## Chapter 3

## Stoichiometry of Formulas \& Equations

- Mole - Mass Relationships in Chemical Systems
- Determining the Formula of an Unknown Compound
- Writing and Balancing Chemical Equations
- Calculating the Amounts of Reactant and Product
- Calculating Limiting Reagent \& Theoretical Yield
- Fundamentals of Solution Stoichiometry


## Stoichiometry

- Stoichiometry - The study of the quantitative relationships between elements, compounds, chemical formulas and chemical reactions
- Each element in a compound has a unique atomic mass (total mass of protons \& neutrons)
> The concept of the "MOLE" was developed to relate the number of entities in a substance to the mass values we determine in the laboratory
> From the relationship between the number of atoms and the mass of a substance we can quantify the relationship between elements and compounds in chemical reactions


## Mass vs. Amount

- The standard unit of mass in the metric system is the gram (or kilogram)
- Each of the 100 or so different elements has a unique mass (atomic weight) expressed as either atomic mass units (amu) or grams determined by the number of protons and neutrons in the nucleus
- The same mass (weight) of two different substances will represent a different number of atoms
- A chemical equation defines the relative number of molecules of each component involved in the reaction
- The "Mole" establishes the relationship between the number of atoms of a given element and the mass of the substance used in a reaction


## Mass vs. Amount

- Amounts in chemistry are expressed by the mole
> mole - quantity of substance that contains the same number of molecules or formula units as exactly 12 g of Carbon-12
> The atomic mass of one atom expressed in atomic mass units (amu) is numerically the same as the mass of 1 mole of the element expressed in grams
- Molar Mass = mass of 1 mole of substance
> One molecule of Carbon (C) has an atomic mass of 12.0107 amu and a molar mass of $12.0107 \mathrm{~g} / \mathrm{mol}$
$>1$ mole of Carbon contains $6.022 \times 10^{23}$ atoms
$>1$ mole of Sodium contains $6.022 \times 10^{23}$ atoms


## Molecular \& Formula Weight

- Molecular Mass (also referred to as Molecular Weight (MW) is the sum of the atomic weights of all atoms in a covalently bonded molecule organic compounds, oxides, etc.
- Formula Mass is sometimes used in a more general sense to include Molecular Mass, but its formal definition refers to the sum of the atomic weights of the atoms in ionic bonded compounds


## Molecular \& Formula Weight

The computation of Molecular (covalent) or Formula (ionic) molar masses is mathematically the same Ex.

Molecular Molar Mass of Methane $\left(\mathrm{CH}_{4}\right)$ (covalent bonds)
$1 \mathrm{~mol} \mathrm{CH}_{4}=1 \mathrm{~mol} \mathrm{C} / \mathrm{mol} \mathrm{CH}_{4} \times 12 \mathrm{~g} / \mathrm{mol} \mathrm{C}=12 \mathrm{~g}$

$$
\begin{aligned}
& 4 \mathrm{~mol} \mathrm{H}
\end{aligned} \mathrm{~mol} \mathrm{CH}_{4} \times 1 \mathrm{~g} / \mathrm{mol} \mathrm{H}=4 \mathrm{~g}, ~\left(16 \mathrm{~g} / \mathrm{mol} \mathrm{CH}_{4}=6.022 \times 10^{23}\right. \text { molecules }
$$

Formula Molar Mass of Aluminum Phosphate ( AlPO $_{4}$ ) (ionic bonds)
$\left.1 \mathrm{~mol} \mathrm{AlPO}_{4}=1 \mathrm{~mol} \mathrm{Al} / \mathrm{mol} \mathrm{AlPO}_{4} \times 27 \mathrm{~g} / \mathrm{mol} \mathrm{Al}\right)=27 \mathrm{~g}$ $1 \mathrm{~mol} \mathrm{P/mol} \mathrm{AlPO}_{4} \times 31 \mathrm{~g} / \mathrm{mol} P=31 \mathrm{~g}$ $\left.4 \mathrm{~mol} \mathrm{O} / \mathrm{mol} \mathrm{AlPO}_{4} \times 16 \mathrm{~g} / \mathrm{mol} \mathrm{O}\right)=64 \mathrm{~g}$ $=122 \mathrm{~g} / \mathrm{mol} \mathrm{AlPO}_{4}=6.022 \times 10^{23}$ molecules

## The Concept of Amount

| Summary of |
| :--- |
| Isotopic Mass |
| Atomic Mass <br> (atomic weight) |

## Mole Relationships: Example Calculations

How many molecules of $\mathrm{H}_{2} \mathrm{O}$ are in 251 kg of water?

251 kg x (1000 g/kg) $=2.51 \times 10^{5} \mathrm{~g} \mathrm{H}_{2} \mathrm{O}$
$2.51 \times 10^{5} \mathrm{~g} \mathrm{H}_{2} \mathrm{O} \times\left(1 \mathrm{~mol} \mathrm{H}_{2} \mathrm{O} / 18.0153 \mathrm{~g}\right)=1.39326 \times 10^{4} \mathrm{~mol} \mathrm{H}_{2} \mathrm{O}$
$1.39326 \times 10^{4} \mathrm{~mol} \times 6.022 \times 10^{23}$ atoms $/ \mathrm{mol}=8.39021 \times 10^{27}$ molecules

How many total atoms are in 251 kg of water?
$8.39021 \times 10^{27}$ molecules $\times$ ( 3 atoms $/ 1$ molecule) $=2.52 \times 10^{28}$ atoms

## Practice Problems

What is the molar mass of Caffeine, $\mathrm{C}_{8} \mathrm{H}_{10} \mathrm{~N}_{4} \mathrm{O}_{2}$ ?

$$
\begin{array}{ll}
\mathrm{C}=12.0107 \mathrm{~g} / \mathrm{mol} & \mathrm{H}=1.00794 \mathrm{~g} / \mathrm{mol} \\
\mathrm{~N}=14.0067 \mathrm{~g} / \mathrm{mol} & \mathrm{O}=15.9994 \mathrm{~g} / \mathrm{mol}
\end{array}
$$

