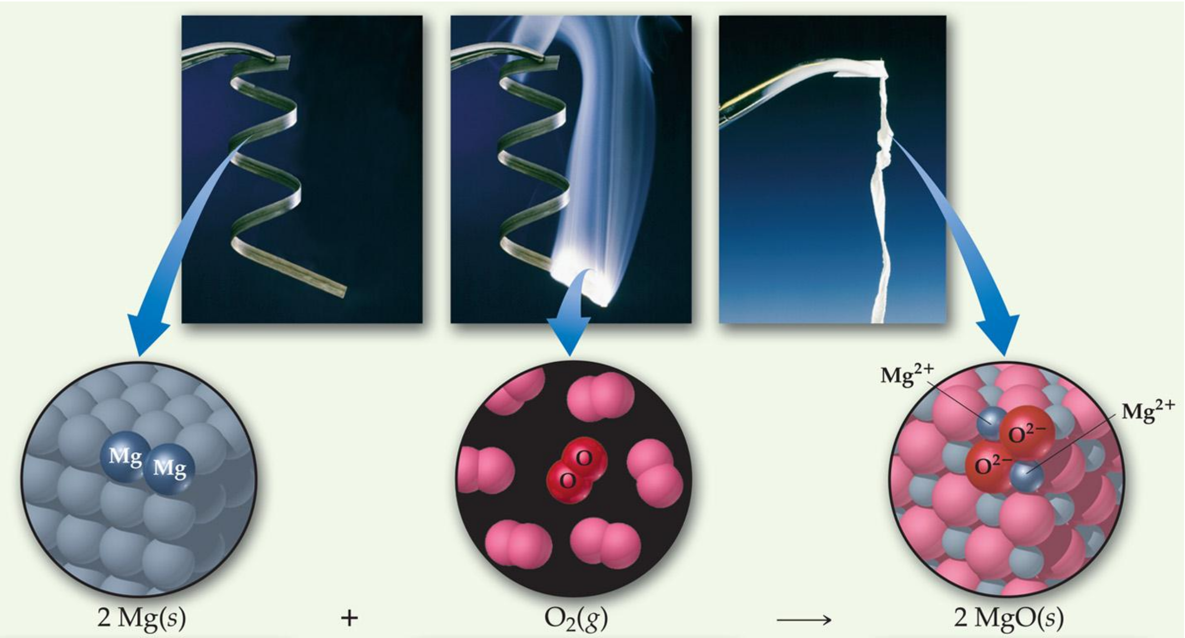
Subscripts and Coefficients Give Different Information



- Subscripts tell the number of atoms of each element in a molecule
- Coefficients tell the number of molecules

Reaction Types

Combination Reactions



- Two or more substances react to form one product

- Examples:

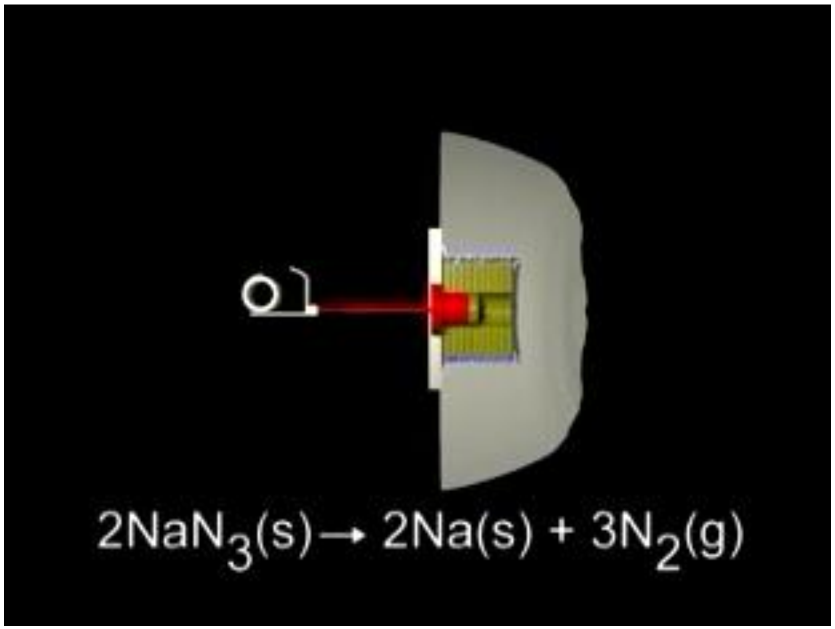
$$N_{2\,(g)} + 3\ H_{2\,(g)} \longrightarrow 2\ NH_{3\,(g)}$$

