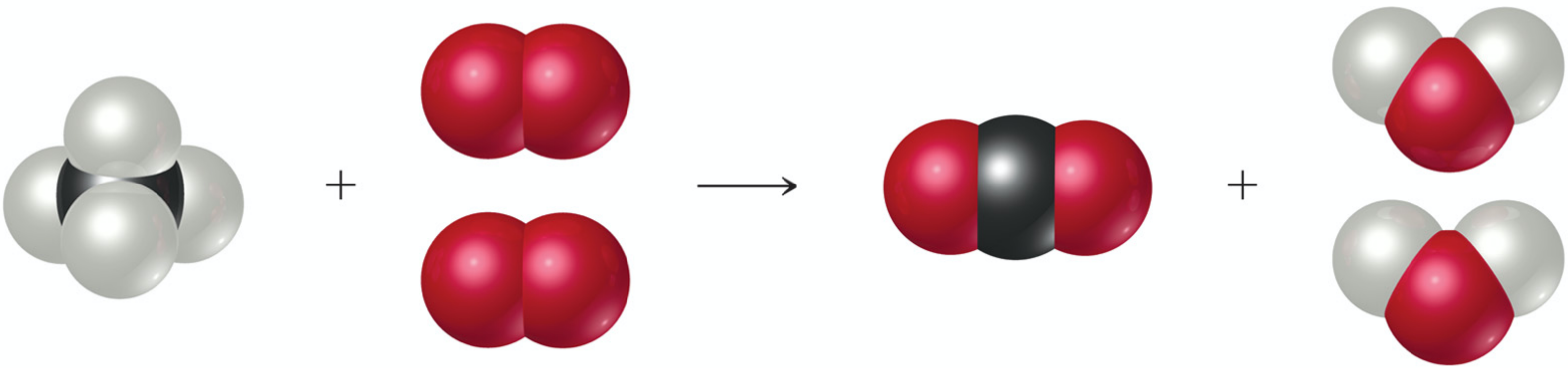
Chapter 3
Stoichiometry:

Calculations with Chemical Formulas and Equations

Anatomy of a Chemical Equation

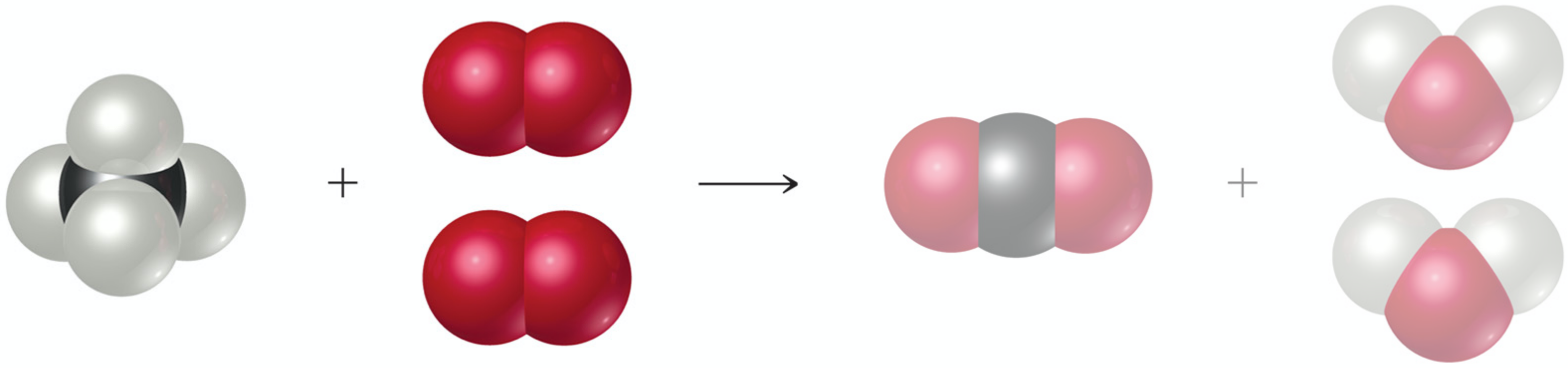
$$CH_{4\,(g)} + 2O_{2\,(g)} \longrightarrow CO_{2\,(g)} + 2\,H_2O_{(g)}$$



$\begin{pmatrix}1\,C\\4\,H\end{pmatrix}$ (4 O) $\begin{pmatrix}1\,C\\2\,O\end{pmatrix}$ $\begin{pmatrix}2\,O\\4\,H\end{pmatrix}$

Anatomy of a Chemical Equation

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

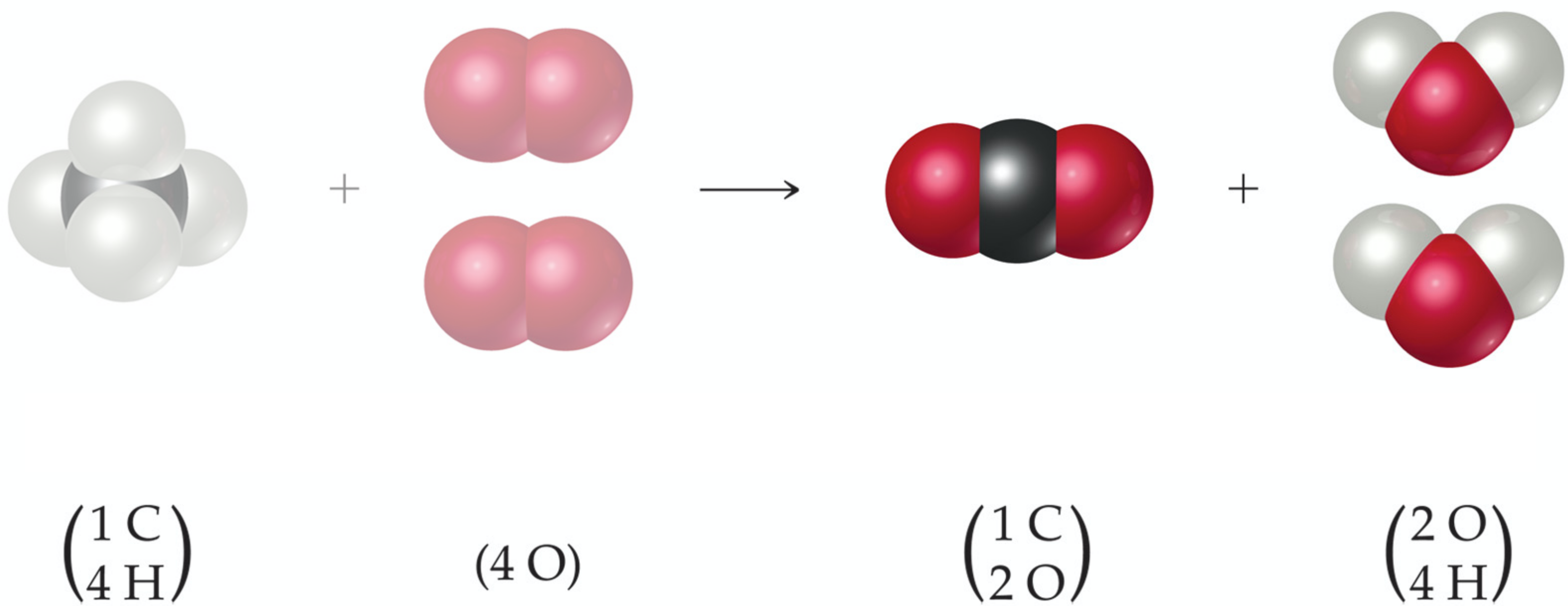


$\binom{1\,C}{4\,H}$ (4 O) $\binom{1\,C}{2\,O}$ $\binom{2\,O}{4\,H}$

Reactants appear on the left side of the equation.