$12.0107 \mathrm{~g} / \mathrm{mql} \mathrm{C} \times 8 \mathrm{~mol} \mathrm{C} / \mathrm{mol} \mathrm{C}_{8} \mathrm{H}_{10} \mathrm{~N}_{4} \mathrm{O}_{2}=96.0856 \mathrm{~g} / \mathrm{mol} \mathrm{C} \mathrm{C}_{8} \mathrm{H}_{10} \mathrm{~N}_{4} \mathrm{O}_{2}$ $1.00794 \mathrm{~g} / \mathrm{mp} / \mathrm{H} \times 10 \mathrm{mq} / \mathrm{H} / \mathrm{mol} \mathrm{C}_{8} \mathrm{H}_{10} \mathrm{~N}_{4} \mathrm{O}_{2}=10.0794 \mathrm{~g} / \mathrm{mol} \mathrm{C}_{8} \mathrm{H}_{10} \mathrm{~N}_{4} \mathrm{O}_{2}$ $14.0067 \mathrm{~g} / \mathrm{mal} \mathrm{N} \times 4 \mathrm{mal} \mathrm{N} / \mathrm{mol} \mathrm{C} \mathrm{C}_{8} \mathrm{H}_{10} \mathrm{~N}_{4} \mathrm{O}_{2}=56.0268 \mathrm{~g} / \mathrm{mol} \mathrm{C} \mathrm{C}_{8} \mathrm{H}_{10} \mathrm{~N}_{4} \mathrm{O}_{2}$ $15.9994 \mathrm{~g} / \mathrm{m} \mathrm{\& l} \mathrm{O} \times 2 \mathrm{~m} \mathrm{\& l} \mathrm{O} / \mathrm{mol} \mathrm{C}_{8} \mathrm{H}_{10} \mathrm{~N}_{4} \mathrm{O}_{2}=31.9988 \mathrm{~g} / \mathrm{mol} \mathrm{C}_{8} \mathrm{H}_{10} \mathrm{~N}_{4} \mathrm{O}_{2}$

Sum of elemental masses = molecular mass of Caffeine $96.0856+10.0794+56.0268+31.9988=$
$194.1906 \mathrm{~g} / \mathrm{mol} \mathrm{C}_{8} \mathrm{H}_{10} \mathrm{~N}_{4} \mathrm{O}_{2}$

## Practice Problem

How many Sulfur atoms are in 25 g of $\mathrm{Al}_{2} \mathrm{~S}_{3}$ ?

$$
\mathrm{Al}=26.9815 \mathrm{~g} / \mathrm{mol} \quad \mathrm{~S}=32.065 \mathrm{~g} / \mathrm{mol}
$$

$\mathrm{Al}_{2} \mathrm{~S}_{3}=26.98915 \mathrm{~g} / \mathrm{mdl} \mathrm{Al}^{2} \times 2 \mathrm{~m} \downarrow \mathrm{Al}+32.065 \mathrm{~g} / \mathrm{md} / \mathrm{S} \times 3 \mathrm{~m} \downarrow \mathrm{~S}$
$=150.158 \mathrm{~g} / \mathrm{mol} \mathrm{Al}_{2} \mathrm{~S}_{3}$
$25 \mathrm{~g} \mathrm{Al}_{2} \mathrm{~S}_{3} / 150.158 \mathrm{~g} / \mathrm{mol} \mathrm{Al}_{2} \mathrm{~S}_{3}=0.166491 \mathrm{~mol} \mathrm{Al}_{2} \mathrm{~S}_{3}$
Compute moles of Sulfur atoms
$0.166491 \mathrm{mo} \not \stackrel{\wedge}{2}_{2} \mathrm{~S}_{3} \times 3 \mathrm{~mol} \mathrm{~S} / 1 \mathrm{~mol} \mathrm{Al}_{2} \mathrm{~S}_{3}=0.499474 \mathrm{~mol} \mathrm{~S}$ atoms
Compute atoms of Sulfur
0.499474 mo\s atoms $\times 6.022 \times 10^{23} \mathrm{~S}$ atoms $/ 1 \mathrm{~mol} \backslash$ atoms $=$ $3.008 \times 10^{23}$ atoms $S$

## Percent Composition

- It is often necessary to determine the mass percentage of a component in a mixture or an element in a compound

$$
\text { Mass } \% \mathrm{~A}=\frac{\text { Mass of A in Whole }}{\text { Mass of Whole }} \times 100
$$

- Example calculation: What are the mass percentages of $\mathrm{C}, \mathrm{H}$ and O in $\mathrm{C}_{2} \mathrm{H}_{4} \mathrm{O}_{2}$ (Acetic Acid)?

1 mol acetic acid $=60.052 \mathrm{~g}$
$\% \mathrm{C}=[2 \mathrm{~mol} \mathrm{C} \times(12.0107 \mathrm{~g} / \mathrm{mol} \mathrm{C})] \div 60.052 \mathrm{~g} / \mathrm{mol} \times 100=40.00 \%$
$\% \mathrm{H}=[4 \mathrm{~mol} \mathrm{H} \times(1.00794 \mathrm{~g} / \mathrm{mol} \mathrm{C})] \div 60.052 \mathrm{~g} / \mathrm{mol} \times 100=6.71 \%$
$\% \mathrm{O}=[2 \mathrm{~mol} \mathrm{O} \times(15.9994 \mathrm{~g} / \mathrm{mol} \mathrm{C})] \div 60.052 \mathrm{~g} / \mathrm{mol} \times 100=53.29 \%$

## Practice Problem

What is the mass percentage of C in in I -Carvone, $\mathrm{C}_{10} \mathrm{H}_{14} \mathrm{O}$, which is the principal component of spearmint?