$$C_3H_{6\,(g)} + Br_{2\,(l)} \longrightarrow C_3H_6Br_{2\,(l)}$$

$$2\ Mg_{(s)} + O_{2\,(g)} \longrightarrow 2\ MgO_{(s)}$$

$$2\ Mg_{(s)} + O_{2\ (g)} \longrightarrow 2\ MgO_{(s)}$$

Decomposition Reactions



- 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

- Rapid reactions that produce a flame
- Most often involve hydrocarbons reacting with oxygen in the air

- 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 Weights

Formula Weight (FW)

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

$$\begin{array}{r} \text{Ca: } 1(40.1 \text{ amu}) \\ \underline{+\text{ Cl: } 2(35.5 \text{ amu})} \\ 111.1 \text{ amu} \end{array}$$

- These 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

$$
\begin{array}{lr}
C: & 2(12.0 \text{ amu}) \\
+ H: & 6(1.0 \text{ amu}) \\
\hline
 & 30.0 \text{ amu}
\end{array}
$$

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 of carbon in ethane is…

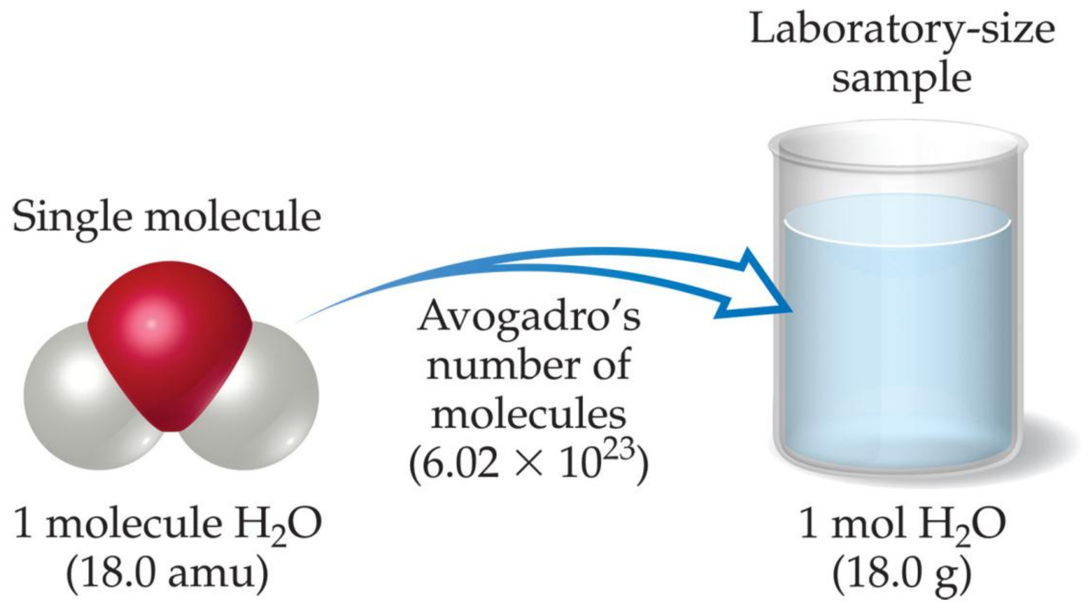
$$\%C = \frac{(2)(12.0\ \text{amu})}{(30.0\ \text{amu})}$$

$$= \frac{24.0\ \text{amu}}{30.0\ \text{amu}} \times 100$$

$$= 80.0\%$$

Moles

Avogadro's Number

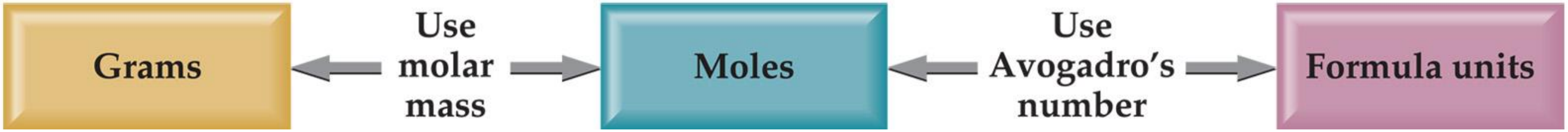


- 6.02×10^{23}
- 1 mole of ^{12}C has a mass of 12 g

Molar Mass

- By definition, these are 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)