Anatomy of a Chemical Equation

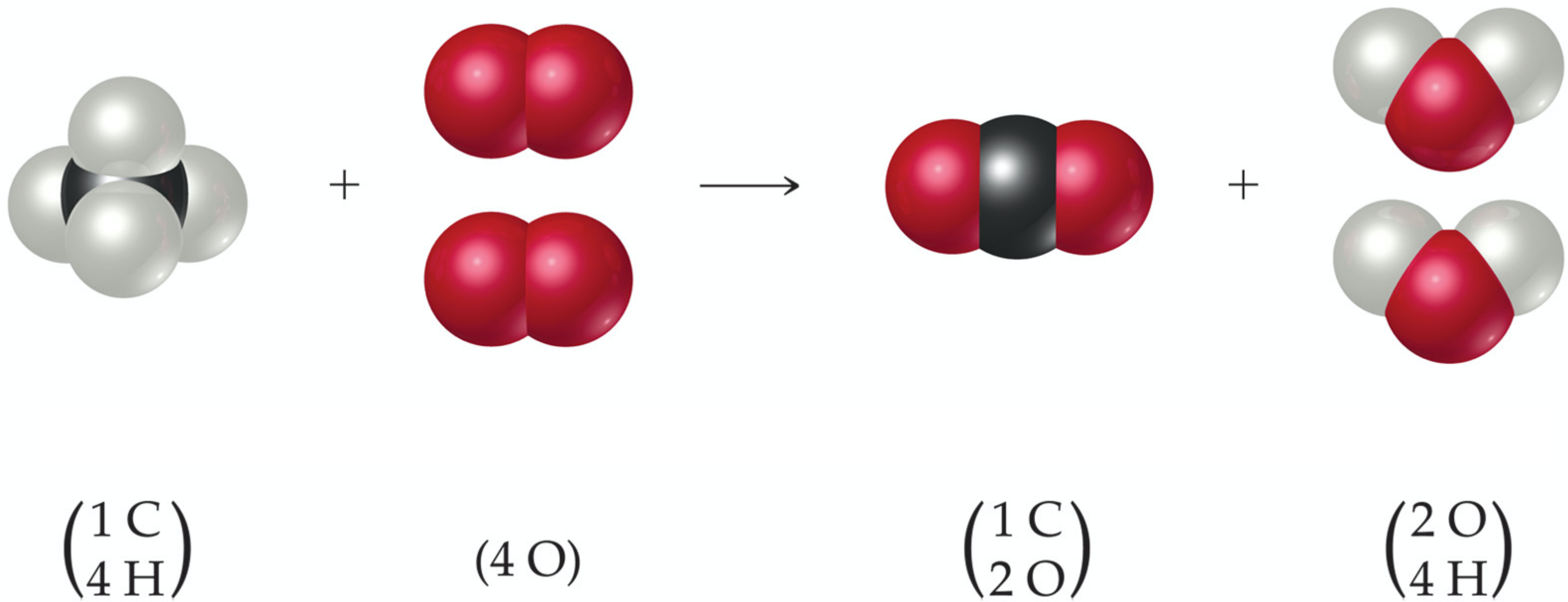
$$CH_{4\,(g)} + 2\,O_{2\,(g)} \longrightarrow CO_{2\,(g)} + 2\,H_2O_{\,(g)}$$



Products appear on the right side of the equation.

Anatomy of a Chemical Equation

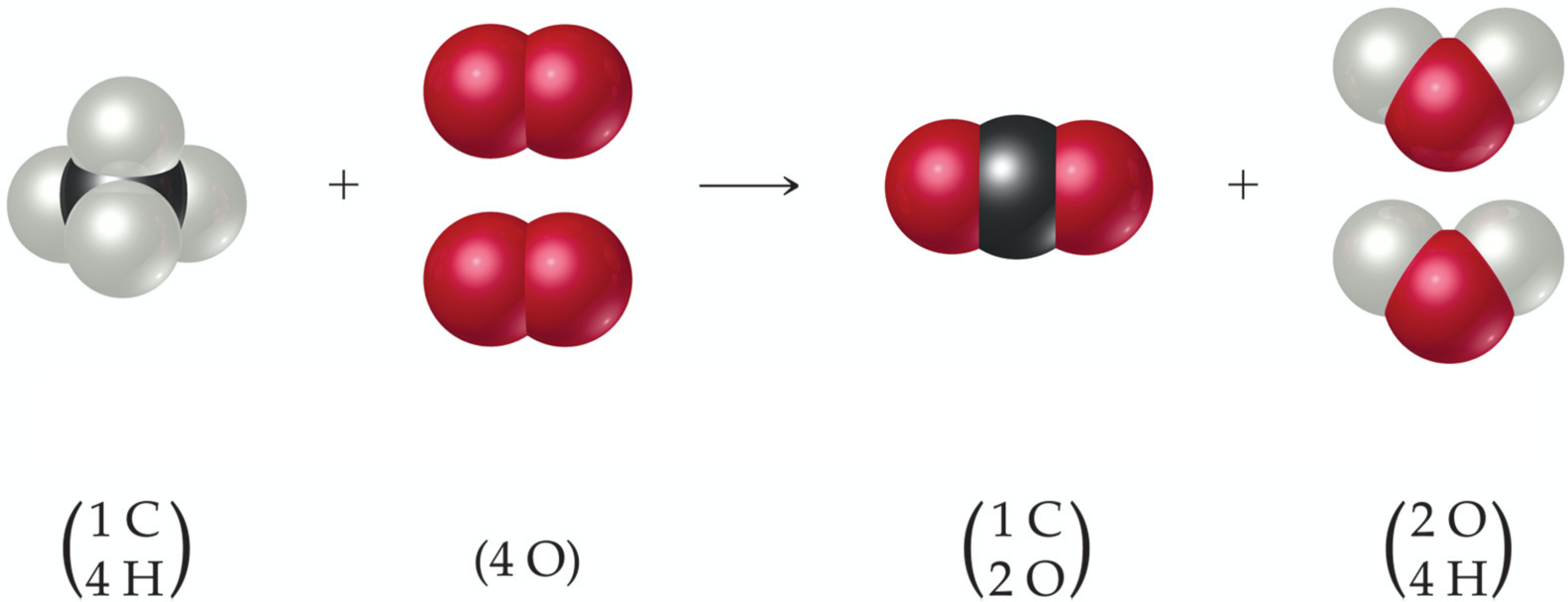
$$CH_{4\,(g)} + 2\ O_{2\,(g)} \longrightarrow CO_{2\,(g)} + 2\ H_2O_{\,(g)}$$



