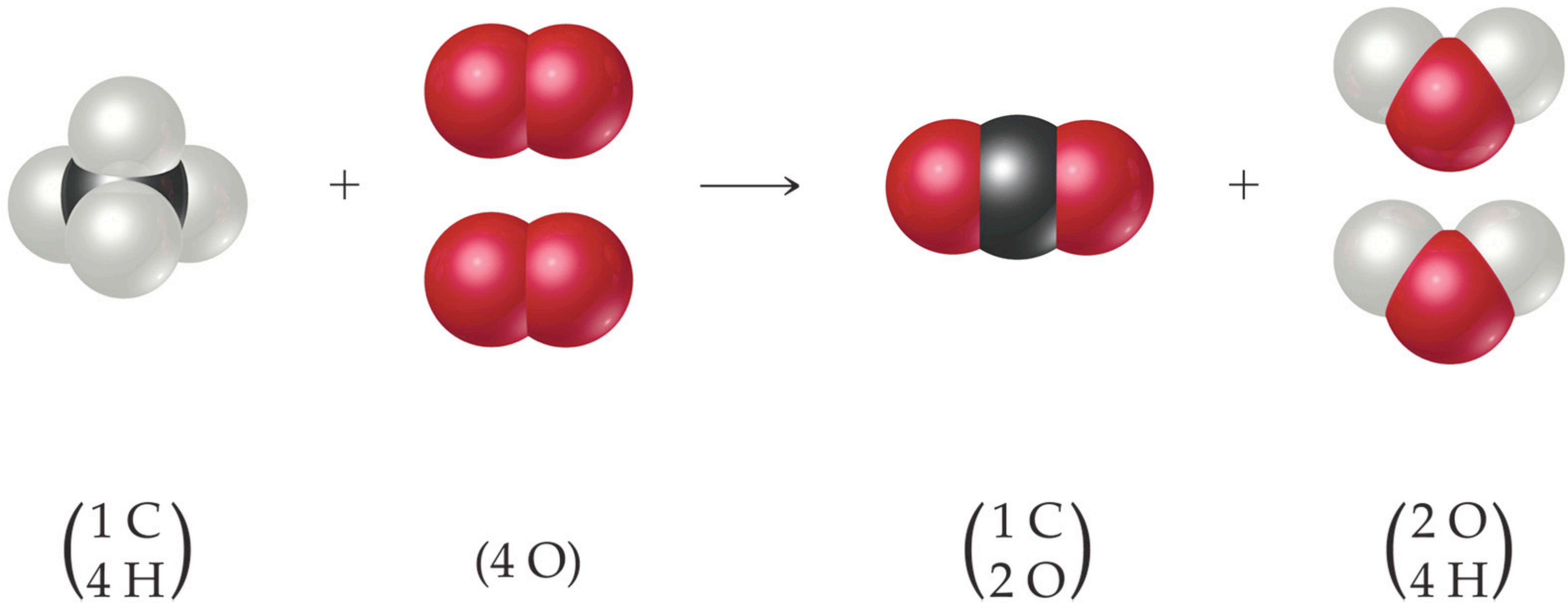
Chapter 3
Stoichiometry:

Calculations with Chemical Formulas and Equations

Anatomy of a Chemical Equation

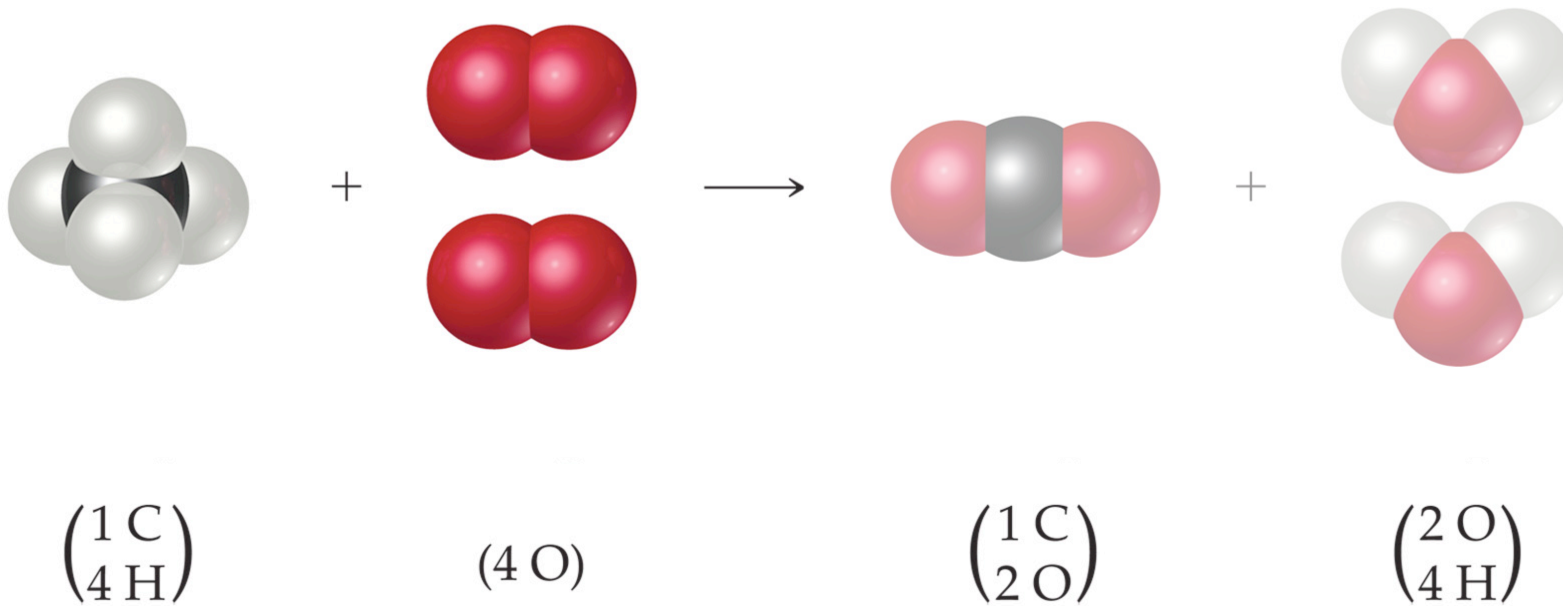
$$CH_{4\,(g)} + 2O_{2\,(g)} \longrightarrow CO_{2\,(g)} + 2\,H_2O_{(g)}$$