$$
\begin{array}{lllll}
C=12.0107 \mathrm{~g} / \mathrm{mol} & \mathrm{H}=1.00794 \mathrm{~g} . \mathrm{mol} & \mathrm{O}=15.9994 \mathrm{~g} / \mathrm{mol} \\
\begin{array}{llll}
\text { a. } 30 \% & \text { b. } 40 \% & \text { c. } 60 \% & \text { d. } 70 \%
\end{array} & \text { e. } 80 \%
\end{array}
$$

Ans: e

Molar Mass C $=12.0170 \mathrm{~g} / \mathrm{mol} \mathrm{C} \mathrm{x} 10 \mathrm{~mol} \mathrm{C}=120.170 \mathrm{~g} \mathrm{C}$

$$
\begin{aligned}
\mathrm{H}=1.00794 \mathrm{~g} / \mathrm{mol} \mathrm{H} \times 14 \mathrm{~mol} \mathrm{H} & =14.1112 \mathrm{~g} \mathrm{H} \\
\mathrm{O}=15.9994 \mathrm{~g} / \mathrm{mol} \mathrm{O} \times 1 \mathrm{~mol} \mathrm{O} & =15.9994 \mathrm{~g} \mathrm{O} \\
\text { Molar Mass C }{ }_{10} \mathrm{H}_{14} \mathrm{O} & =150.218 \mathrm{~g} / \mathrm{mol}
\end{aligned}
$$

Mass \% C = $120.170 / 150.218 \times 100=79.9971$ ( $80 \%$ )

## Empirical \& Molecular Formulas

- Empirical formula - formula of a substance written with the smallest whole number subscripts
- EF of Acetic Acid = $\mathrm{C}_{2} \mathrm{H}_{5} \mathrm{O}_{2}$
- For small molecules, empirical formula is identical to the molecular formula: formula for a single molecule of substance
- For Succinic acid, its molecular formula is: $\mathrm{C}_{4} \mathrm{H}_{6} \mathrm{O}_{4}$
Its empirical formula is: $\quad \mathrm{C}_{2} \mathrm{H}_{3} \mathrm{O}_{2}(\mathrm{n}=2)$
- Molecular weight $=n \times$ empirical formula weight ( $\mathrm{n}=$ number of empirical formula units in the molecule)


## Practice Problem

Of the following, the only empirical formula is
a. $\mathrm{C}_{2} \mathrm{H}_{4}$
b. $\mathrm{C}_{5} \mathrm{H}_{12}$
C. $\mathrm{N}_{2} \mathrm{O}_{4}$
d. $\mathrm{S}_{8}$
e. $\mathrm{N}_{2} \mathrm{H}_{4}$

Ans: b

Subscript (5) cannot be further divided into whole numbers

## Molecular Formula from Elemental Analysis:

A moth repellant, para-dichlorobenzene, has the composition 49.1\% C, $2.7 \% \mathrm{H}$ and $48.2 \% \mathrm{Cl}$. Its molecular weight is determined from mass spectrometry (next slide). What is its molecular formula?

Assume a sample mass of 100 grams

$$
\begin{aligned}
& 49.1 \mathrm{~g} \mathrm{C} \mathrm{x} 1 \mathrm{molC} / 12.0107 \mathrm{~g} \mathrm{C}=4.0880 \mathrm{~mol} \mathrm{C} \\
& 2.7 \mathrm{~g} \mathrm{H} \mathrm{x} 1 \mathrm{~mol} \mathrm{H} / 1.00794 \mathrm{~g} \mathrm{H}=2.6787 \mathrm{~mol} \mathrm{H} \\
& 48.2 \mathrm{~g} \mathrm{Cl} \times 1 \mathrm{~mol} \mathrm{Cl}
\end{aligned}
$$

Convert Mole values to "Whole" numbers (divide each value by smallest)
$4.0880 / 1.3595=3.01(3 \mathrm{~mol} \mathrm{C})$
$2.6787 / 1.3595=1.97(2 \mathrm{~mol} \mathrm{H})$
$1.3595 / 1.3595=1.00(1 \mathrm{~mol} \mathrm{Cl})$
$\therefore$ Empirical Formula is: $\mathrm{C}_{3} \mathrm{H}_{2} \mathrm{Cl}$

Molecular Formula from Elemental Analysis: An Example Calculation (Con't)
Empirical formula $=\mathrm{C}_{3} \mathrm{H}_{2} \mathrm{Cl}$
Compute Empirical Formula Weight (EFW)

$$
\begin{aligned}
& \text { Carbon } \begin{array}{l}
\text { Hydrogen Chlorine } \\
\text { EFW }
\end{array}=3 \times 12.01+2 \times 1.01+1 \times 35.45=73.51 \mathrm{amu} \\
& \text { EFW }=73.51 \mathrm{~g} / \mathrm{mol}
\end{aligned}
$$

Molecular weight ( $\mathrm{M}^{+}$ion from mass spectrum) $=146 \mathrm{amu}$

$$
n=146 / 73.51=1.99=2
$$

$\therefore$ Molecular Formula $=\mathrm{C}_{6} \mathrm{H}_{4} \mathrm{Cl}_{2}$

## Empirical Formula from Mole Fraction

- A sample of an unknown compound contains:

$$
0.21 \mathrm{~mol} \mathrm{Zn} \quad 0.14 \mathrm{~mol} \mathrm{P} \quad 0.56 \mathrm{~mol} \mathrm{O}
$$

What is the Empirical Formula?
Ans: Express preliminary formula using mole fraction values

$$
\mathrm{Zn}_{0.21} \mathrm{P}_{0.14} \mathrm{O}_{0.56}
$$

Divide Each Fraction Value by the Smallest Fraction value

$$
\begin{aligned}
& 0.21 / 0.14=1.5 \\
& 0.14 / 0.14=1.0 \\
& 0.56 / 0.14=4.0
\end{aligned} \quad \mathrm{Zn}_{1.5} \mathrm{P}_{1.0} \mathrm{P}_{4.0}
$$

Multiply through by the smallest integer that turns all subscripts into whole number integers

$$
\mathrm{Zn}_{(1.5 \times 2)} \mathrm{P}_{1.0 \times 2)} \mathrm{P}_{(4.0 \times 2)}=\mathrm{Zn}_{3} \mathrm{P}_{2} \mathrm{O}_{8}
$$

