

> - Conversion between moles and entities
> [ $1 \mathbf{~ m o l}$ entities $/ 6.022 \times 10^{23}$ entities]
> Example:
> 1) How many molecules of water are present in 2.7 mol of water?
> 2) How many atoms of hydrogen are present in 2.7 mol of water?
> $2.7 \mathrm{~mol} \mathrm{H}_{2} \mathrm{O}\left(\frac{6.022 \times 10^{23} \text { molec. } \mathrm{H}_{2} \mathrm{O}}{1 \mathrm{molH}_{2} \mathrm{O}^{-}}\right)=1.6 \times 10^{24}$ molec. $\mathrm{H}_{2} \mathrm{O}$
> $1.6 \times 10^{24}$ molec. $\mathrm{H}_{2} \mathrm{O}\left(\frac{2 \text { atoms } \mathrm{H}}{1 \text { molec. } \mathrm{H}_{2} \mathrm{O}}\right)=3.3 \times 10^{24}$ atoms H

## Molar Mass (M)

- Mass of a substance per 1 mol of its entities - element $\rightarrow$ atoms (or molecules for $\mathrm{H}_{2}, \mathrm{O}_{2}, \mathrm{P}_{4}, \ldots$ )
- molecular compound $\rightarrow$ molecules
- ionic compound $\rightarrow$ formula units
- Units of $\boldsymbol{M} \rightarrow \mathbf{g} / \mathbf{m o l}$
- $M=m_{\text {particle }} \times N_{A}$

Example:
What is the molar mass of ${ }^{1} \mathrm{H}$, if the mass of 1 atom ${ }^{1} \mathrm{H}$ is $1.673 \times 10^{-24} \mathrm{~g}$ ?
$M=1.673 \times 10^{-24} \mathrm{~g} \times 6.022 \times 10^{23} / \mathrm{mol}=1.007 \mathrm{~g} / \mathrm{mol}$

## Stoichiometry

- Studies the quantitative aspects of chemical reactions


### 3.1 The Mole

- Unit for amount of substance in terms of the number of entities (atoms, molecules, ...) in it.
1 mol of entities $\rightarrow$ \# of atoms in 12 g of ${ }^{12} \mathrm{C}$
1 atom of ${ }^{12} \mathrm{C} \rightarrow 1.99265 \times 10^{-23} \mathrm{~g}^{12} \mathrm{C}$ (mass spectrometry)
$12 \mathrm{~g}^{12} \mathrm{C} \times\left[1\right.$ atom $\left./ 1.99265 \times 10^{-23} \mathrm{~g}^{12} \mathrm{C}\right]=6.022 \times 10^{23}$ atoms
$\Rightarrow \mathbf{1} \mathbf{~ m o l}$ of entities $\boldsymbol{\rightarrow} \mathbf{6 . 0 2 2} \times 10^{\mathbf{2 3}}$ entities
- Avogadro's number $\left(N_{A}\right)$ - number of entities per $1 \mathrm{~mol} \rightarrow N_{A}=\mathbf{6 . 0 2 2} \times \mathbf{1 0}^{\mathbf{2 3}} / \mathbf{m o l}$
- The atomic mass (in $a m u$ ) of an element is numerically equal to the mass (in $g$ ) of 1 mol of the element
$-{ }^{12} \mathrm{C} \rightarrow 12 \mathrm{amu} \quad 1 \mathrm{~mol}{ }^{12} \mathrm{C} \rightarrow 12 \mathrm{~g}$ (definitions)
$-\mathrm{C} \rightarrow 12.01 \mathrm{amu} \quad 1 \mathrm{~mol} \mathrm{C} \rightarrow 12.01 \mathrm{~g}$
$-\mathrm{H} \rightarrow 1.008 \mathrm{amu} \quad 1 \mathrm{~mol} \mathrm{H} \rightarrow 1.008 \mathrm{~g}$
$-\mathrm{O} \rightarrow 16.00 \mathrm{amu} \quad 1 \mathrm{~mol} \mathrm{O} \rightarrow 16.00 \mathrm{~g}$
- The molecular (formula) mass (in $a m u$ ) of a compound is numerically equal to the mass (in $g$ ) of 1 mol of the compound
$-\mathrm{CO}_{2} \rightarrow 44.01 \mathrm{amu} \quad 1 \mathrm{~mol} \mathrm{CO}_{2} \rightarrow 44.01 \mathrm{~g}$
$\Rightarrow 1 \mathrm{~mol}$ of a substance has a fixed mass (can be used to measure moles of substances by weighing them)
- $\boldsymbol{M}$ is numerically equal to the atomic, molecular, or formula mass of the substance
- For elements, $\boldsymbol{M}=$ atomic mass (from per. table)
-For molecular compounds and molecular elements, $\boldsymbol{M}=$ molecular mass
- For ionic compounds, $\boldsymbol{M}=$ formula mass
$\Rightarrow$ For compounds and molecular elements, $\boldsymbol{M}$
equals the sum of the molar (atomic) masses of the elements in the formula