Using Moles



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

Mole Relationships

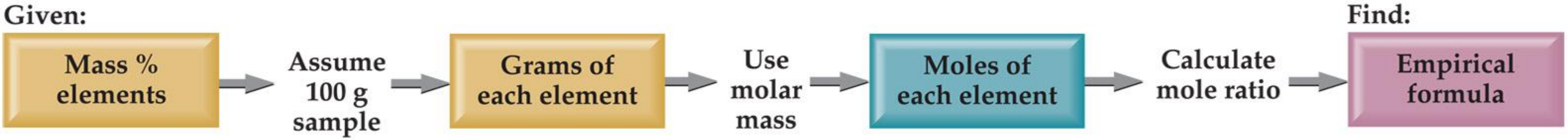
Name of substance	Formula	Formula Weight (amu)	Molar Mass (g/mol)	Number and Kind of Particles in One Mole
Atomic nitrogen	N	14.0	14.0	6.022×10^{23} N atoms
Molecular nitrogen	N_2	28.0	28.0	6.022×10^{23} N_2 molecules $2(6.022 \times 10^{23})$ N atoms
Silver	Ag	107.9	107.9	6.022×10^{23} Ag atoms
Silver ions	Ag^+	107.9[a]	107.9	6.022×10^{23} Ag^+ ions
Barium chloride	$BaCl_2$	208.2	208.2	6.022×10^{23} $BaCl_2$ units 6.022×10^{23} Ba^{2+} ions $2(6.022 \times 10^{23})$ Cl^- ions

[a]Recall that the electron has negligible mass; 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

Finding Empirical Formulas

Calculating Empirical Formulas



One can calculate the empirical formula from the percent composition

Calculating Empirical Formulas

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,

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

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

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

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

Calculating Empirical Formulas

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

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

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

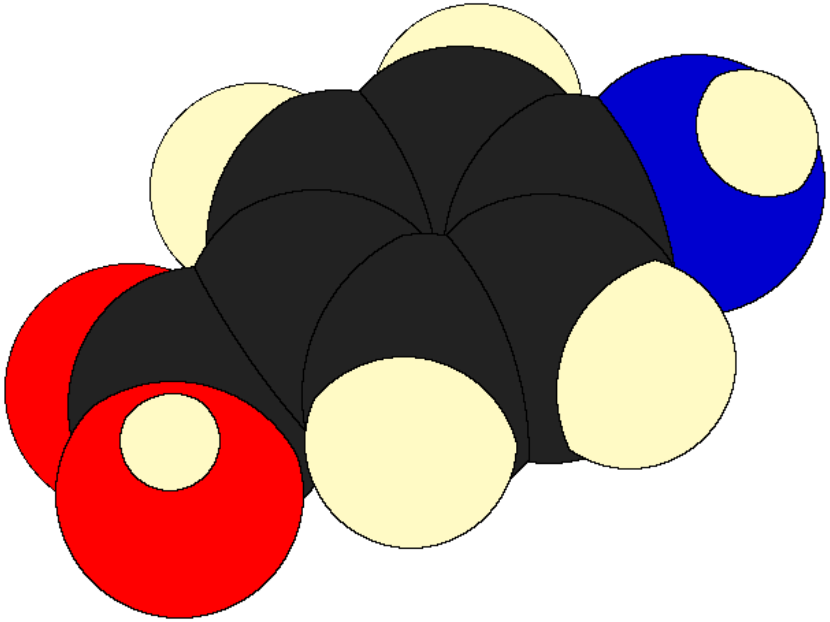
N: $\frac{0.7288 \text{ mol}}{0.7288 \text{ mol}} = 1.000$