Stoichiometry

Anatomy of a Chemical Equation

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

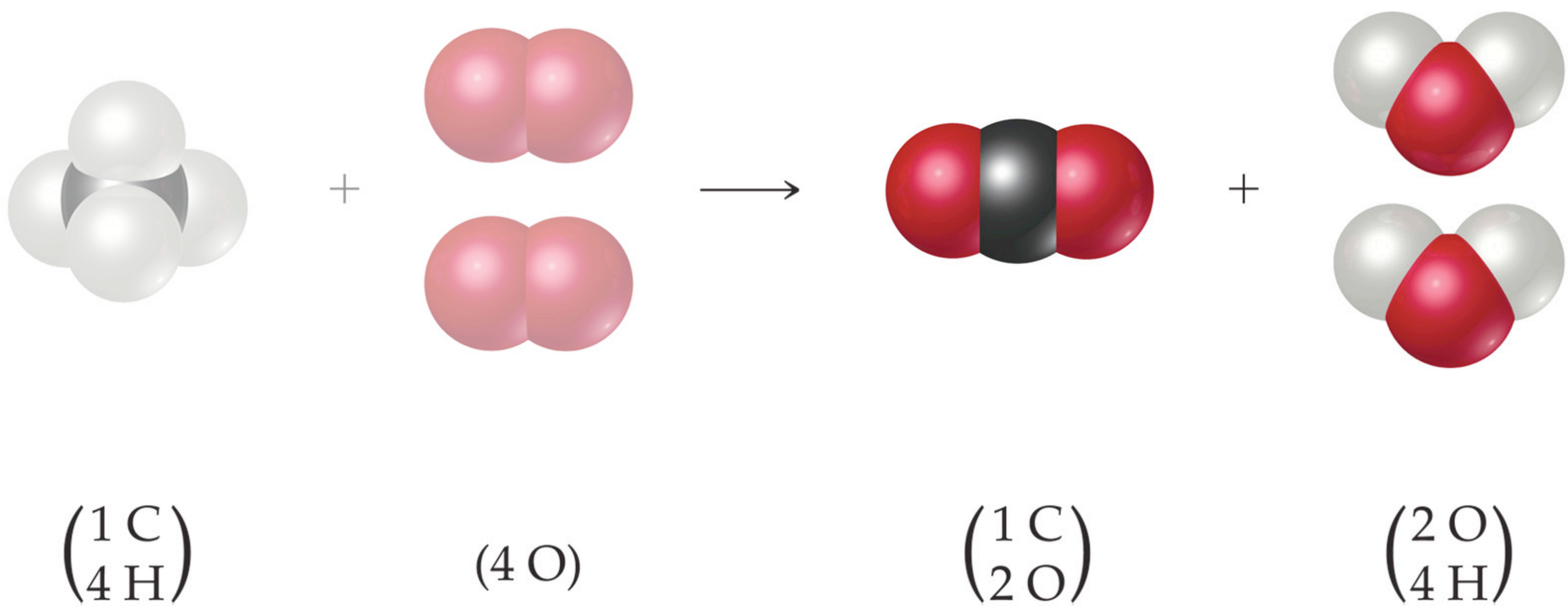


Reactants appear on the left side of the equation.

Stoichiometry

Anatomy of a Chemical Equation

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

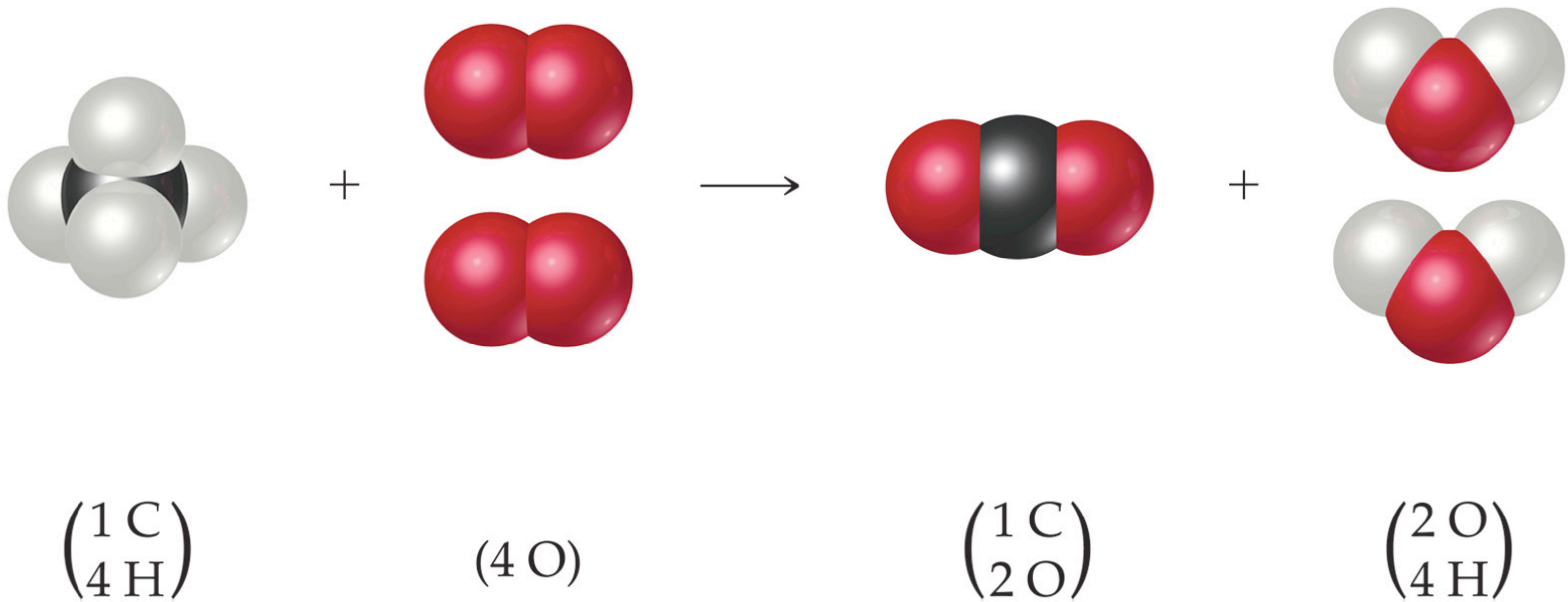


Products appear on the right side of the equation.