## The Chemical Equation

A chemical equation is the representation of the reactants and products in a chemical reaction in terms of chemical symbols and formulas

The subscripts represent the number of atoms of an element in the compound

The coefficients in front of the compound represents the number of moles of each compound required to balance the equation

## The Chemical Equation

A balanced equation will have an equal number of atoms of each element on both sides of equation

(4 atoms on each side)
1 mole nitrogen +1 mole oxygen yields 2 moles nitrogen monoxide

Phase representations in Chemical Equations
$\rightarrow$ = yields, or forms (g) = gas phase
(I) = liquid phase (s) = Solid phase

## The Chemical Equation

## - Example Problem

Balance the following reaction

$$
\mathrm{C}_{8} \mathrm{H}_{18}+\mathrm{O}_{2} \rightarrow \mathrm{CO}_{2}+\mathrm{H}_{2} \mathrm{O}
$$

$1 \mathrm{C}_{8} \mathrm{H}_{18}+\mathrm{O}_{2} \rightarrow 8 \mathrm{CO}_{2}+\mathrm{H}_{2} \mathrm{O}$
$1 \mathrm{C}_{8} \mathrm{H}_{18}+\mathrm{O}_{2} \rightarrow 8 \mathrm{CO}_{2}+9 \mathrm{H}_{2} \mathrm{O}$
$1 \mathrm{C}_{8} \mathrm{H}_{18}+25 / 2 \mathrm{O}_{2} \rightarrow 8 \mathrm{CO}_{2}+9 \mathrm{H}_{2} \mathrm{O}$
$2 \mathrm{C}_{8} \mathrm{H}_{18}+25 \mathrm{O}_{2} \rightarrow 16 \mathrm{CO}_{2}+18 \mathrm{H}_{2} \mathrm{O}$

## Stoichiometry in Chemical Equations

When Dinitrogen Pentoxide, $\mathrm{N}_{2} \mathrm{O}_{5}$ a while solid, is heated, it decomposes to Nitrogen Dioxide and Oxygen $2 \mathrm{~N}_{2} \mathrm{O}_{5}(\mathrm{~s}) \rightarrow 4 \mathrm{NO}_{2}(\mathrm{~g})+\mathrm{O}_{2}(\mathrm{~g}) \quad$ Molar Ratio 2:4:1 If a sample of $\mathrm{N}_{2} \mathrm{O}_{5}$ produces 1.315 g of $\mathrm{O}_{2}$, how many grams of $\mathrm{NO}_{2}$ are formed? How many grams of $\mathrm{N}_{2} \mathrm{O}_{5}$ are consumed?

## Strategy:

1. Compute actual no. of moles of oxygen produced
2. Determine molar ratio of $\mathrm{NO}_{2} \& \mathrm{~N}_{2} \mathrm{O}_{5}$ relative to $\mathrm{O}_{2}$
(4:1 \& 2:1)
3. Compute mass of $\mathrm{NO}_{2}$ produced from molar ratio and actual moles $\mathrm{O}_{2}$

$$
0.04109 \mathrm{~mol}_{2} \times\left(4 \mathrm{~mol} \mathrm{NO}_{2} / 1 \mathrm{~mol}_{2}\right) \times\left(46.01 \mathrm{~g} \mathrm{NO}_{2} / 1 \mathrm{moN}_{2}\right)=7.563 \mathrm{~g} \mathrm{NO}_{2}
$$

4. Compute mass of $\mathrm{N}_{2} \mathrm{O}_{5}$ from molar ratio and actual moles $\mathrm{O}_{2}$

$$
0.04109 \mathrm{~mol}_{2} \times\left(2 \mathrm{~mol}_{2} \mathrm{O}_{5} / 1 \mathrm{~mol}_{2}\right) \times\left(108.0 \mathrm{~g} \mathrm{~N}_{2} \mathrm{O}_{5} / \mathrm{mol}_{2} \mathrm{O}_{5}\right)=8.834 \mathrm{~g} \mathrm{~N}_{2} \mathrm{O}_{5}
$$

## Stoichiometry in Chemical Equations

How many grams of HCl are required to react with 5.00 grams Manganese Dioxide $\left(\mathrm{MnO}_{2}\right)$ according to the equation? $4 \mathrm{HCl}(\mathrm{aq})+\mathrm{MnO}_{2}(\mathrm{~s}) \rightarrow 2 \mathrm{H}_{2} \mathrm{O}(\mathrm{l})+\mathrm{MnCl}_{2}(\mathrm{aq})+\mathrm{Cl}_{2}(\mathrm{~g})$ Strategy: 1. Determine the Molar Ratio of HCL to $\mathrm{MnO}_{2}$
2. Compute the no. moles $\mathrm{MnO}_{2}$ actually used
3. Use actual moles $\mathrm{MnO}_{2}$ \& Molar ratio to compute mass HCL

Molar Ratio $\mathrm{HCl}: \mathrm{MnO}_{2}=4: 1$
$5.00 \mathrm{~g}_{\mathrm{gnnO}}^{2}$ x $\left(1 \mathrm{~mol} \mathrm{MnO} / 86.9368 \mathrm{~g} / \mathrm{MnO}_{2}\right)=0.575 \mathrm{~mol}_{\mathrm{MnO}}^{2}$
$\left.0.575 \mathrm{~mol}^{\mathbf{~} \mathrm{MnO}_{2} \times(4 \mathrm{~mol} \mathrm{ACl} / 1 \mathrm{~mol}} \mathrm{MnO}_{2}\right) \times(36.461 \mathrm{~g} \mathrm{HCl} / \mathrm{moN} \AA \mathrm{HCl})$
$=8.39 \mathrm{~g} \mathrm{HCl}$