## Example:

Calculate the molar masses of $\mathrm{O}_{2}$ and $\mathrm{Li}_{2} \mathrm{O}$.
$M\left(\mathrm{O}_{2}\right)=2 \times 16.00=32.00 \mathrm{~g} / \mathrm{mol}$
$M\left(\mathrm{Li}_{2} \mathrm{O}\right)=2 \times 6.941+1 \times 16.00=29.88 \mathrm{~g} / \mathrm{mol}$

- $\boldsymbol{M}$ can be used as a conversion factor
- Conversion between moles ( $\boldsymbol{n}$ ) and mass ( $\boldsymbol{m}$ )

$$
m=n \times M \quad \leftrightarrow \quad n=m / M
$$



$$
\frac{\text { Grams }}{\text { Molar mass }(\mathrm{g} / \mathrm{mol})}=\text { grams } \times \frac{\text { moles }}{\text { grams }}=\text { moles }
$$

- Conversion between moles ( $\boldsymbol{n}$ ) and masses (m) of compounds (same as for elements)


## Example:

Calculate the number of moles of urea, $\left(\mathrm{NH}_{2}\right)_{2} \mathrm{CO}$, in $2.3 \times 10^{5} \mathrm{~kg}$ of this compound.
$M=2 \times 14.00+4 \times 1.008+1 \times 12.01+1 \times 16.00=60.04 \mathrm{~g} / \mathrm{mol}$
$2.3 \times 10^{5} \mathrm{~kg}$ urea $\times\left(\frac{10^{3} \text { g urea }}{1 \text { kg urea }}\right) \times\left(\frac{1 \text { mol urea }}{60.04 \text { g urea }}\right)$
$=3.8 \times 10^{6} \mathrm{~mol}$ urea

- Conversion between moles ( $\boldsymbol{n}$ ) and masses (m) of elements


## Example:

What is the mass of 1.221 mol Kr ?
$m=1.221 \mathrm{~mol} \times \mathbf{8 3 . 8 0} \mathrm{g} / \mathrm{mol}=\mathbf{1 0 2 . 3} \mathrm{g}$

## Example:

How many moles of atoms are present in 1.23 g of Kr ?
$1.23 \mathrm{~g} \mathrm{Kr} \times\left(\frac{1 \mathrm{~mol} \mathrm{Kr}}{83.80 \mathrm{~g} \mathrm{Kr}}\right)=1.47 \times 10^{-2} \mathrm{~mol} \mathrm{Kr}$

- Conversion between masses and number of entities of elements and compounds


## Example:

Calculate the number of $\mathrm{CO}_{2}$ molecules and oxygen atoms in $\mathbf{1 5 . 8} \mathbf{g}$ of $\mathrm{CO}_{2}$.
$M\left(\mathrm{CO}_{2}\right)=12.01+\mathbf{2 \times 1 6 . 0 0}=\mathbf{4 4 . 0 1} \mathrm{g} / \mathrm{mol}$
$15.8 \mathrm{~g} \mathrm{CO}_{2}\left(\frac{1 \mathrm{molCO}_{2}}{44.01 \mathrm{gCO}_{2}}\right)\left(\frac{6.022 \times 10^{23} \mathrm{molec}^{2} \mathrm{CO}_{2}}{1 \mathrm{molCO}_{2}}\right)$
$=2.16 \times 10^{23}$ molec. $\mathrm{CO}_{2}$
$2.16 \times 10^{23}$ molec. $\mathrm{CO}_{2}\left(\frac{2 \text { atoms }}{1 \text { molec. } \mathrm{CO}_{2}}\right)=4.32 \times 10^{23}$ atoms O

> - Conversion between masses of compounds and masses of their elements using chemical formulas (The subscripts in formulas refer to individual atoms as well as to moles of atoms) Example: What is the mass of H in $\mathbf{5 . 0 0} \mathbf{g ~ C H}$ 4 ?