Stoichiometry

Anatomy of a Chemical Equation

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

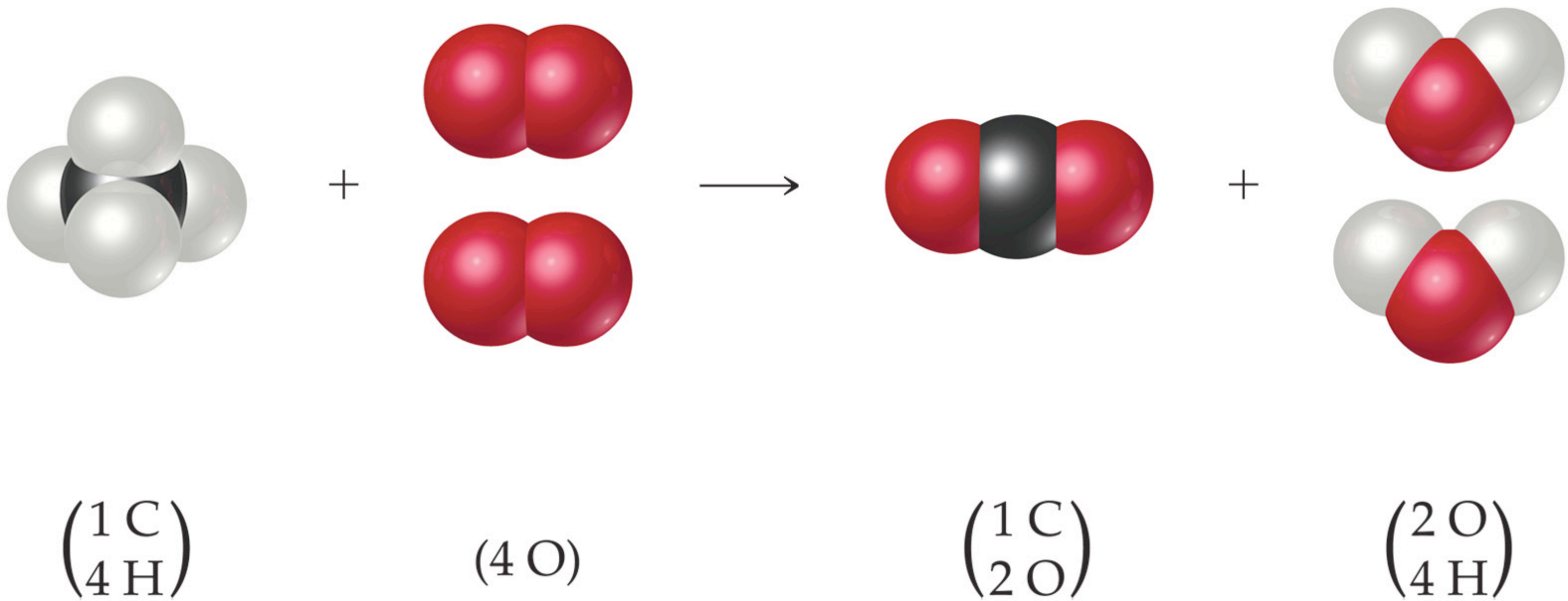


The states of the reactants and products are written in parentheses to the right of each compound.

Stoichiometry

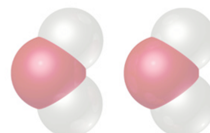
Anatomy of a Chemical Equation

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



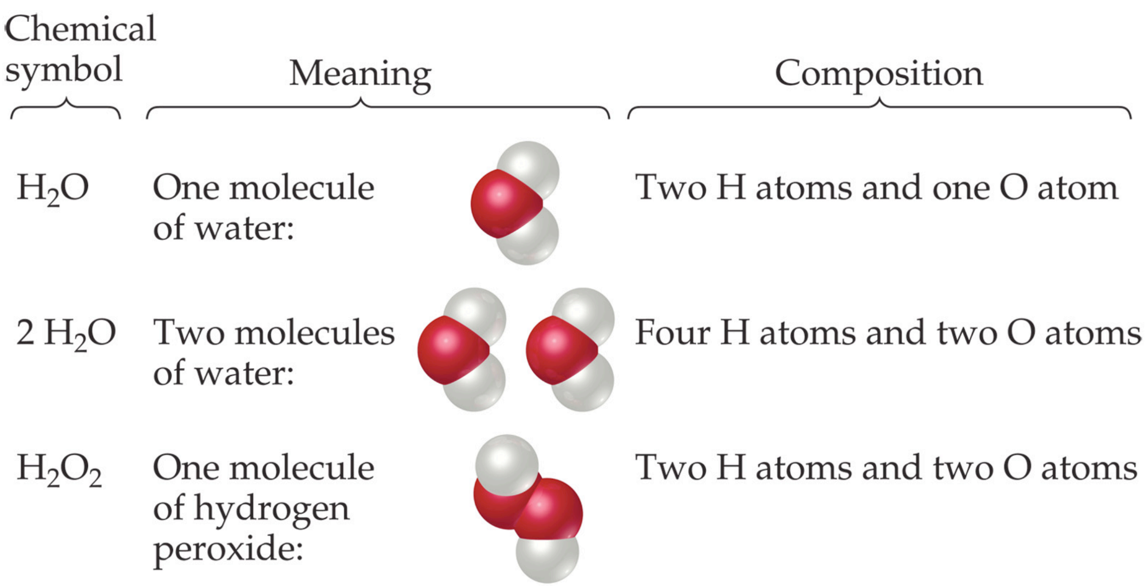
Coefficients are inserted to balance the equation.

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
H_2O_2	One molecule of hydrogen peroxide:		Two H atoms and two O atoms