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

Anatomy of a Chemical Equation

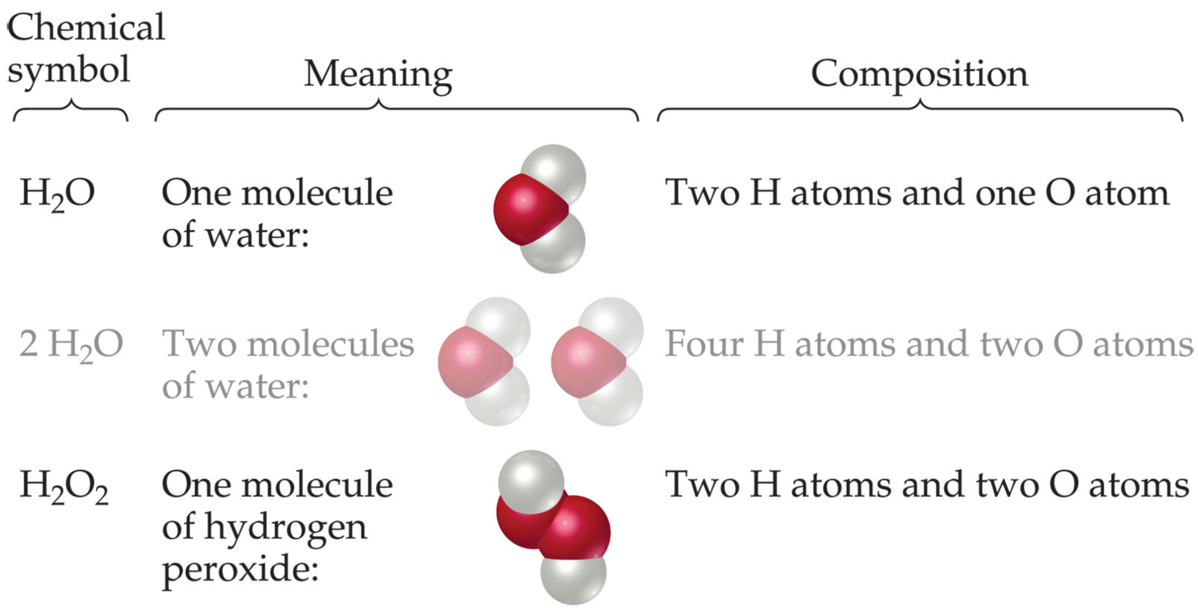
$$CH_{4\,(g)} + 2\,O_{2\,(g)} \longrightarrow CO_{2\,(g)} + 2\,H_2O_{\,(g)}$$



Coefficients are inserted to ***balance*** the equation.

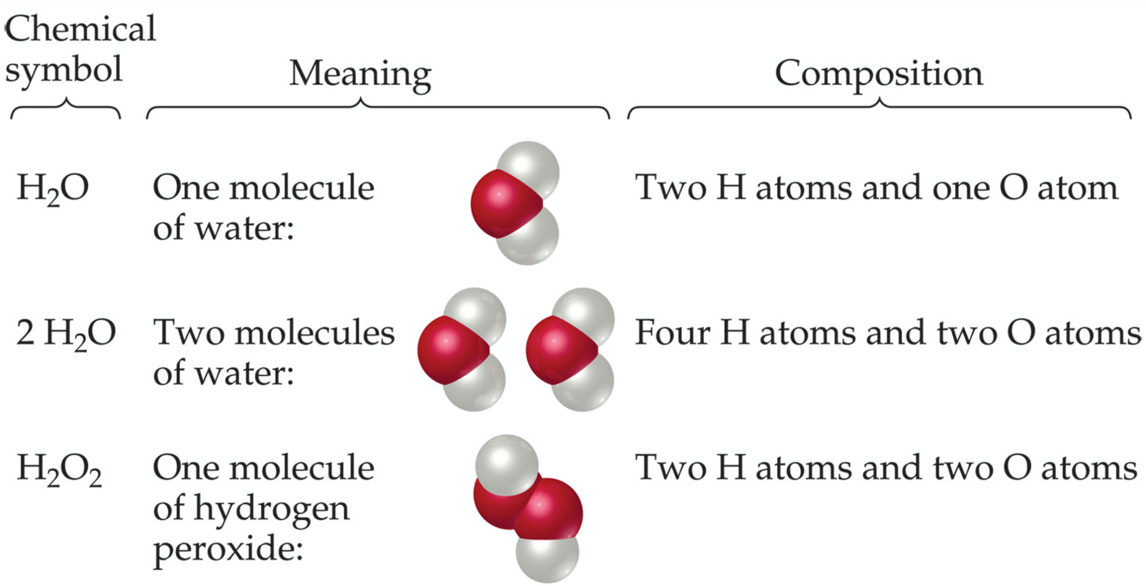
Balance: making the reaction agree with the conservation of mass.

Subscripts and Coefficients Give Different Information



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

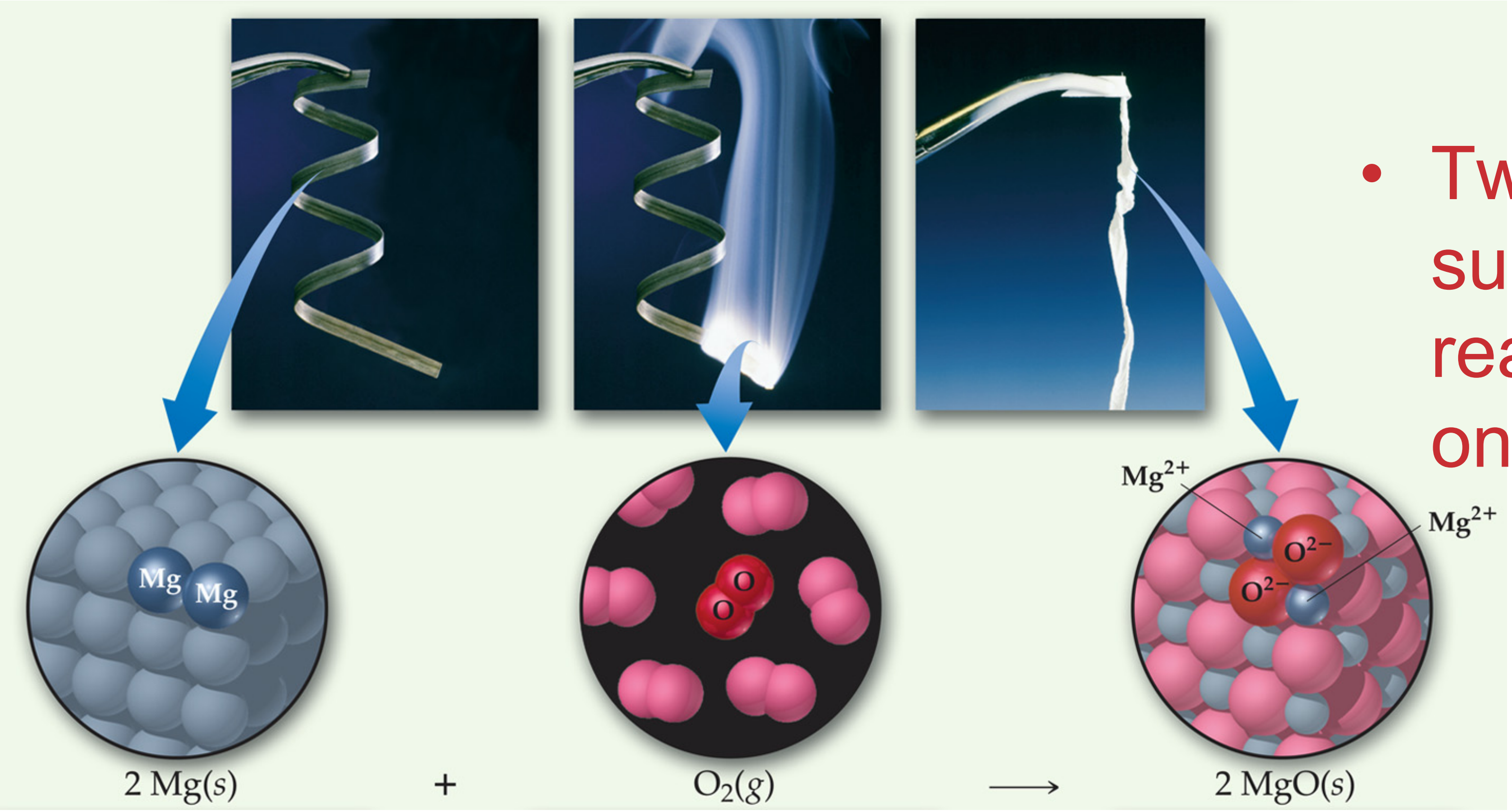
Subscripts and Coefficients Give Different Information