## Mass Percentage Composition

- Percentage by mass of each element in a compound

Mass\% $=\left[\mathrm{m}_{\text {element }} / \mathrm{m}_{\text {compound }}\right] \times \mathbf{1 0 0 \%}$

- Calculation of Mass\% from chemical formulas
- Consider 1 mol of a compound
$\mathbf{m}_{\text {comp }}=\boldsymbol{M}$ of comp
$\mathbf{m}_{\text {elem }}=(\#$ moles of elem in 1 mol of comp $) \times(\boldsymbol{M}$ of elem $)$
Note: The \# of moles of the element in 1 mol of the compound equals the \# of atoms of the element in the formula of the compound
- Calculation of Mass\% from chemical analysis


## Example:

Calculate the mass percentage of C in nicotine, if analysis shows that 5.00 g of nicotine contain $3.70 \mathrm{~g} \mathrm{C}, 0.44 \mathrm{~g} \mathrm{H}$ and 0.86 g N .

Mass $\% \mathrm{C}=\left(\frac{3.70 \mathrm{~g} \mathrm{C}}{5.00 \mathrm{~g} \text { nicotine }}\right) \times 100 \%=74.0 \%$

## Determining Empirical Formulas

- Elemental analysis - gives the masses of the elements in a given mass of the compound or the Mass\% composition
- EF from Mass\% data

1. Consider 100 g of the compound
2. The masses of the elements equal their mass\%
3. Convert the masses of the elements to moles
4. Determine the relative number of moles (mol ratio)
5. Simplify the mole ratio to whole numbers

- EF from mass data
- Omit steps 1 and 2 above

Mass\% of element
$\left[\frac{(\text { \# atoms of element in formula })(M \text { of element })}{(M \text { of compound })}\right] \times 100 \%$

## Example:

Calculate the Mass\% of O in $\mathrm{CO}_{2}$.
$\mathrm{CO}_{2} \rightarrow M=1 \times 12.01+2 \times 16.00=44.01 \mathrm{~g} / \mathrm{mol}$ $\mathrm{O} \rightarrow M=16.00 \mathrm{~g} / \mathrm{mol}$

Mass $\% \mathrm{O}=\left(\frac{2 \times 16.00 \mathrm{~g} / \mathrm{mol}}{44.01 \mathrm{~g} / \mathrm{mol}}\right) \times 100 \%=72.71 \%$

### 3.2 Determination of Chemical Formulas

- Molecular formulas - numbers of atoms of each element in a molecule
- Empirical formulas - relative numbers of atoms of each element using the smallest whole numbers


## Example:

acetic acid $\rightarrow \mathrm{C}_{2} \mathrm{H}_{4} \mathrm{O}_{2}(\mathrm{MF}) \rightarrow \mathrm{CH}_{2} \mathrm{O}$ (EF)
formaldehyde $\rightarrow \mathrm{CH}_{2} \mathrm{O}$ (MF) $\rightarrow \mathrm{CH}_{2} \mathrm{O}$ (EF) glucose $\rightarrow \mathrm{C}_{6} \mathrm{H}_{12} \mathrm{O}_{6}(\mathrm{MF}) \rightarrow \mathrm{CH}_{2} \mathrm{O}$ (EF)

## Example:

- Determine the EF of nicotine, if the mass\% of $\mathrm{C}, \mathrm{H}$ and N in it are $74.0,8.7$ and $17.3 \%$, respectively.

1. Consider 100 g nicotine
2. $74.0 \mathrm{~g} \mathrm{C}, 8.7 \mathrm{~g} \mathrm{H}, \mathbf{1 7 . 3} \mathbf{g ~ N}$
3. Convert masses to moles:
$74.0 \mathrm{~g} \mathrm{C} \times(1 \mathrm{~mol} \mathrm{C} / 12.01 \mathrm{~g} \mathrm{C})=6.16 \mathrm{~mol} \mathrm{C}$
$8.7 \mathrm{~g} \mathrm{H} \times(1 \mathrm{~mol} \mathrm{H} / 1.008 \mathrm{~g} \mathrm{H})=8.6 \mathrm{~mol} \mathrm{H}$
$17.3 \mathrm{~g} \mathrm{~N} \times(1 \mathrm{~mol} \mathrm{~N} / 14.01 \mathrm{~g} \mathrm{~N})=1.23 \mathrm{~mol} \mathrm{~N}$
4. Mol ratio:
$\mathbf{6 . 1 6 ~ m o l ~ C ~ : ~} \mathbf{8 . 6} \mathbf{~ m o l ~ H : ~} \mathbf{1 . 2 3} \mathbf{~ m o l ~ N}$
5. Simplify the mole ratio:
(divide by the smallest number, and if necessary, multiply by a factor to get whole numbers)
6.16/1.23 $=5.01 \cong 5$
8.6/1.23 = $7.0 \cong 7$
$1.23 / 1.23=1.00 \cong 1$
$\rightarrow$ simplest whole-number ratio:

## $\mathbf{5} \mathbf{~ m o l ~ C ~ : ~} \mathbf{7} \mathbf{m o l ~ H : \mathbf { 1 ~ m o l ~ N }}$

$\rightarrow \mathrm{EF}$ :

$$
\mathrm{C}_{5} \mathrm{H}_{7} \mathbf{N}
$$

## Example:

- The empirical formula of nicotine is $\mathbf{C}_{5} \mathbf{H}_{7} \mathbf{N}$ and its molar mass is $162.23 \mathrm{~g} / \mathrm{mol} . \mathrm{MF}=$ ?

$$
\begin{aligned}
& M_{E F} \rightarrow 5 \times 12.01+7 \times 1.008+1 \times 14.01=81.12 \mathrm{~g} / \mathrm{mol} \\
& \quad \mathrm{n}=\frac{M}{M_{E F}}=\frac{162.23 \mathrm{~g} / \mathrm{mol}}{81.12 \mathrm{~g} / \mathrm{mol}}=2.000 \cong 2 \\
& \Rightarrow M F=2 \times E F \\
& M F \rightarrow C_{10} \mathrm{H}_{14} \mathrm{~N}_{2}
\end{aligned}
$$

## Determining Molecular Formulas

- The MF is a whole-number multiple of the EF

$$
\Rightarrow M=M_{E F} \times \mathbf{n}
$$

$-\boldsymbol{M} \rightarrow$ molar mass
$-\boldsymbol{M}_{\boldsymbol{E F}} \rightarrow$ EF mass
$-\mathbf{n} \rightarrow$ whole number (number of EFs per molecule)

$$
\Rightarrow \mathbf{n}=M / M_{E F}
$$

- Determining MFs from EFs and molar masses


## Combustion Analysis

- A method for elemental analysis of combustible organic compounds through their combustion in excess $\mathrm{O}_{2}$
- The $\mathbf{C}$ in the sample is converted to $\mathbf{C O}$ which is absorbed in a NaOH absorber and weighed
- The $\mathbf{H}$ in the sample is converted to $\mathbf{H}_{2} \mathbf{O}$ which is absorbed in a $\mathrm{P}_{4} \mathrm{O}_{10}$ absorber and weighed
- If a third element ( $\mathrm{O}, \mathrm{N}, \ldots$ ), it passes through the absorbers

$$
1 \mathrm{~mol} \mathrm{C} \text { from the sample } \rightarrow 1 \mathrm{~mol} \mathrm{CO}_{2}
$$

$2 \mathbf{m o l ~ H}$ from the sample $\rightarrow \mathbf{1} \mathbf{~ m o l ~} \mathrm{H}_{2} \mathrm{O}$

## Example:

When 0.236 g aspirin is burned in excess $\mathbf{O}_{2}$, $0.519 \mathrm{~g} \mathrm{CO}_{2}$ and $0.0945 \mathrm{~g} \mathrm{H}_{\mathbf{2}} \mathbf{O}$ are formed. Determine the mass $\%$ of $\mathrm{C}, \mathrm{H}$ and O in aspirin.
$>$ Calculate the masses of C and H in the sample based on the masses of $\mathrm{CO}_{2}$ and $\mathrm{H}_{2} \mathrm{O}$ :
$>$ Calculate the mass of O by subtracting the masses of $C$ and $H$ from the total mass of the sample
$\times\left(\frac{12.01 \mathrm{~g} \mathrm{C}}{1 \mathrm{~mol} \mathrm{C}}\right)=0.142 \mathrm{~g} \mathrm{C}$
$0.0945 \mathrm{~g} \mathrm{H}_{2} \mathrm{O} \times\left(\frac{1 \mathrm{~mol} \mathrm{H}_{2} \mathrm{O}}{18.02 \mathrm{~g} \mathrm{H}_{2} \mathrm{O}}\right) \times\left(\frac{2 \mathrm{~mol} \mathrm{H}}{1 \mathrm{~mol} \mathrm{H}_{2} \mathrm{O}}\right) \times$
$\times\left(\frac{1.008 \mathrm{~g} \mathrm{H}}{1 \mathrm{~mol} \mathrm{H}}\right)=0.0106 \mathrm{~g} \mathrm{H}$

$$
0.236-0.142-0.0106=0.084 \mathrm{~g} \mathrm{O}
$$

$$
\begin{aligned}
& \% \mathrm{C}=\left(\frac{0.142 \text { g C }}{0.236 \text { g sample }}\right) \times 100 \%=60.0 \% \\
& \% \mathrm{H}=\left(\frac{0.0106 \text { g H }}{0.236 \text { g sample }}\right) \times 100 \%=4.48 \% \\
& \% \mathrm{O}=\left(\frac{0.084 \text { g O }}{0.236 \text { g sample }}\right) \times 100 \%=35.5 \%
\end{aligned}
$$