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

Subscripts and Coefficients Give Different Information



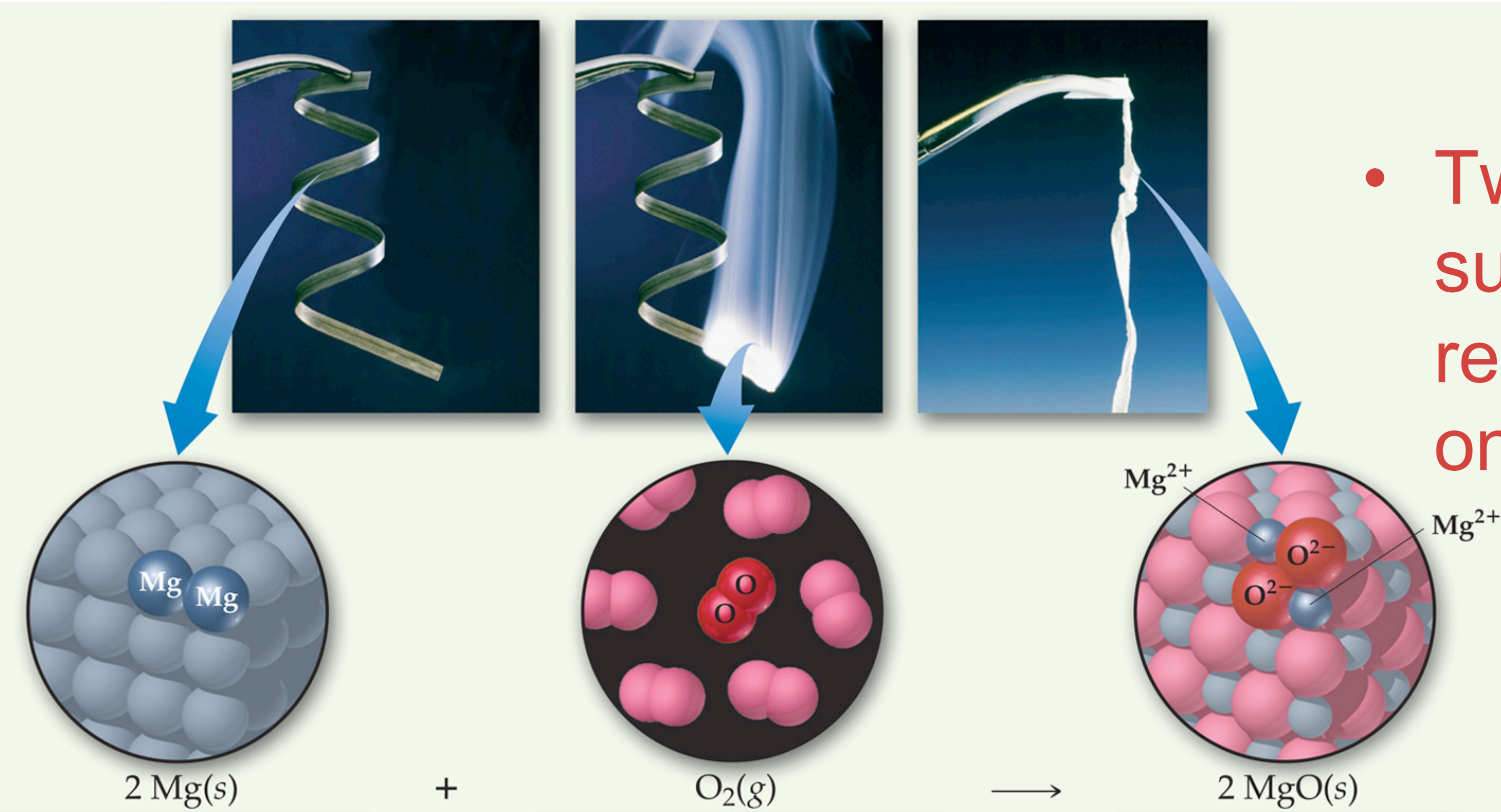
- Subscripts tell the number of atoms of each element in a molecule
- Coefficients tell the number of molecules (compounds).

Stoichiometry

Reaction Types

Stoichiometry

Combination Reactions



- Two or more substances react to form one product

- Examples:

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

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

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

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

Stoichiometry

Decomposition Reactions

- One substance breaks down into two or more substances

- Examples:

$$CaCO_{3\,(s)} \longrightarrow CaO_{\,(s)} + CO_{2\,(g)}$$

$$2\ KClO_{3\,(s)} \longrightarrow 2\ KCl_{\,(s)} + O_{2\,(g)}$$

$$2\ NaN_{3\,(s)} \longrightarrow 2\ Na_{\,(s)} + 3\ N_{2\,(g)}$$

Stoichiometry

Combustion Reactions

- Rapid reactions that have oxygen as a reactant sometimes produce a flame
- Most often involve hydrocarbons reacting with oxygen in the air to produce CO_2 and H_2O.

- Examples:

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

$$C_3H_{8\,(g)} + 5\,O_{2\,(g)} \longrightarrow 3\,CO_{2\,(g)} + 4\,H_2O_{\,(g)}$$

$$2H_2 + O_2 \dashrightarrow 2H_2O$$

Stoichiometry

Formula Weights

Stoichiometry

The amu unit

- Defined (since 1961) as:

- 1/12 mass of the ^{12}C isotope.
- ^{12}C = 12 amu

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

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

- 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

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

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 and hydrogen in ethane (C_2H_6, molecular mass = 30.0) is:

$$\%C = \frac{(2)(12.0\ \text{amu})}{(30.0\ \text{amu})} = \frac{24.0\ \text{amu}}{30.0\ \text{amu}} \times 100 = 80.0\%$$

$$\%H = \frac{(6)(1.01\ \text{amu})}{(30.0\ \text{amu})} = \frac{6.06\ \text{amu}}{30.0\ \text{amu}} \times 100 = 20.0\%$$

Stoichiometry

Moles

Atomic mass unit and the mole

- amu definition: ^{12}C = 12 amu.
- The atomic mass unit is defined this way.
- 1 amu = 1.6605×10^{-24} g
- How many ^{12}C atoms weigh 12 g?
- **6.02×10^{23} ^{12}C weigh 12 g.**
- Avogadro's number
- The mole

Stoichiometry

Atomic mass unit and the mole

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- How many ^{12}C atoms weigh 12 g?
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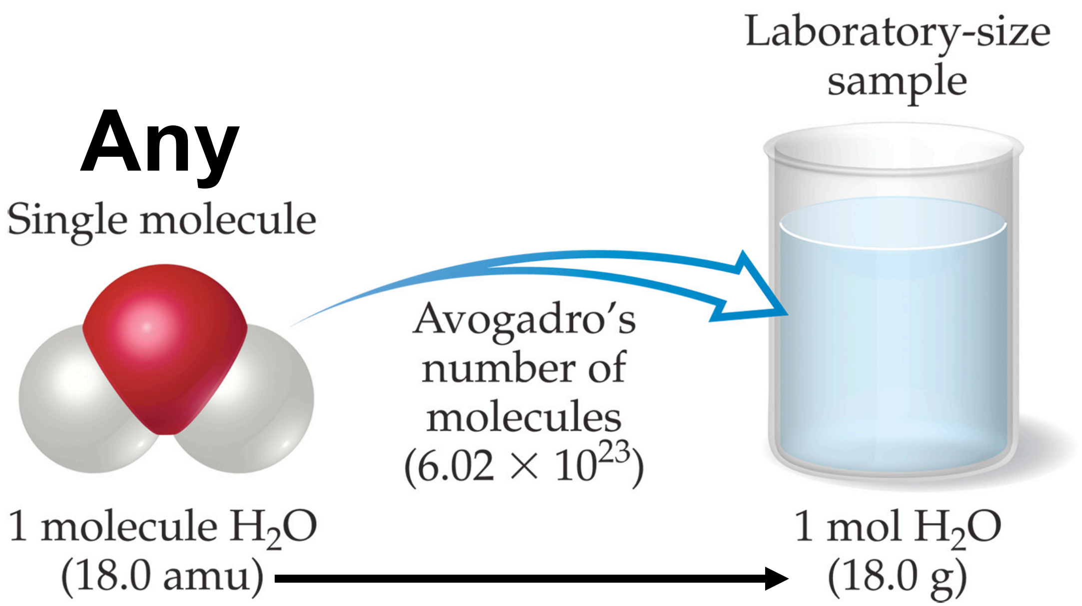
- Avogadro's number
- The mole