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

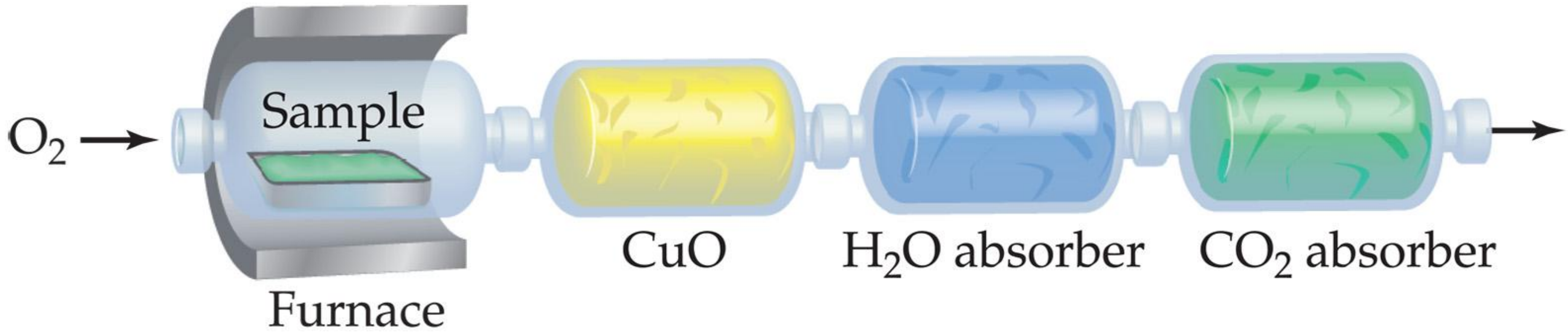
Calculating Empirical Formulas

These are the subscripts for the empirical formula:

$C_7H_7NO_2$



Combustion Analysis

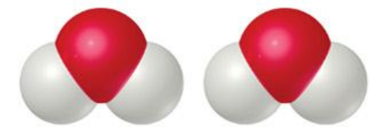


- Compounds containing C, H and O are routinely analyzed through combustion in a chamber like this
  - C is determined from the mass of CO_2 produced
  - H is determined from the mass of H_2O produced
  - O is determined by difference after the C and H have been determined

Elemental Analyses

Compounds containing other elements are analyzed using methods analogous to those used for C, H and O

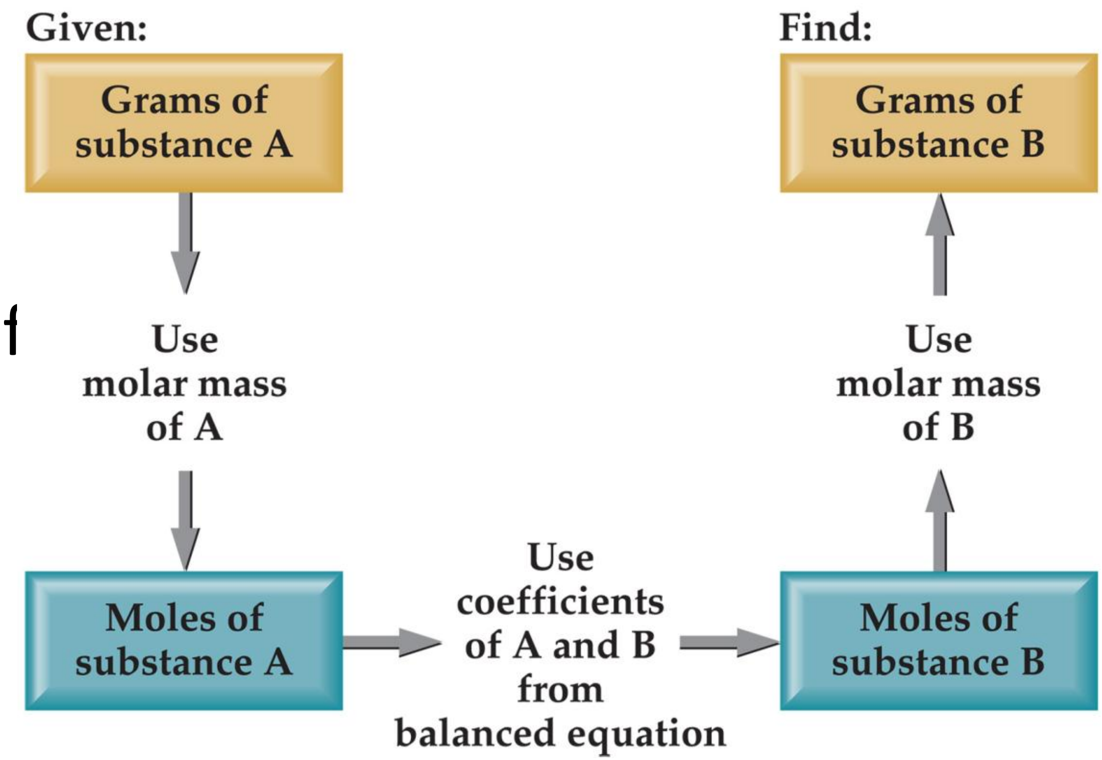
Stoichiometric Calculations

Equation:	**$2\ H_2(g)$**	**+**	**$O_2(g)$**	**$\longrightarrow$**	**$2\ H_2O(l)$**
Molecules:	2 molecules H_2	+	1 molecule O_2	$\longrightarrow$	2 molecules H_2O
					