# Reactions that Occur in a Sequence 

- In many situations, a product of one reaction becomes a reactant for the next
- For stoichiometric purposes, when the same (common) substance forms in one reaction and reacts (used up) in the next, it is eliminated in the overall reaction
- Steps in the addition of reactions:
> Write the sequence of balanced equations
> Adjust the equations arithmetically to cancel the common substance
> Add the adjusted equations together to obtain the overall balanced equation


## Reactions that Occur in a Sequence

- Ex. Write the two balanced equations

$$
\begin{aligned}
2 \mathrm{Cu}_{2} \mathrm{~S}(\mathrm{~s})+3 \mathrm{O}_{2}(\mathrm{~g}) & \rightarrow 2 \mathrm{Cu}_{2} \mathrm{O}(\mathrm{~s})+2 \mathrm{SO}_{2}(\mathrm{~g}) \\
\mathrm{Cu}_{2} \mathrm{O}(\mathrm{~s})+\mathrm{C}(\mathrm{~s}) & \rightarrow 2 \mathrm{Cu}(\mathrm{~s})+\mathrm{CO}(\mathrm{~g})
\end{aligned}
$$

- Adjust Coefficients - Multiply $2^{\text {nd }}$ equation by 2

$$
\begin{aligned}
& 2 \mathrm{Cu}_{2} \mathrm{~S}(\mathrm{~s})+3 \mathrm{O}_{2}(\mathrm{~g}) \rightarrow 2 \mathrm{Cu}_{2} \mathrm{Q}(\mathrm{~s})+2 \mathrm{SO}_{2}(\mathrm{~g}) \\
& 2 \mathrm{Cu}_{2} \mathrm{Q}(\mathrm{~s})+2 \mathrm{C}(\mathrm{~s}) \rightarrow 4 \mathrm{Cu}(\mathrm{~s})+2 \mathrm{CO}(\mathrm{~g})
\end{aligned}
$$

$\left.2 \mathrm{Cu}_{2} \mathrm{~S}(\mathrm{~s})+3 \mathrm{O}_{2}(\mathrm{~g})+2 \mathrm{C}(\mathrm{s}) \rightarrow 4 \mathrm{Cu}(\mathrm{s})+2 \mathrm{CO}(\mathrm{g})\right)+2 \mathrm{SO}_{2}(\mathrm{~g})$
The common compound in both reactions $\left(\mathrm{Cu}_{2} \mathrm{O}\right)$ is eliminated
Biological systems have many examples of Multistep reaction sequences called "Metabolic Pathways"

## Limiting Reactants and Yields

 Limiting Reagent \& Theoretical Yield> The "Limiting Reagent" is that reactant whose mass (on a molar equivalent basis) actually consumed in the reaction is less than the amount of the other reactant, i.e., the reactant in excess
>From the Stoichiometric balanced equation determine the molar ratio among the reactants and products, i.e., how many moles of reagent A react with how many moles of reagent $B$ to yield how many moles of product C, D, etc.

# Limiting Reactants and Yields 

$>$ If the ratio of moles of A to moles of B actually used is greater than the Stoichiometric molar ratio of $A$ to $B$, then

reagent A is in "Excess"<br>reagent $B$ is "Limiting"

> If, however, the actual molar ratio of A to B used is less than the Stoichiometric molar ratio, then B is in excess and A is "Limiting"
$>$ The moles of product(s) (theoretical yield) is determined by the moles of 'limiting Reagent" on a molar equivalent basis

## Limiting Reactants and Yields

Example 1

$$
\mathrm{A}+\mathrm{B} \rightarrow \mathrm{C} \quad \text { Molar Ratio } \mathrm{A}: \mathrm{B}=1
$$

Moles actually used: $\mathrm{A}=0.345$

$\therefore$ On a molar equivalent basis (1/1) there is not enough reagent A ( 0.345 mol ) to react with reagent $B(0.498 \mathrm{~mol})$; therefore reagent $B$ is in excess \& reagent A is Limiting
$\therefore$ Since 1 mol "A" produces 1 mol " $\mathrm{C}^{\prime}$
Theoretical Yield of "C" $=0.345$ moles

## Limiting Reactants and Yields

## Example 2

$$
A+B \rightarrow C
$$

Stoichiometric Molar ratio $A: B=1: 1$
Moles actually used:
$A=0.20$
Ratio of Moles actually used (A/B):

$$
0.20 / 0.12=1.67
$$

The ratio of $A: B$ is greater than 1.00
$A$ is in excess and $B$ is limiting
Only 0.12 moles of the 0.2 moles of " $A$ " would be required to react with the 0.12 moles of B

The reaction would have a theoretical yield of:

$$
0.12 \text { moles of "C" (Molar Ratio of } \mathrm{B}: \mathrm{C}=1: 1 \text { ) }
$$

## Limiting Reactants and Yields

## Example 3

$$
\mathrm{A}+2 \mathrm{~B} \rightarrow \mathrm{C}
$$

Stoichiometric Molar ratio $A: B=1: 2=0.5$
Moles actually used: $\quad A=0.0069 ; B=0.023$
Ratio of Moles actually used $(A / B)$ :
$0.0069 / 0.023=0.30<0.5$
$\therefore$ "A" is limiting
Only $0.0069 \bullet 2=0.0138$ moles of the 0.023 moles of B are required to react with the 0.0069 moles of A

Since $0.0138<0.023$ " $B$ " is in excess, " $A$ " is limiting
The reaction would have a theoretical yield of:

$$
0.0069 \text { moles of } \mathrm{C} \quad \text { (Molar Ratio of } \mathrm{A}: \mathrm{C}=1: 1 \text { ) }
$$

## Limiting Reactants and Yields

Theoretical Yield \& Percent Yield

- The Theoretical Yield, in grams, is computed from the number of moles of the "Limiting Reagent", the Stoichiometric Molar Ratio, and the Molecular Weight of the product
Yield $=$ mol (Lim) $\times$ Mol Ratio Prod/Lim $\times$ Mol Wgt Product
- The Percent Yield of a product obtained in a "Synthesis" experiment is computed from the amount of product actually obtained in the experiment and the Theoretical Yield
\% Yield = Actual Yield / Theoretical Yield $\times 100$
Note: The yield values can be expressed in either grams or moles