- #atoms = (1 atom/12 amu)(1 amu/1.66×10^{-24} g)(12g) = **6.02×10^{23} ^{12}C weigh 12 g**

Therefore:



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

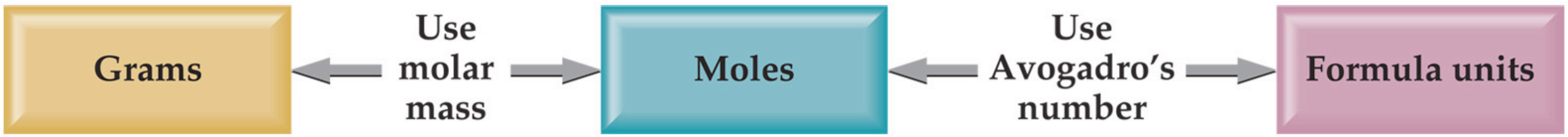
The mole

- The mole is just a number of things
- 1 dozen = 12 things
- 1 pair = 2 things
- 1 mole = 6.022141×10^{23} things

Molar Mass
The trick:

- By definition, this 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)

Using Moles



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

The number of moles correspond to the number of molecules. 1 mole of any substance has the same number of molecules.

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.

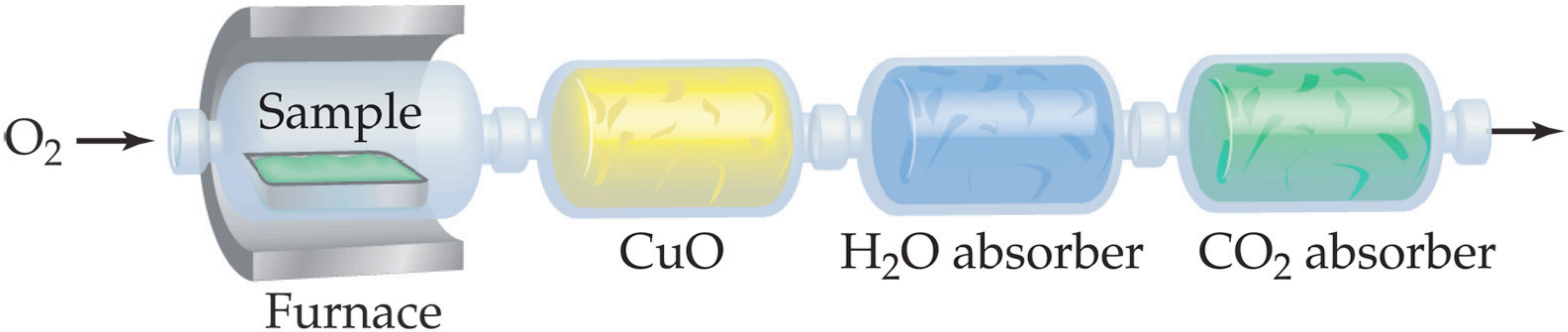
- One mole of atoms, ions, or molecules contains Avogadro's number of those particles
- One mole of molecules or formula units contains Avogadro's number times the number of atoms or ions of each element in the compound

Stoichiometry

Finding Empirical Formulas

Stoichiometry

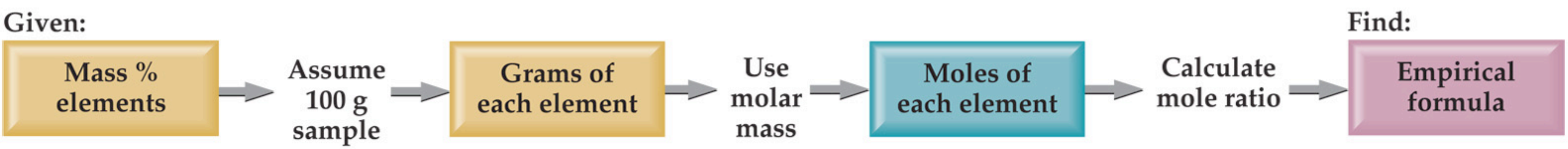
Combustion Analysis gives % composition



$$C_nH_nO_n + O_2 \longrightarrow nCO_2 + 1/2nH_2O$$

- 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

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,

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

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

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

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

Calculating Empirical Formulas

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

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

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

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

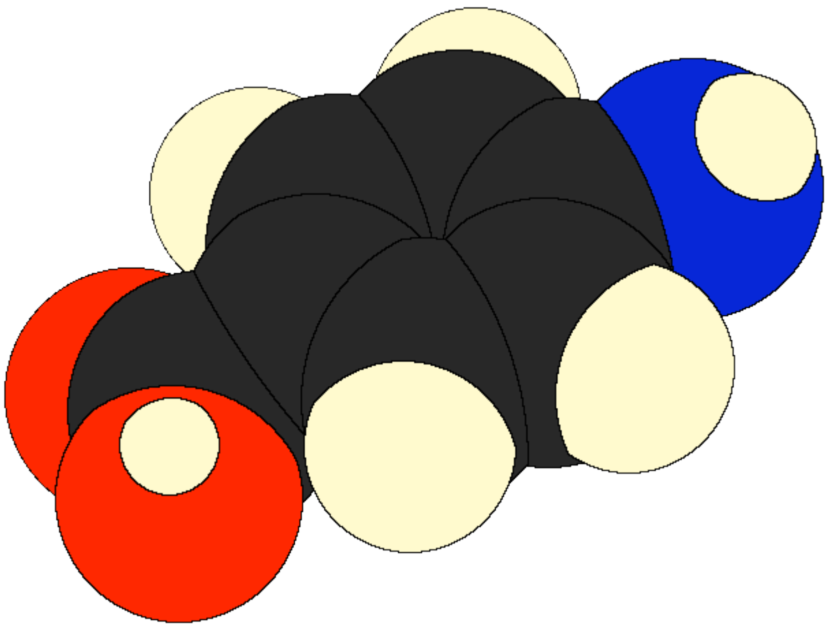
$$\text{O:} \quad \frac{1.458\ \cancel{\text{mol}}}{0.7288\ \cancel{\text{mol}}} = 2.001 \approx 2$$