Mass (amu):	4.0 amu H_2	+	32.0 amu O_2	$\longrightarrow$	36.0 amu H_2O
Amount (mol):	2 mol H_2	+	1 mol O_2	$\longrightarrow$	2 mol H_2O
Mass (g):	4.0 g H_2	+	32.0 g O_2	$\longrightarrow$	36.0 g H_2O

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

Stoichiometric Calculations

From 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)



Stoichiometric Calculations

$C_6H_{12}O_6 + 6\ O_2 \rightarrow 6\ CO_2 + 6\ H_2O$

Starting with 1.00 g of $C_6H_{12}O_6$…

we calculate the moles of $C_6H_{12}O_6$…

use the coefficients to find the moles of H_2O…

and then turn the moles of water to grams

Limiting Reactants

How Many Cookies Can I Make?

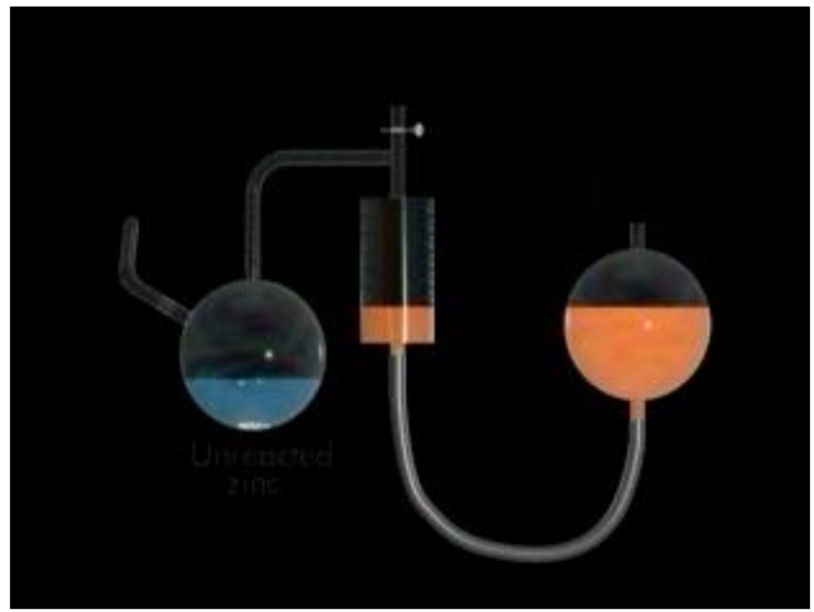
- You can make cookies until you run out of one of the ingredients
- Once this family runs out of sugar, they will stop making cookies (at least any cookies you would want to eat)

How Many Cookies Can I Make?

- In this example the sugar would be the limiting reactant, because it will limit the amount of cookies you can make