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

Examples of Reactions

Combination Reactions



- Two or more substances react to form one product

- Examples:

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

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

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

Decomposition Reactions
One reactant decomposes to more than one or more products

- 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 have **oxygen** as a reactant
- sometimes produces a flame
- Most often involve hydrocarbons reacting with oxygen in the air to produce CO_2 and H_2O.
- For our purposes combustion will mean:
- Oxygen reacting with something to form CO_2 and H_2O

- Examples:

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

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

$$2H_2 \quad + \quad O_2 \quad \text{-------}\!\!\rightarrow \quad 2H_2O$$

Formula Weights

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

Ca:	1(40.1 amu)
+ Cl:	2(35.5 amu)
	111.1 amu

- 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

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

Percent Composition

The percent composition by element:

$$\% \text{ element} = \frac{(\#\text{ of atoms of element})(\text{atomic weight})}{(\text{FW or MW of the compound})} \times 100$$

Percent Composition

So the percentage of carbon and hydrogen in ethane (C_2H_6, molecular mass = 30.0) is:

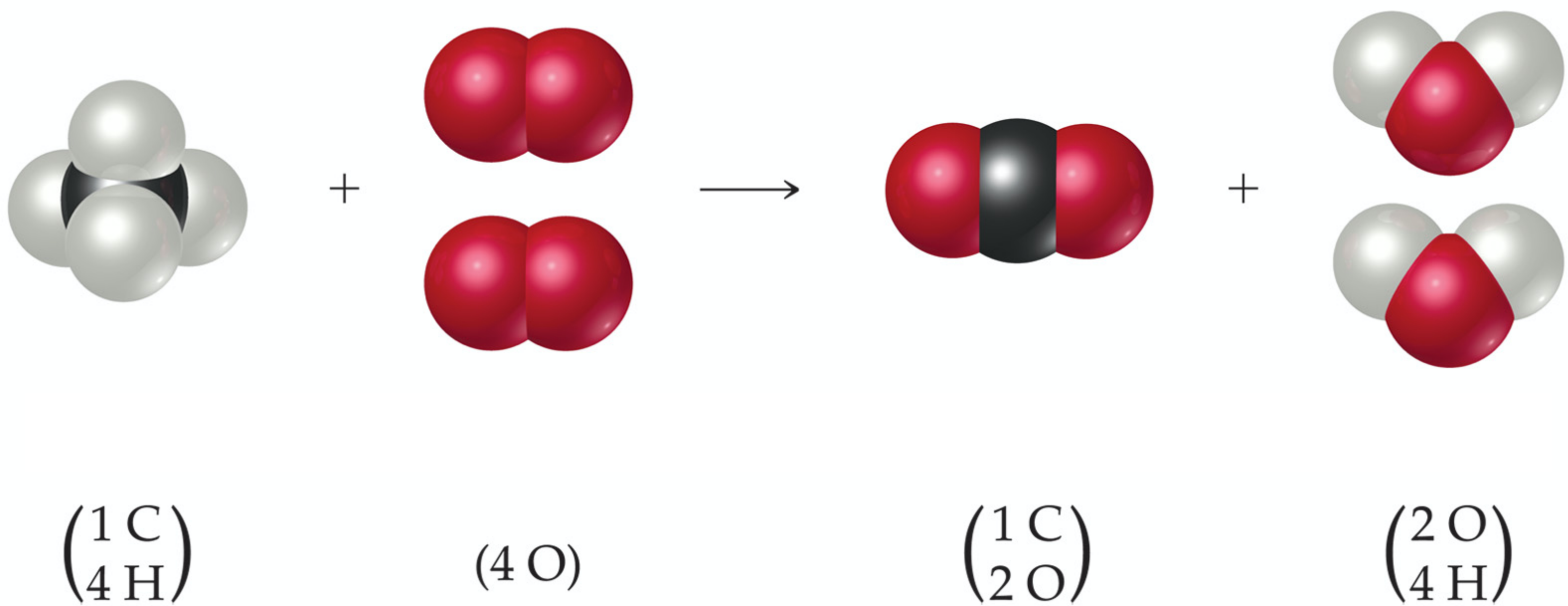
$$\%C = \frac{(2)(12.0\ \text{amu})}{(30.0\ \text{amu})} = \frac{24.0\ \text{amu}}{30.0\ \text{amu}} \times 100 = 80.0\%$$

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

Moles

Making a Chemical Equation

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



How do I know how much methane and oxygen I need?
My scale says grams, not number of atoms or molecules.x

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?
- **$6.02221409 \times 10^{23}$ ^{12}C weigh 12 g.**
- Avogadro’s number
- *The mole*

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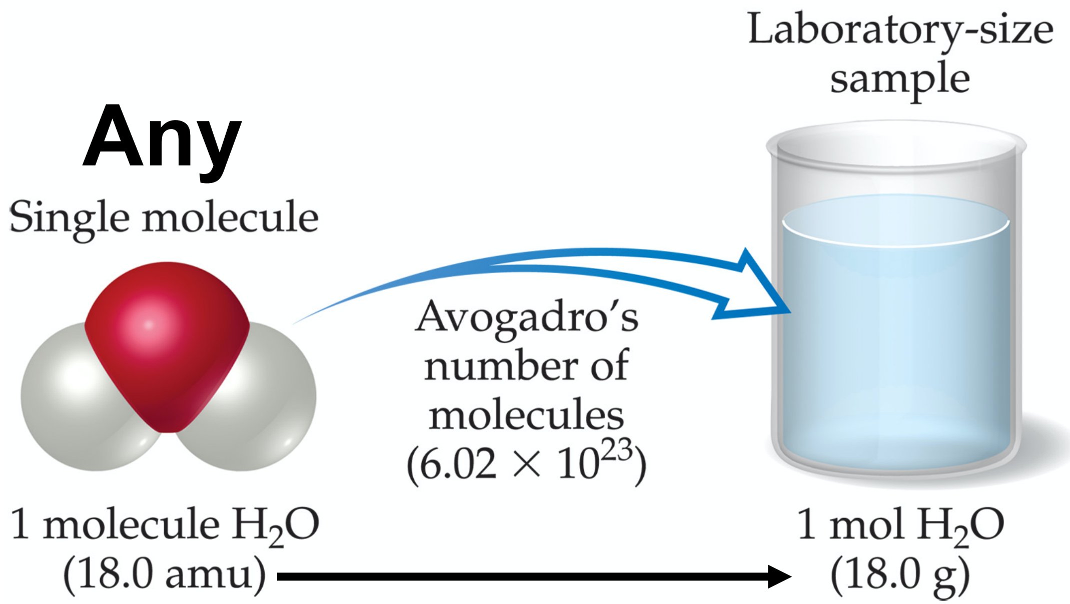
- 1 amu = 1.6605×10^{-24} g
- How many ^{12}C atoms weigh 12 g?
- **6.0221409×10^{23} ^{12}C weigh 12 g.**
- Avogadro's number
- The mole