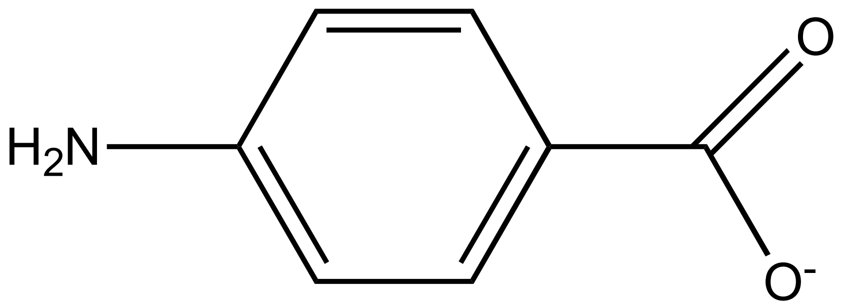
Stoichiometry

Calculating Empirical Formulas

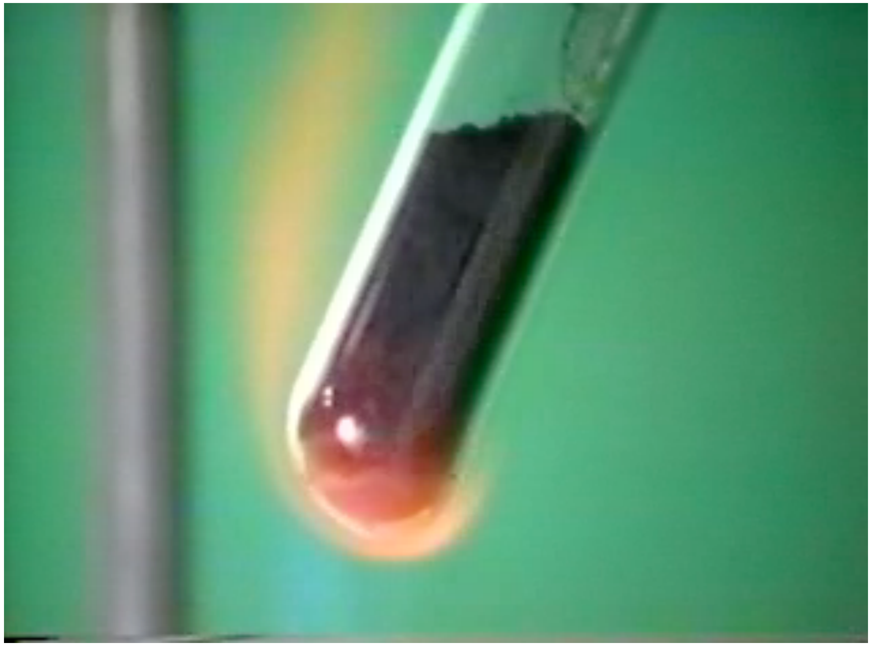
These are the subscripts for the empirical formula:

$C_7H_7NO_2$





Elemental Analyses



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

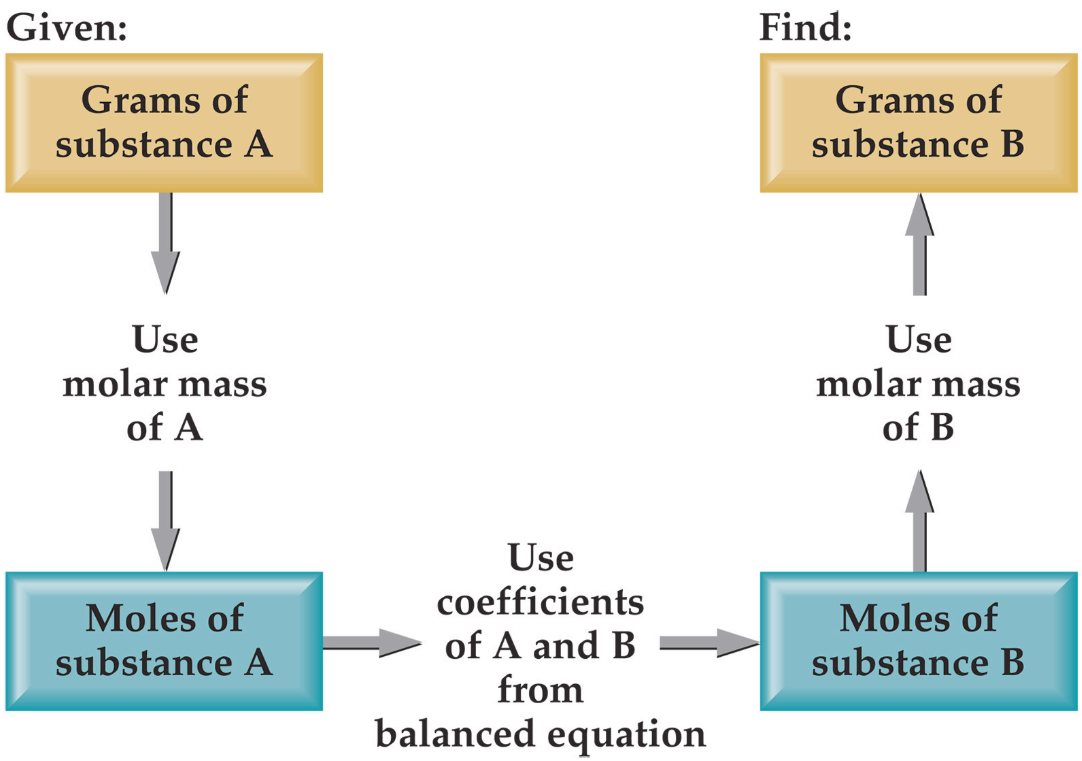
Stoichiometric Calculations

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

Example: 10 grams of glucose ($C_6H_{12}O_6$) react in a combustion reaction. How many grams of each product are produced?

$$C_6H_{12}O_{6(s)} + 6\ O_{2(g)} \rightarrow 6\ CO_{2(g)} + 6\ H_2O_{(l)}$$

$$10.g \longrightarrow \ ? \quad + \quad ?$$

Starting with 10. 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 & CO_2

and then turn the moles to grams

Stoichiometry

Stoichiometric calculations

	$C_6H_{12}O_6$ + $6O_2$ →	$6CO_2$ +	$6H_2O$
	10.g →	? +	?
MW:	180g/mol	44 g/mol	18g/mol
#mol:	10.g(1mol/180g)		
	0.055 mol	6(.055)	6(.055mol)
		6(.055mol)44g/mol	6(.055mol)18g/mol
#grams:		15g	5.9 g

Stoichiometry

Limiting Reactants

Stoichiometry

How Many Cookies Can I Make?