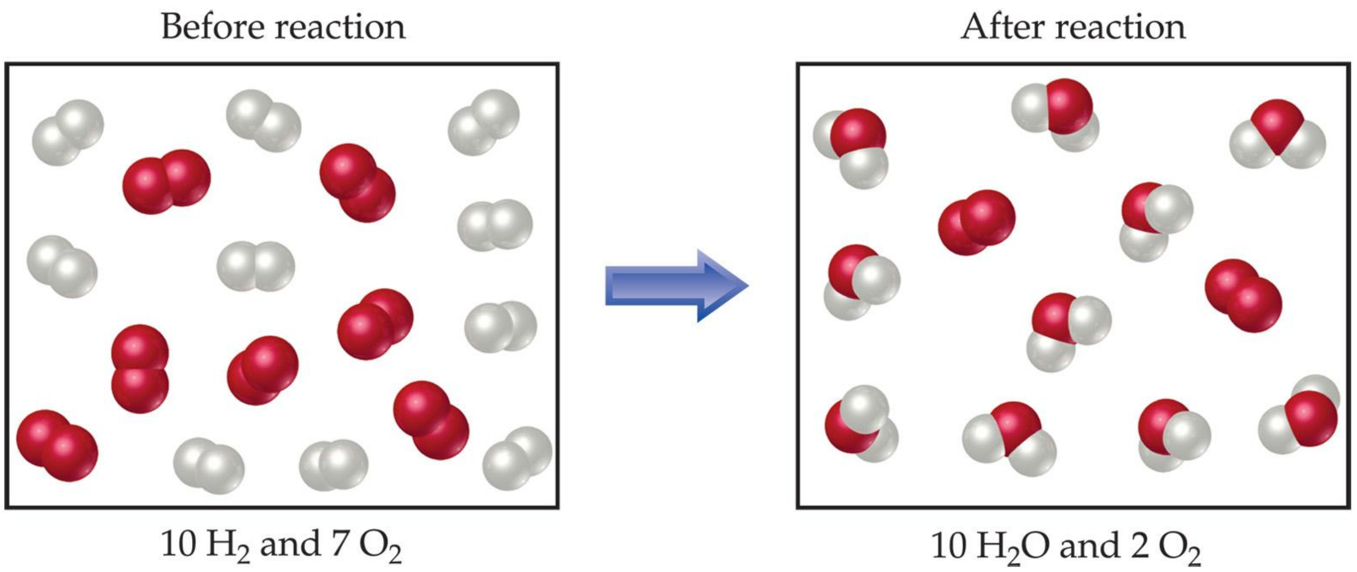
Limiting Reactants

The limiting reactant is the reactant present in the smallest stoichiometric amount



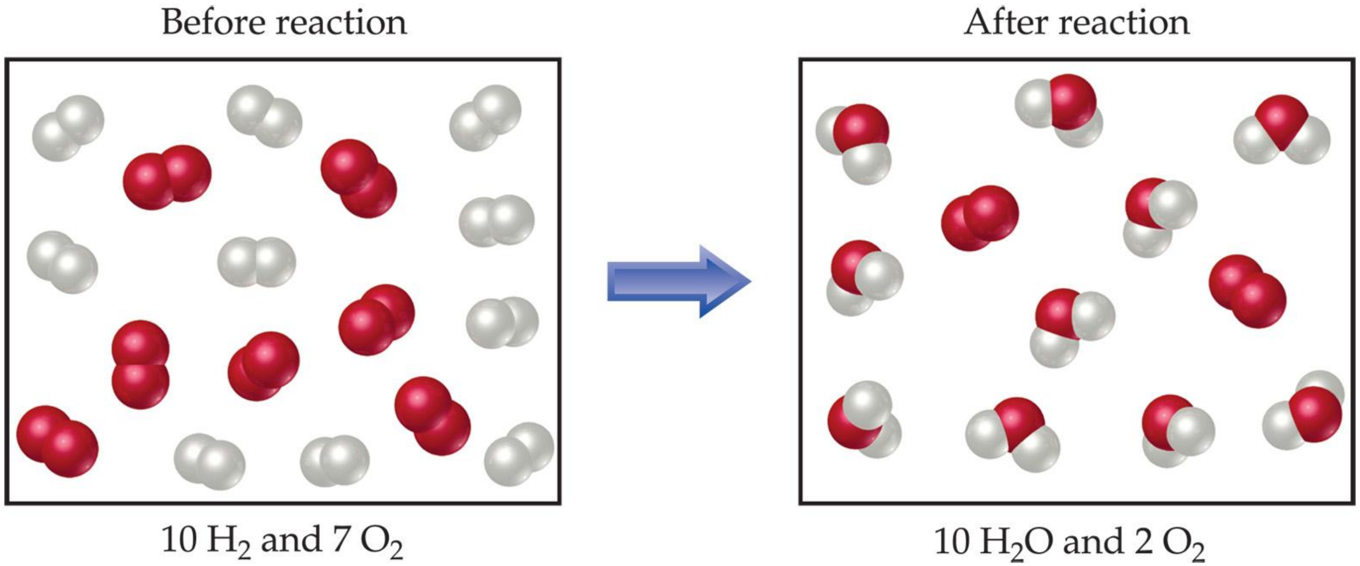
Limiting Reactants

- 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



Theoretical Yield

- The theoretical yield is the 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, the amount one actually produces and measures

Percent Yield

A comparison of the amount actually obtained to the amount it was possible to make

$$\text{Percent Yield} = \frac{\text{Actual Yield}}{\text{Theoretical Yield}} \times 100$$