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

Therefore:



- 6.02×10^{23}
- 1 mole of ^{12}C has a mass of 12 g
- 1 mole of H_2O has a mass of 18.0 g!

The mole

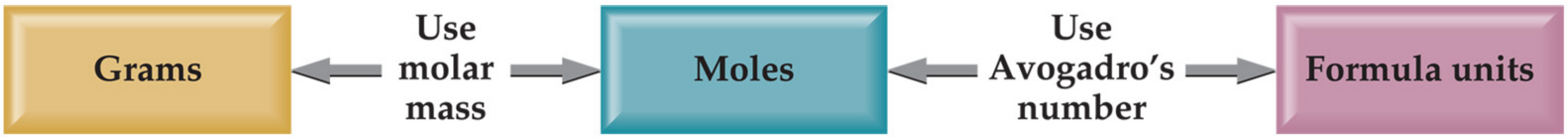
- The mole is just a number of things
- 1 dozen = 12 things
- 1 pair = 2 things
- 1 mole = 6.022141×10^{23} things

- 6.022141×10^{23}atoms/mole
- SO
- 1 mole C atoms = 6.022×10^{23} C atoms

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

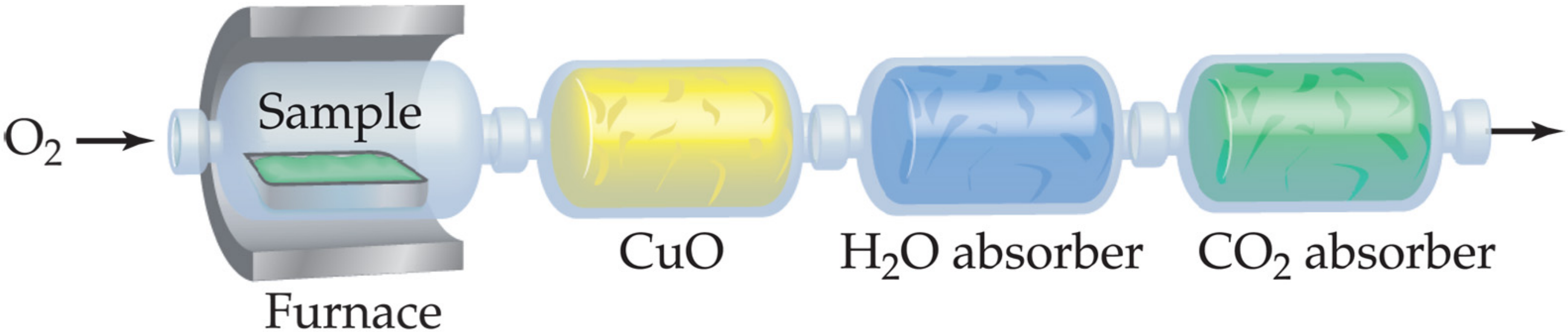
Name of substance	Formula	Formula Weight (amu)	Molar Mass (g/mol)	Number and Kind of Particles in One Mole
Atomic nitrogen	N	14.0	14.0	6.022×10^{23} N atoms
Molecular nitrogen	N_2	28.0	28.0	6.022×10^{23} N_2 molecules; $2(6.022 \times 10^{23})$ N atoms
Silver	Ag	107.9	107.9	6.022×10^{23} Ag atoms
Silver 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

Finding Empirical Formulas

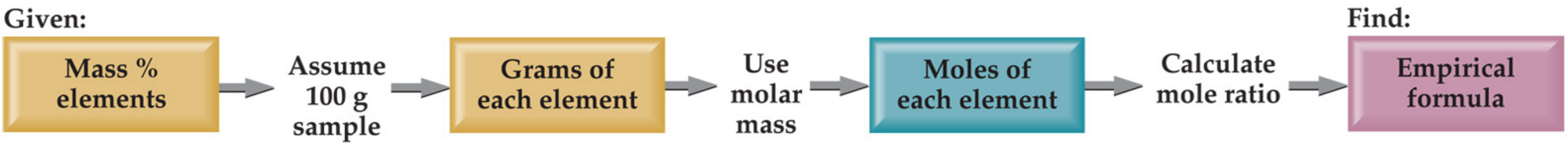
Combustion Analysis
gives % composition



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

- 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

1. Assuming 100.00 g of *para*-aminobenzoic acid, find out how many moles of each element are in that 100 g.:

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

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

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

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

Calculating Empirical Formulas

2. Calculate the mole ratio by dividing moles of each element by the number of moles of the element with the least number of moles:

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

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

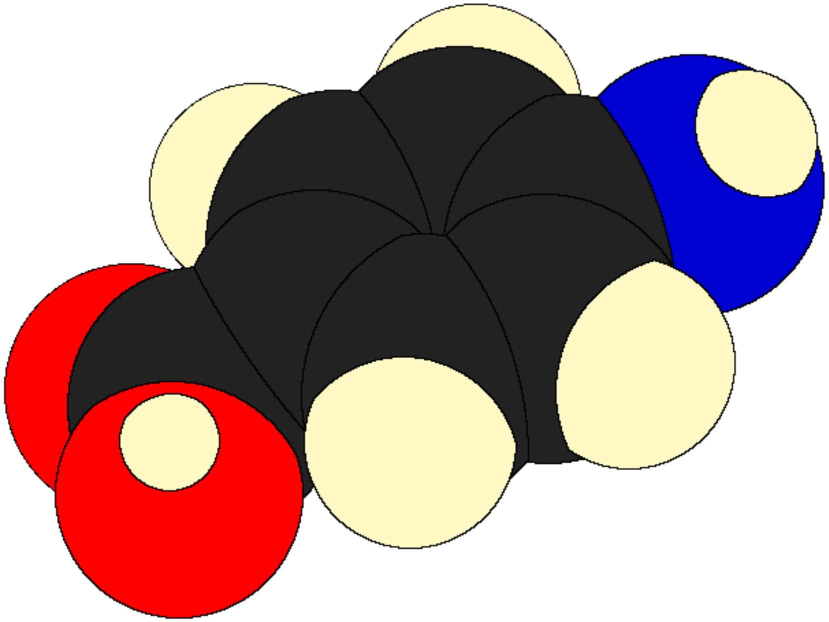
$$\text{N:} \quad \frac{0.7288 \cancel{\text{mol}}}{0.7288 \cancel{\text{mol}}} = 1.000$$