- You can make cookies until you run out of one of the ingredients
- Once you run out of sugar, you will stop making cookies

Stoichiometry

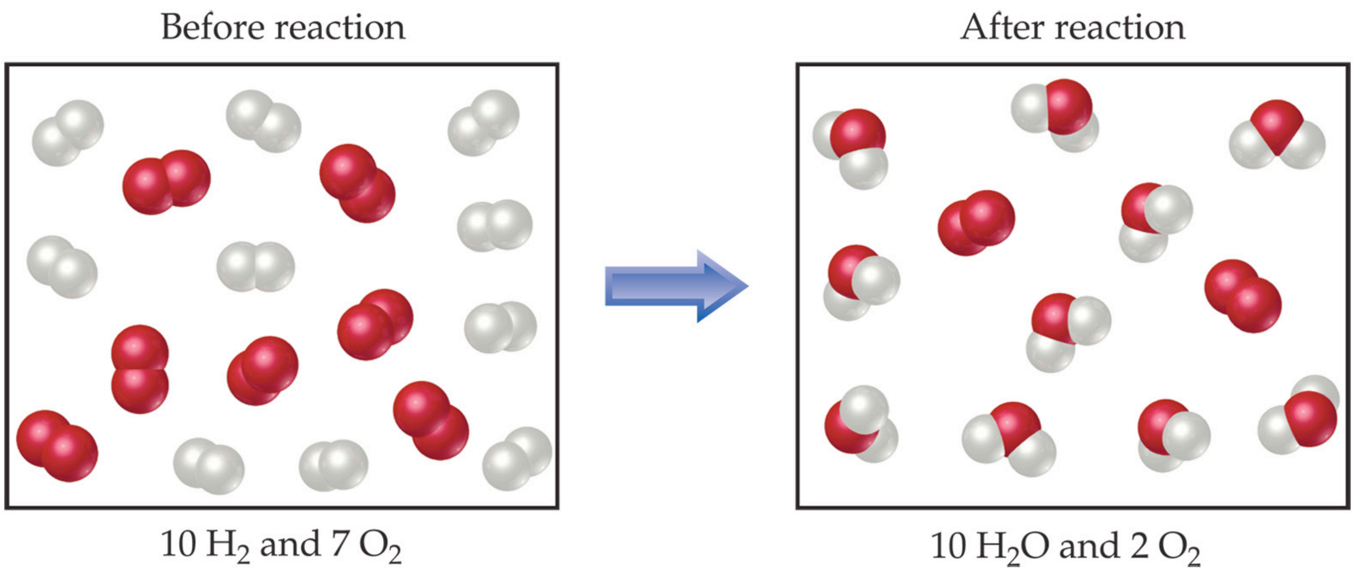
How Many Cookies Can I Make?

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

Stoichiometry

Limiting Reactants

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

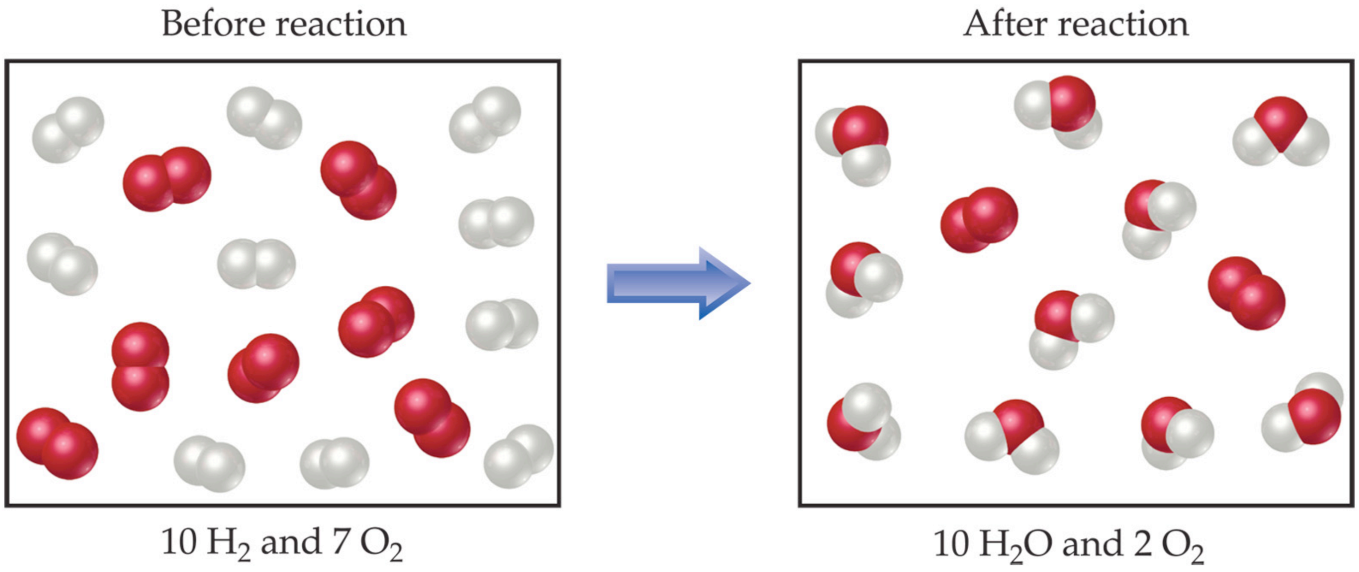


	$2H_2$	+	O_2	-------->	$2H_2O$
#moles	~~14~~		7		
	10		5		10
Left:	0		2		10

Stoichiometry

Limiting Reactants

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



Limiting reagent, example:

Soda fizz comes from sodium bicarbonate and citric acid ($H_3C_6H_5O_7$) reacting to make carbon dioxide, sodium citrate ($Na_3C_6H_5O_7$) and water. If 1.0 g of sodium bicarbonate and 1.0g citric acid are reacted, which is limiting? How much carbon dioxide is produced?

$3NaHCO_{3(aq)}$ + $H_3C_6H_5O_{7(aq)}$ ------> $3CO_2(g)$ + $3H_2O(l)$ + $Na_3C_6H_5O_7(aq)$

1.0g	1.0g	
84g/mol	192g/mol	44g/mol
1.0g(1mol/84g)	1.0(1mol/192g)	
0.012 mol	0.0052 mol	

(if citrate limiting)

0.0052(3)=~~0.016~~ 0.0052 mol

So bicarbonate limiting:

0.012 mol   0.012(1/3)=.0040mol   0.012 moles CO_2

44g/mol(0.012mol)=0.53g CO_2

.0052-.0040=.0012mol left

0.0012 mol(192 g/mol)=

0.023 g left.