## Example Yield Calculation

Methyl Salicylate (MSA) is prepared by heating Salicylic Acid (SA), $\mathrm{C}_{7} \mathrm{H}_{6} \mathrm{O}_{3}$, with Methanol (ME), $\mathrm{CH}_{3} \mathrm{OH}$

$$
\mathrm{C}_{7} \mathrm{H}_{6} \mathrm{O}_{3}+\mathrm{CH}_{3} \mathrm{OH} \rightarrow \mathrm{C}_{8} \mathrm{H}_{8} \mathrm{O}_{3}+\mathrm{H}_{2} \mathrm{O}
$$

1.50 g of Salicylic acid (SA) is reacted with 11.20 g of Methanol (ME). The yield of Methyl Salicylate is 1.27 g . What is the limiting reactant? What is the percent yield of Methyl Salicylate (MSA)?

Molar Ratio: 1 mole SA reacts with 1 mole ME to produce 1 mole MSA
Moles SA: $\quad 1.50 \mathrm{~g} \mathrm{SA} \times(1 \mathrm{~mol} \mathrm{SA} / 138.12 \mathrm{~g} \mathrm{SA})=0.0109 \mathrm{~mol} \mathrm{SA}$

$0.0109 \mathrm{~mol} \mathrm{SA} \times(1 \mathrm{~mol} \mathrm{SA} / 1 \mathrm{~mol}$ ME $)<0.350 \mathrm{~mol}$ ME
$\therefore$ Salicylic acid (SA) is limiting; Methanol (ME) is in "Excess"

Theoretical Yield $=0.0109 \mathrm{~mol} \mathrm{SA} \times(1 \mathrm{~mol} \mathrm{MSA} / 1 \mathrm{~mol} \mathrm{SA}) \times$

$$
(152.131 \mathrm{~g} \mathrm{MSA} / 1 \mathrm{~mol} \text { MSA })=1.66 \mathrm{~g} \text { MSA }
$$

## Example Yield Calculation

Hydrogen $\left(\mathrm{H}_{2}\right)$ is a possible clean fuel because it reacts with Oxygen (O) to form non-polluting water $\left(\mathrm{H}_{2} \mathrm{O}\right)$

$$
2 \mathrm{H}_{2}(\mathrm{~g})+\mathrm{O}_{2}(\mathrm{~g}) \rightarrow 2 \mathrm{H}_{2} \mathrm{O}(\mathrm{~g})
$$

If the yield of this reaction is $87 \%$ what mass of Oxygen is required to produce 105 kg of Water?
Molar Ratio: 2 mol $\mathrm{H}_{2}$ reacts with $1 \mathrm{~mol} \mathrm{O}_{2}$ to form 2 mol Water $\left(\mathrm{H}_{2} \mathrm{O}\right)$
Moles $\mathrm{H}_{2} \mathrm{O}: 105 \mathrm{~kg} \mathrm{H}_{2} \mathrm{O} \times(1000 \mathrm{~g} / 1 \mathrm{~kg}) \times\left(1 \mathrm{~mol} \mathrm{H}_{2} \mathrm{O} / 18.01 \mathrm{~g} / \mathrm{mol} \mathrm{H}_{2} \mathrm{O}\right)$
$=5,830 \mathrm{~mol} \mathrm{H} \mathrm{H}_{2}$
Moles $\mathrm{O}_{2}=\left(1 \mathrm{~mol} \mathrm{O}_{2} / 2 \mathrm{~mol} \mathrm{H} \mathrm{O}\right) \times 5,830 \mathrm{~mol} \mathrm{H}_{2} \mathrm{O}=2,915 \mathrm{~mol} \mathrm{O}_{2}$
Mass $\mathrm{O}_{2}=2,915 \mathrm{~mol}_{2} \times\left(32.0 \mathrm{~g} \mathrm{O}_{2} / 1 \mathrm{~mol} \mathrm{O}_{2}\right) \times(1 \mathrm{~kg} / 1000 \mathrm{~g})$
$=93.2 \mathrm{~kg} \mathrm{O}_{2}$ required to produce $105 \mathrm{~kg} \mathrm{H}_{2} \mathrm{O}(100 \%)$
At $87 \%$ efficiency: $93.2 \mathrm{~kg} \times 100 \% / 87 \%=107 \mathrm{~kg} \mathrm{O}_{2}$ required

## Sample Problem

In the study of the following reaction:

$$
2 \mathrm{~N}_{2} \mathrm{H}_{4}(\mathrm{I})+\mathrm{N}_{2} \mathrm{O}_{4}(\mathrm{I}) \rightarrow 3 \mathrm{~N}_{2}(\mathrm{~g})+4 \mathrm{H}_{2} \mathrm{O}(\mathrm{~g})
$$

the yield of $N_{2}$ was less than expected
It was then discovered that a $2^{\text {nd }}$ side reaction also occurs:

$$
\left.\left.\mathrm{N}_{2} \mathrm{H}_{4}(\mathrm{I})+2 \mathrm{~N}_{2} \mathrm{O}_{4}(\mathrm{I}) \rightarrow 6 \mathrm{NO}(\mathrm{~g})+2 \mathrm{H}_{2} \mathrm{O}\right) \mathrm{~g}\right)
$$

In one experiment, 10.0 g of NO formed when 100.0 g of each reactant was used

What is the highest percent yield of $\mathrm{N}_{2}$ that can be expected?