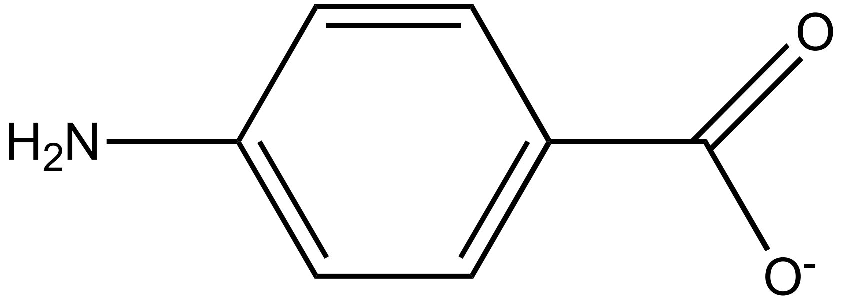
$$\text{O:} \quad \frac{1.458 \cancel{\text{mol}}}{0.7288 \cancel{\text{mol}}} = 2.001 \approx 2$$

Calculating Empirical Formulas

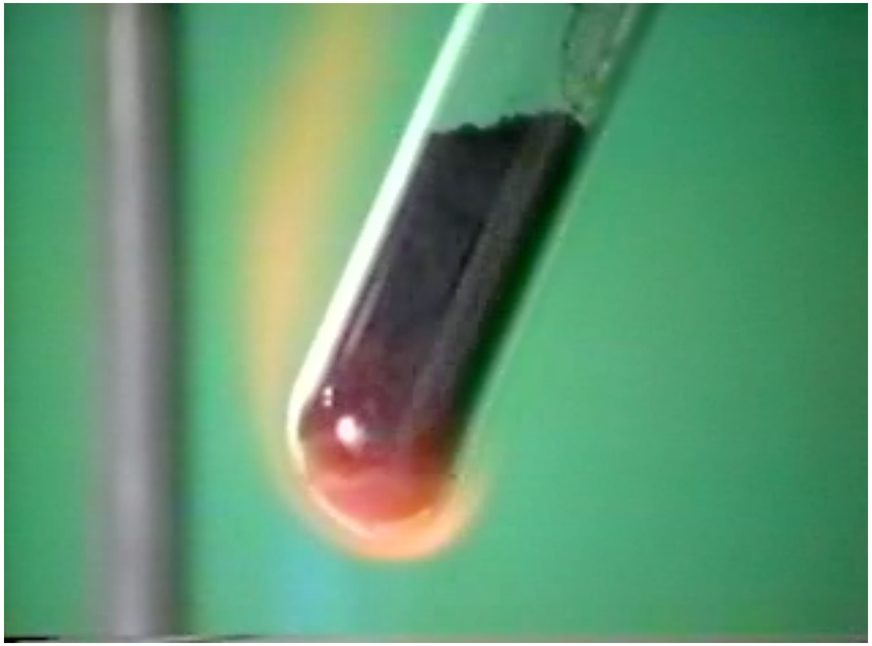
These are the subscripts for the empirical formula:

$C_7H_7NO_2$



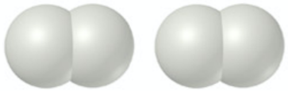
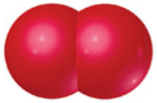
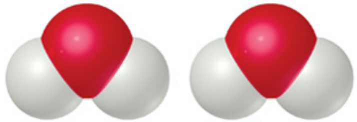


Elemental Analyses



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

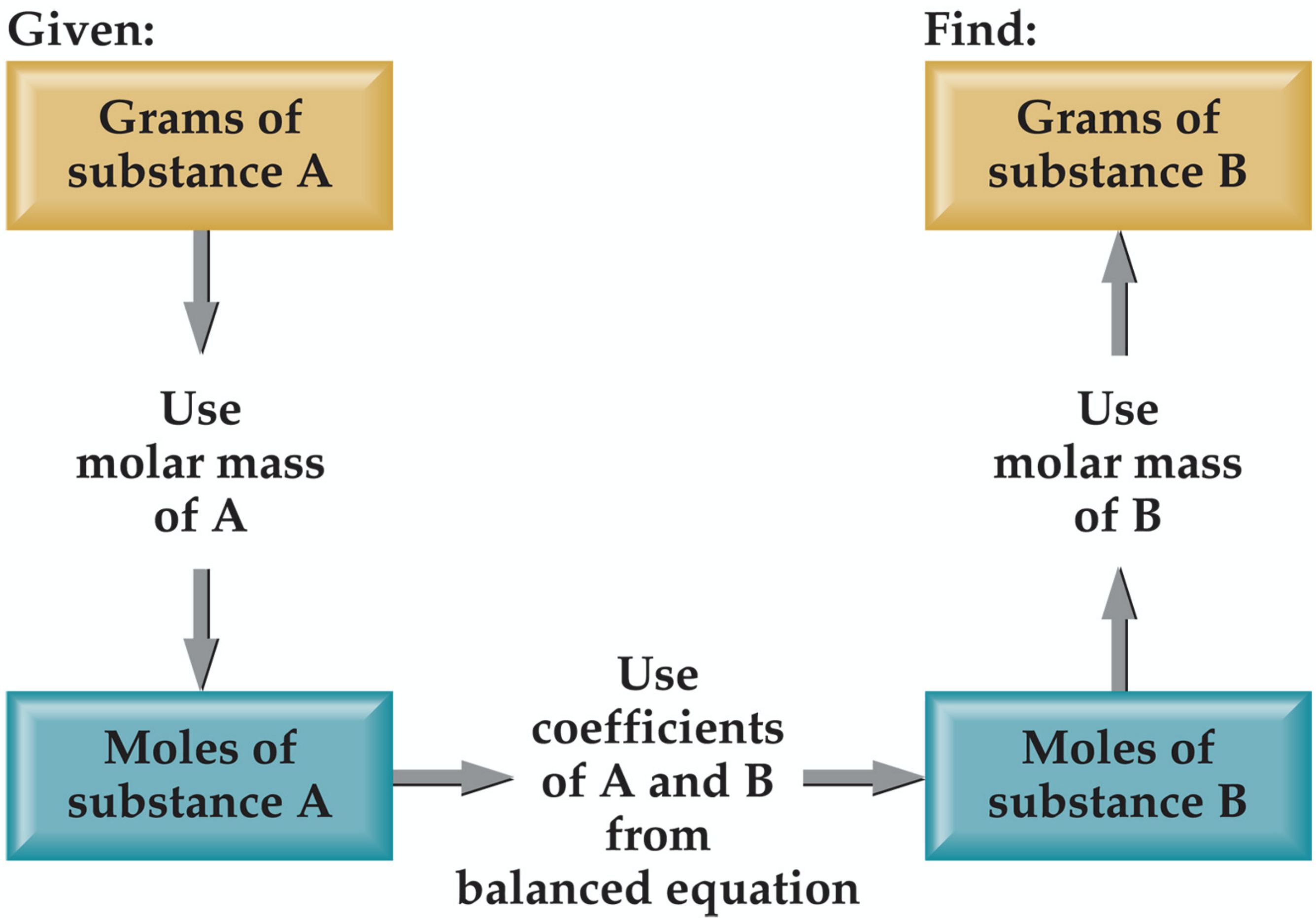
Stoichiometric Calculations

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

$$A_{(g)} + 2B_{(g)} \longrightarrow C_{(g)} + 2D_{(g)}$$



Stoichiometric Calculations

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

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

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

Starting with 10. g of $C_6H_{12}O_6$…

1. calculate the moles of $C_6H_{12}O_6$…
2. use the coefficients to find the moles of H_2O & CO_2
3. then turn the moles to grams of H_2O & CO_2

Stoichiometric calculations

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

10.g $\longrightarrow$? + ?