Stoichiometry

Theoretical Yield

- The theoretical yield is the amount of product that can be made
  - In other words it's the amount of product **possible** from stoichiometry. The "perfect reaction."
- 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

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

Example

Benzene (C_6H_6) reacts with Bromine to produce bromobenzene (C_6H_6Br) and hydrobromic acid. If 30. g of benzene reacts with 65 g of bromine and produces 56.7 g of bromobenzene, what is the percent yield of the reaction?

C_6H_6 +	Br_2 ------>	C_6H_5Br +	HBr
30.g	65 g	56.7 g	
78g/mol	160.g/mol	157g/mol	
30.g(1mol/78g)	65g(1mol/160g)		
0.38 mol	0.41 mol		
(If Br_2 limiting)			
~~0.41 mol~~	0.41 mol		
(If C_6H_6 limiting)			
0.38 mol	0.38 mol	0.38mol(157g/1mol) = 60.g	
		56.7g/60.g(100)=94.5%=95%	

Stoichiometry

Example, one more

React 1.5 g of NH_3 with 2.75 g of O_2. How much NO and H_2O is produced? What is left?

$4NH_3$ +	$5O_2$ -------->	$4NO$ +	$6H_2O$
1.5g	2.75g	?	?
17g/mol	32g/mol	30.g/mol	18g/mol
1.5g(1mol/17g)=	2.75g(1mol/32g)=		
.088mol	.086		
(If NH_3 limiting):			
.088mol	.088(5/4)= ~~.11~~		
O_2 limiting:			
.086(4/5)=	.086 mol	.086 mol(4/5)=	.086(6/5)=
.069mol		.069 mol	.10mol
.069mol(17g/mol)		.069mol(30.g/mol)	.10mol(18g/mol)
1.2g	2.75g	2.1 g	1.8g

Stoichiometry

Stoichiometry

Gun powder reaction

- $10KNO_{3(s)} + 3S_{(s)} + 8C_{(s)} \dashrightarrow 2K_2CO_{3(s)} + 3K_2SO_{4(s)} + 6CO_{2(g)} + 5N_{2(g)}$
- Salt peter   sulfur   charcoal

And heat.

What is interesting about this reaction?
What kind of reaction is it?
What do you think makes it so powerful?

Gun powder reaction

Oxidizing agent — Oxidizing agent — Reducing agent

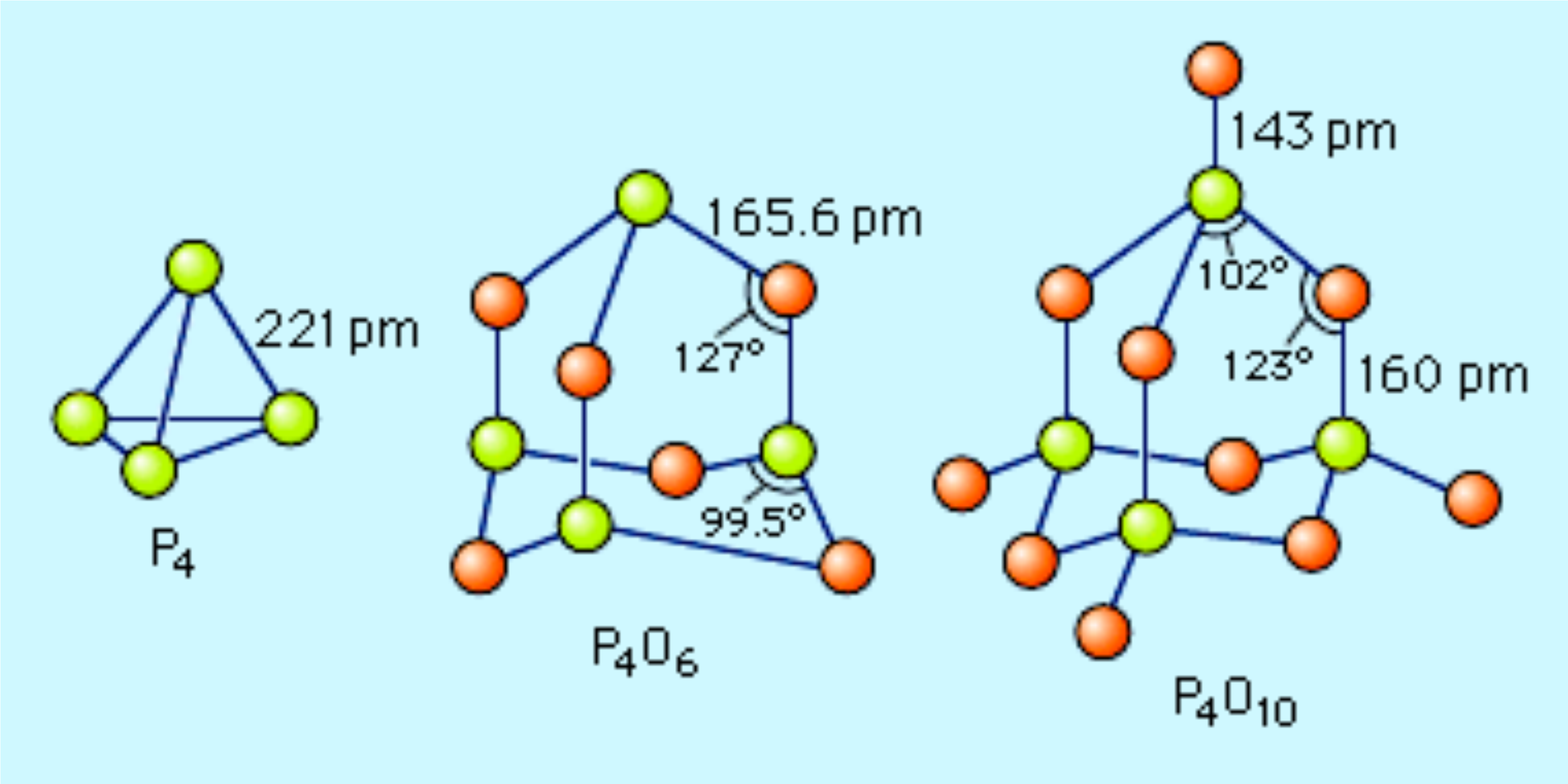
- $10KNO_{3(s)} + 3S_{(s)} + 8C_{(s)} \rightarrow 2K_2CO_{3(s)} + 3K_2SO_{4(s)} + 6CO_{2(g)} + 5N_{2(g)}$
- Salt peter sulfur charcoal
-

And heat.

What is interesting about this reaction?
Lots of energy, no oxygen
What kind of reaction is it?
Oxidation reduction
What do you think makes it so powerful and explosive?
Makes a lot of gas!!!!

Stoichiometry

White phosphorous and Oxygen under water



Stoichiometry