## Sample Problem

Ans:
If 100.0 g of Dinitrogen Tetroxide $\left(\mathrm{N}_{2} \mathrm{O}_{4}\right)$ reacts with 100.0 g of Hydrazine $\left(\mathrm{N}_{2} \mathrm{H}_{4}\right)$, what is the theoretical yield of Nitrogen if no side reaction takes place?
First, we need to identify the limiting reactant!
The limiting reactant is used to calculate the theoretical yield Determine the amount of limiting reactant required to produce 10.0 grams of NO
Reduce the amount of limiting reactant by the amount used to produce NO
The reduced amount of limiting reactant is then used to calculate an "actual yield"
The "actual" and theoretical yields will give the maximum percent yield

## Sample Problem (con't)

Solution (con't):
Determining the limiting reagent:
$\mathrm{N}_{2}$ from $\mathrm{N}_{2} \mathrm{O}_{4}=\left(100.0 \mathrm{~g} \mathrm{~N}_{2} \mathrm{O}_{4}\right)\left(\frac{1 \mathrm{~mol} \mathrm{~N}_{2} \mathrm{O}_{4}}{92.02 \mathrm{~g} \mathrm{~N}_{2} \mathrm{O}_{4}}\right)\left(\frac{3 \mathrm{~mol} \mathrm{~N}_{2}}{1 \mathrm{~mol} \mathrm{~N}_{2} \mathrm{O}_{4}}\right)=3.26016 \mathrm{~mol} \mathrm{~N}$
$\mathrm{N}_{2}$ from $\mathrm{N}_{2} \mathrm{H}_{4}=\left(100.0 \mathrm{~g} \mathrm{~N}_{2} \mathrm{H}_{4}\right)\left(\frac{1 \mathrm{~mol} \mathrm{~N}_{2} \mathrm{H}_{4}}{32.05 \mathrm{~g} \mathrm{~N}_{2} \mathrm{H}_{4}}\right)\left(\frac{3 \mathrm{~mol} \mathrm{~N}}{2}\right.$ $\left.2 \mathrm{~mol} \mathrm{~N}_{2} \mathrm{H}_{4}\right)=4.68019 \mathrm{~mol} \mathrm{~N}_{2}$

Molar Ratio $=\frac{3.26016 \mathrm{~mol} \mathrm{~N}_{2}}{4.68019 \mathrm{~mol} \mathrm{~N}_{2}}=0.696779<1.0$
$\therefore \mathrm{N}_{2} \mathrm{O}_{4}$ is the limiting reagent-Produces $3.26016 \mathrm{~mol} \mathrm{~N}_{2}$ vs. $4.68019 \mathrm{~mol} \mathrm{~N}_{2}$ from $\mathrm{N}_{2} \mathrm{H}_{2}$

Theoretical Yield of $\mathrm{N}_{2}=\left(100.0 \mathrm{~g} \mathrm{~N}_{2} \mathrm{O}_{4}\right)\left(\frac{1 \mathrm{~mol} \mathrm{~N}_{2} \mathrm{O}_{4}}{92.02 \mathrm{~g} \mathrm{~N}_{2} \mathrm{O}_{4}}\right)\left(\frac{3 \mathrm{~mol} \mathrm{~N}_{2}}{1 \mathrm{~mol} \mathrm{~N}_{2} \mathrm{O}_{4}}\right)\left(\frac{28.02 \mathrm{~g} \mathrm{~N}_{2}}{1 \mathrm{~mol} \mathrm{~N}_{2}}\right)=91.3497 \mathrm{~g} \mathrm{~N}_{2}$

## Sample Problem (con't)

## Soln (con't)

How much limiting reagent $\left(\mathrm{N}_{2} \mathrm{O}_{4}\right)$ is used to produce 10.0 g NO ?
Grams $\mathrm{N}_{2} \mathrm{O}_{4}$ used $=(10.0 \mathrm{~g} \mathrm{NO})\left(\frac{1 \mathrm{~mol} \mathrm{NO}}{30.01 \mathrm{~g} \mathrm{NO}}\right)\left(\frac{2 \mathrm{~mol} \mathrm{~N}_{2} \mathrm{O}_{4}}{6 \mathrm{~mol} \mathrm{NO}}\right)\left(\frac{92.02 \mathrm{~g} \mathrm{~N}_{2} \mathrm{O}_{4}}{1 \mathrm{~mol} \mathrm{~N}_{2} \mathrm{O}_{4}}\right)=10.221 \mathrm{~g} \mathrm{~N}_{2} \mathrm{O}_{4}$
Determine the actual yield

Initial amount of $\mathrm{N}_{2} \mathrm{O}_{4}$ available $=100.0 \mathrm{~g}$

Mass of $\mathrm{N}_{2} \mathrm{O}_{4}$ remaining to produce Nitrogen $\left(\mathrm{N}_{2}\right)$

$$
100.0 \mathrm{~g}-10.221 \mathrm{~g}=89.779 \mathrm{~g} \mathrm{~N}_{2} \mathrm{O}_{4}
$$

Actual yield of $\mathrm{N}_{2}=\left(89.779 \mathrm{~g} \mathrm{~N}_{2} \mathrm{O}_{4}\left(\frac{1 \mathrm{~mol} \mathrm{~N}_{2} \mathrm{O}_{4}}{92.02 \mathrm{~g} \mathrm{~N}_{2} \mathrm{O}_{4}}\right)\left(\frac{3 \mathrm{~mol} \mathrm{~N}_{2}}{1 \mathrm{~mol} \mathrm{~N}_{2} \mathrm{O}_{4}}\right)\left(\frac{28.02 \mathrm{~g} \mathrm{~N}_{2}}{1 \mathrm{~mol} \mathrm{~N}_{2}}\right)=82.01285 \mathrm{~g} \mathrm{~N}_{2}\right.$

## Solution Stoichiometry

- Solute - A substance dissolved in another substance
- Solvent - The substance in which the "Solute" is dissolved
- Concentration - The amount of solute dissolved in a given amount of solvent
- Molarity (M) - Expresses the concentration of a solution in units of moles solute per liter of solution

$$
\text { Molarity }=\frac{\text { moles of solute }}{\text { liters of solution }} \quad \mathbf{M}=\frac{\text { mol solute }}{\mathrm{L} \text { soln }}
$$

- Molality (m) - Expresses the number of moles dissolved in 1000 g (1KG) of solvent.

$$
\text { Molality }=\frac{\text { Moles Solute }}{\text { Kilogram Solvent }}=\mathrm{m}=\frac{\mathrm{mol} \text { solute }}{\mathrm{Kg} \text { solvent }}
$$

## Solution Volume vs. Solvent Volume

- The Volume term in the denominator of the molarity expression is the solution volume not the volume of the solvent
- 1 mole of solute dissolved in 1 Liter of a solvent does not produce a 1 molar (M) solution.
- The Mass term in the denominator of the molality expression is the Mass of solvent


## Solution Stoichiometry

- (Mole - Mass) Conversions involving Solutions

Calculating the Mass of a substance given the Volume and Molarity

Ex. How many grams of Sodium Hydrogen Phosphate $\left(\mathrm{Na}_{2} \mathrm{HPO}_{4}\right)$ are in 1.75 L of a 0.460 M solution?