MW: 180g/mol 44 g/mol 18g/mol. 1. (what 's known)

How many grams of oxygen reacted?

Stoichiometric calculations

$C_6H_{12}O_6$ + $6O_2$ → $6CO_2$ + $6H_2O$

10.g ⟶ ? + ?

MW: 180g/mol 44 g/mol 18g/mol. 1. (what 's known)

#mol: 10.g(1mol/180g) (Calc. moles)

0.055 mol

How many grams of oxygen reacted?

Stoichiometric calculations

$C_6H_{12}O_6$ + $6O_2$ → $6CO_2$ + $6H_2O$

10.g → ? + ?

MW: 180g/mol 44 g/mol 18g/mol. 1. (what 's known)

#mol: 10.g(1mol/180g) (Calc. moles)

0.055 mol

6(.055) 6(.055mol) (use coefficients calculate moles of others)

How many grams of oxygen reacted?

Stoichiometric calculations

	$C_6H_{12}O_6$ +	$6O_2$ →	$6CO_2$	+	$6H_2O$	
	10.g	→	?	+	?	
MW:	180g/mol		44 g/mol		18g/mol. 1.	(what 's known)
#mol:	10.g(1mol/180g)					(Calc. moles)
	0.055 mol		6(.055)		6(.055mol)	(other moles)
			6(.055mol)44g/mol		6(.055mol)18g/mol	
#grams:			**15g**		**5.9 g**	**(calc. grams)**

How many grams of oxygen reacted?

Stoichiometric calculations

$C_6H_{12}O_6$ + $6O_2$ → $6CO_2$ + $6H_2O$

	10.g	⟶	?	+	?
MW:	180g/mol		44 g/mol		18g/mol. 1. (what 's known)
#mol:	10.g(1mol/180g)				(Calc. moles)
	0.055 mol		6(.055)		6(.055mol) (other moles)
			6(.055mol)44g/mol		6(.055mol)18g/mol
#grams:			**15g**		**5.9 g (calc. grams)**

How many grams of oxygen reacted?

15 + 5.9 -10 = 10.9 g

Limiting Reactants

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

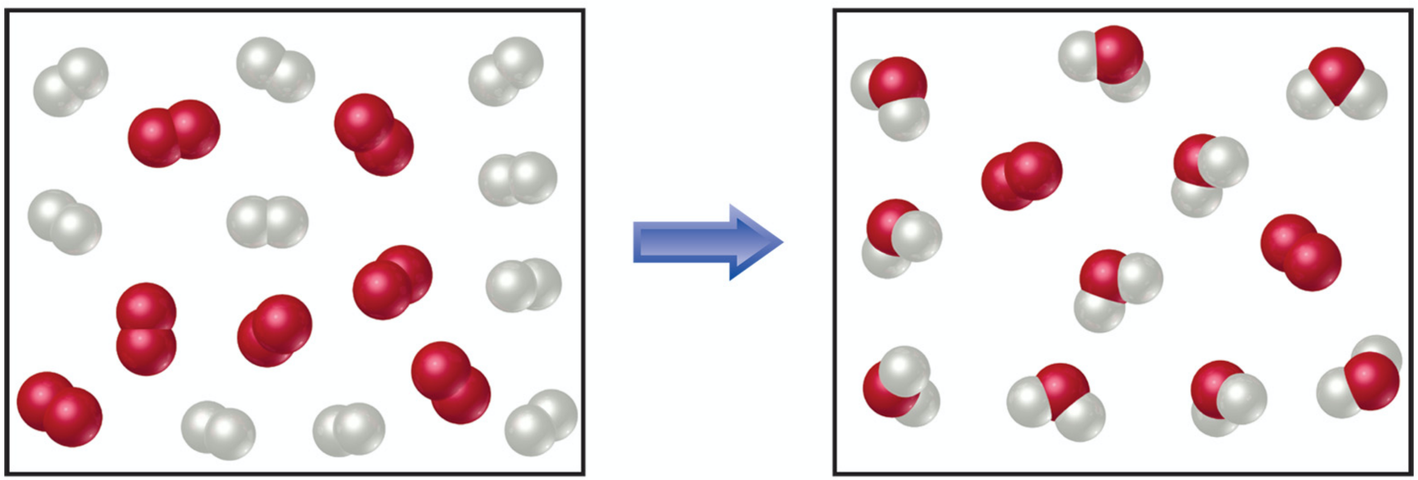
How Many Cookies Can I Make?

- 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

Before reaction | After reaction

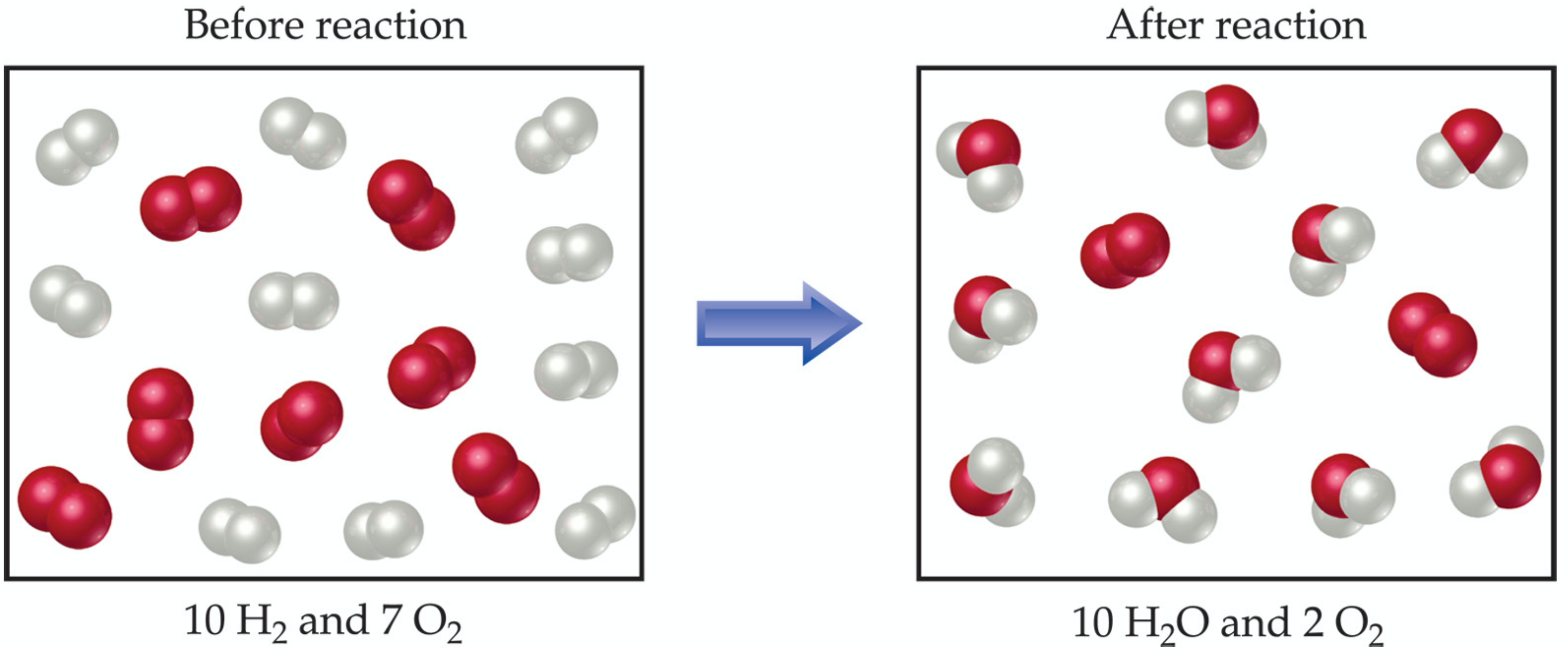


$10\ H_2$ and $7\ O_2$ | $10\ H_2O$ and $2\ O_2$

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

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 1.0 g 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.	(knowns)

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1.0g	1.0g		
84g/mol	192g/mol	44g/mol.	(knowns)
1.0g(1mol/84g)	1.0g(1mol/192g)		
0.012 mol	0.0052 mol		(calculate moles)

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 1.0 g citric acid are reacted, which is limiting? How much carbon dioxide is produced?

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1.0g 1.0g

84g/mol 192g/mol 44g/mol. (knowns)

1.0g(1mol/84g) 1.0g(1mol/192g)

0.012 mol 0.0052 mol (calculate moles)

(Make an assumption)

(i**f citrate limiting**)

0.0052(3)=~~0.016~~ moles bicarbonate, but only have 0.012 moles

Bummer, wrong assumption.

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

(i**f citrate limiting**)

0.0052(3)=~~0.016~~ moles bicarbonate, but only have 0.012 moles

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)=	
	0.23 g left.	

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."
- The ***actual yield*** is the amount actually produced.

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_5Br) 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	(knowns)	
78g/mol		160.g/mol	157g/mol		
30.g(1mol/78g)		65g(1mol/160g).			
0.38 mol		0.41 mol		(moles)	
(If Br_2 limiting)					
~~0.41 mol~~		0.41 mol		(assumption)	
(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%		

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**

1.5 g – 1.2 g=**.3g**

Barking Dog

$$2HNO_3 + 2Cu \text{ -------> } NO + NO_2 + 2Cu^{2+} + 2H^+$$

$$3\ NO + CS_2 \text{ -> } 3/2\ N_2 + CO + SO_2 + 1/8\ S_8$$

$$4\ NO + CS_2 \text{ -> } 2\ N_2 + CO_2 + SO_2 + 1/8\ S_8$$

Gun powder reaction

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

And heat.

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

Gun powder reaction

Oxidizing agent | Oxidizing agent | Reducing agent

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

And heat.

What is interesting about this reaction?

Lots of energy, no oxygen

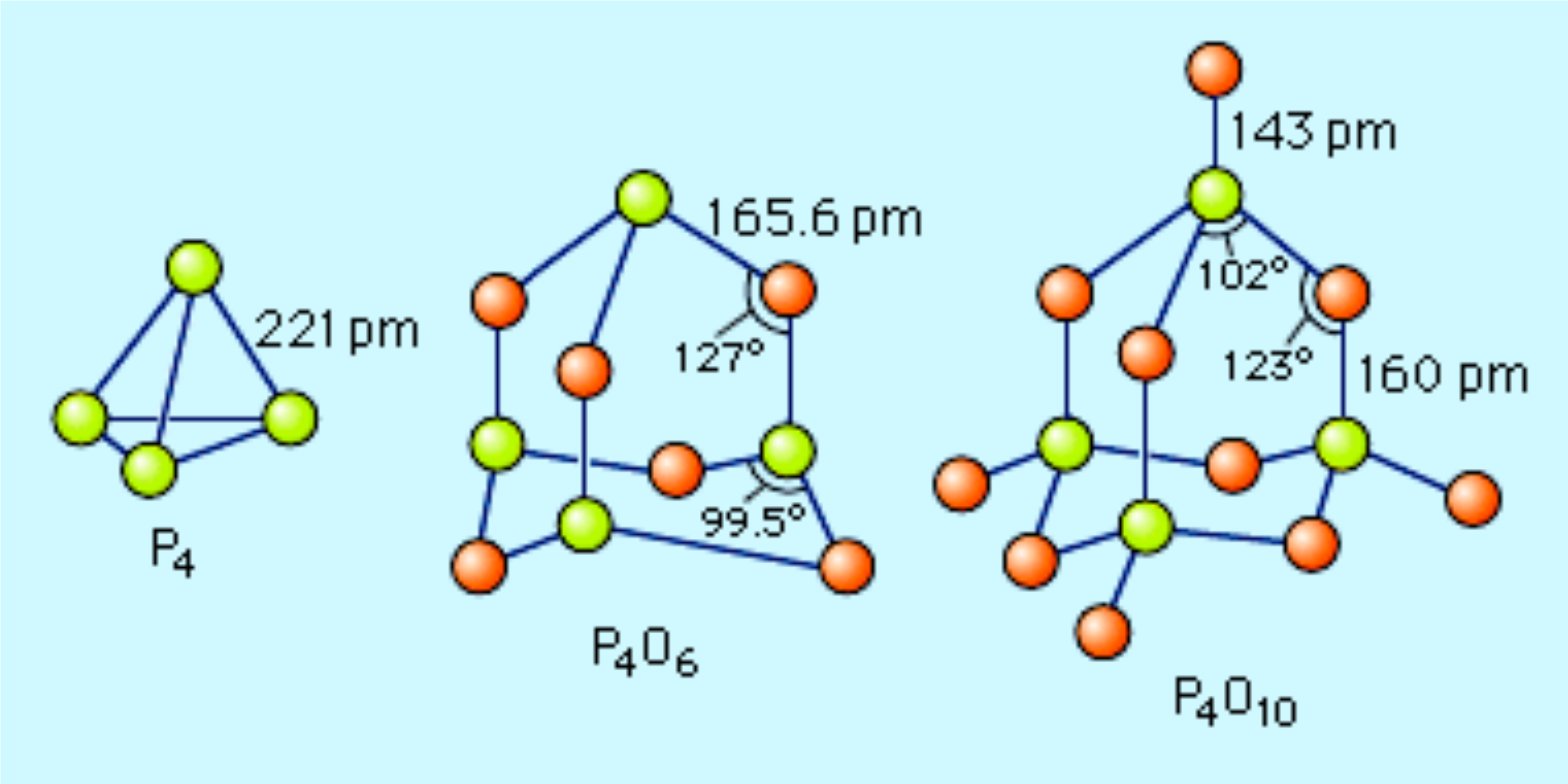
What kind of reaction is it?

Oxidation reduction

What do you think makes it so powerful and explosive?

Makes a lot of gas!!!!

White phosphorous and Oxygen under water



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