Moles $\mathrm{Na}_{2} \mathrm{HPO}_{4}=1.754 \times 0.460 \mathrm{~mol} \mathrm{Na} 2 \mathrm{HPO}_{4} / 1$ ¿soln

$$
=0.805 \mathrm{~mol} \mathrm{Na}_{2} \mathrm{HPO}_{4}
$$

Mass $\mathrm{Na}_{2} \mathrm{HPO}_{4}=0.805$ trol $\times 141.96 \mathrm{~g} \mathrm{Na}_{2} \mathrm{HPO}_{4} / \mathrm{mol}_{\mathrm{Na}}^{2} \mathrm{HPO}_{4}$

$$
=114 . \mathrm{g}
$$

## Practice Problem

- Calculate the volume of a 3.30 M Sucrose solution containing 135 g of solute.
(FW Sucrose - $342.30 \mathrm{~g} / \mathrm{mol}$ )

Ans:

## moles solute

135 g sucrose $\times 1 \mathrm{~mol}$ sucrose $/ 342.30 \mathrm{~g}$ sucrose $=0.3944 \mathrm{~mol}$

Vol soln
0.3944 mol sucrose $\times 1.00 \mathrm{~L}$ solution $/ 3.30 \mathrm{~mol}$ sucrose $=0.120 \mathrm{~L}$

## Dilution

- The amount of solute in a solution is the same after the solution is diluted with additional solvent
- Dilution problems utilize the following relationship between the molarity (M) and volume (V)

$$
\mathbf{M}_{\text {dil }} \times \mathbf{V}_{\text {dil }}=\text { number of moles }=\mathbf{M}_{\text {conc }} \times \mathbf{V}_{\text {conc }}
$$

## Practice Problem

- Calculate the Molarity of the solution prepared by diluting 37.00 mL of 0.250 M Potassium Chloride $(\mathrm{KCl})$ to 150.00 mL .

Ans: Dilution problem $\left(M_{1} V_{1}=M_{2} V_{2}\right)$

$$
\left.\begin{array}{llll}
\mathrm{M}_{1} & =0.250 \mathrm{M} \mathrm{KCl} & \mathrm{~V}_{1} & =37.00 \mathrm{~mL} \\
\mathrm{M}_{2} & =? & \mathrm{~V}_{2} & =150.00 \mathrm{~mL} \\
\mathrm{M}_{1} \mathrm{~V}_{1} & =\mathrm{M}_{2} \mathrm{~V}_{2} & \therefore & \mathrm{M}_{2}
\end{array}=\mathrm{M}_{1} \mathrm{~V}_{1} / \mathrm{V}_{2}\right)
$$

## Practice Problem

- How many liters (L) of stomach acid ( 0.10 M HCl$)$ react with (neutralize) 0.10 grams (g) of Magnesium Hydroxide (antacid)

```
Mg(OH)2(s)}+2\mathbf{2HCl}(\textrm{aq})->=\mp@subsup{MgCl}{2}{(aq)}+2\mp@subsup{\mathbf{H}}{2}{}\mathbf{O}(\textrm{l}
```

- Convert mass (g) of $\mathrm{Mg}(\mathrm{OH})_{2}$ to moles

$$
\mathrm{mol} \mathrm{Mg}(\mathrm{OH})_{2}=0.1 \mathrm{~g} \mathrm{Mg}(\mathrm{OH})_{2} \times \frac{1 \mathrm{~mol} \mathrm{Mg}(\mathrm{OH})_{2}}{58.33 \mathrm{~g} \mathrm{Mg}(\mathrm{OH})_{2}}=1.7 \times 10^{-3} \mathrm{~mol}
$$

- Convert from moles of $\mathrm{Mg}(\mathrm{OH})_{2}$ to moles of HCl

$$
\mathrm{mol} \mathrm{HCl}=1.7 \times 10^{-3} \mathrm{~mol} \mathrm{Mg}(\mathrm{OH})_{2} \times \frac{2 \mathrm{~mol} \mathrm{HCl}}{1 \mathrm{~mol} \mathrm{Mg}(\mathrm{OH})_{2}}=3.4 \times 10^{-3} \mathrm{~mol} \mathrm{HCl}
$$

- Convert moles HCl to volume (L)

$$
\operatorname{Vol}(\mathrm{L}) \mathrm{HCL}=3.4 \times 10^{-3} \mathrm{~mol} \mathrm{HCl} \times \frac{1 \mathrm{~L}}{0.10 \mathrm{~mol} \mathrm{HCl}}=3.4 \times 10^{-2} \mathrm{~L}
$$

## Equation summary

$$
\text { Molarity }=\frac{\text { moles of solute }}{\text { liters of solution }}
$$

$$
\mathbf{M}=\frac{\text { mol solute }}{\mathrm{L} \text { soln }}
$$

$$
\text { Molality }=\frac{\text { Moles Solute }}{\text { Kilogram Solvent }}
$$

$$
\mathrm{m}=\frac{\mathrm{mol} \text { solute }}{\mathrm{Kg} \text { solvent }}
$$

$\mathbf{M}_{\mathrm{dil}} \times \mathbf{V}_{\mathrm{dil}}=$ number of moles $=\mathbf{M}_{\text {conc }} \times \mathbf{V}_{\text {conc }}$