The empirical formula can be determined from the percentage composition in a subsequent step

## - Balanced chemical equations

- same number of atoms of each element appear on each side of the equation
- stoichiometric coefficients - needed to balance the equations

$$
2 \mathrm{H}_{2}+\mathrm{O}_{2} \rightarrow 2 \mathrm{H}_{2} \mathrm{O}
$$

- Microscopic view
( $\mathbf{2}$ molec. $\mathbf{H}_{2}+1$ molec. $\mathrm{O}_{2} \rightarrow \mathbf{2}$ molec. $\mathrm{H}_{2} \mathrm{O}$ ) - Macroscopic view
$\left(\mathbf{2} \mathbf{~ m o l ~ H} \mathbf{2}+1 \mathbf{~ m o l ~ O} \mathbf{O}_{2} \mathbf{2} \mathbf{~ m o l ~ H} \mathbf{H}_{2} \mathrm{O}\right)$
$\left(4.032 \mathrm{~g} \mathrm{H}_{2}+32.00 \mathrm{~g} \mathrm{O}_{2} \rightarrow 36.032 \mathrm{~g} \mathrm{H}_{2} \mathrm{O}\right)$


### 3.3 Chemical Equations

- Represent chemical reactions


## Reactants $\rightarrow$ Products

- Skeletal equations - show identities of reactants and products

$$
\mathrm{H}_{2}+\mathrm{O}_{2} \rightarrow \mathrm{H}_{2} \mathrm{O}
$$

- Law of conservation of mass
- Atoms are neither created nor destroyed (they only change bonding partners)
- Same atoms are present in the reactants as in the products
- The stoichiometric coefficients can be treated as relative number of moles of reactants and products
- Physical state symbols
- (s) solid; (l) liquid; (g) gas; (aq) aqueous solution
$\mathbf{2 K}(\mathrm{s})+\mathbf{2} \mathrm{H}_{2} \mathrm{O}(\mathrm{l}) \rightarrow \mathbf{2 K O H}(\mathrm{aq})+\mathbf{H}_{\mathbf{2}}(\mathrm{g})$


## Balancing Chemical Equations

- Balancing by inspection (only simple cases)
- Change stoichiometric coefficients only
- Never change subscripts in formulas
- Never add other substances to the equation
- Systematic method

1. Write the skeletal equation
2. Balance one element at a time using coefficients

- Start with the elements in the most complex substance and finish with those in the least complex one
- Alternatively, start with the element present in the fewest number of formulas and finish with the element present in the greatest number of formulas
- Use fractional coefficients if necessary

3. If necessary multiply the whole equation by a factor to clear the fractional coefficients
4. Verify that the equation is balanced and the coefficients are the smallest whole numbers
5. Specify physical states

Example: Write the balanced equation for the combustion of ethane, $\mathrm{C}_{2} \mathrm{H}_{6}$, to carbon dioxide and liquid water.
$\begin{array}{ll}\mathrm{C}_{2} \mathrm{H}_{6}+\mathrm{O}_{2} \rightarrow \mathrm{CO}_{2}+\mathrm{H}_{2} \mathrm{O} & \text { skeletal } \\ \mathrm{C}_{2} \mathbf{H}_{6}+\mathrm{O}_{2} \rightarrow 2 \mathrm{CO}_{2}+\mathrm{H}_{2} \mathrm{O} & \text { for } \mathrm{C} \\ \mathrm{C}_{2} \mathbf{H}_{6}+\mathrm{O}_{2} \rightarrow 2 \mathrm{CO}_{2}+3 \mathrm{H}_{2} \mathrm{O} & \text { for } \mathrm{H} \\ \mathrm{C}_{2} \mathrm{H}_{6}+(7 / 2) \mathrm{O}_{2} \rightarrow 2 \mathrm{CO}_{2}+3 \mathrm{H}_{2} \mathrm{O} & \text { for } \mathrm{O}\end{array}$
multiply eq. by 2

$$
\begin{aligned}
2 \mathrm{C}_{2} \mathrm{H}_{6}+7 \mathrm{O}_{2} & \rightarrow 4 \mathrm{CO}_{2}+6 \mathrm{H}_{2} \mathrm{O} \\
2 \mathrm{C}_{2} \mathrm{H}_{6}(\mathrm{~g})+7 \mathrm{O}_{2}(\mathrm{~g}) & \rightarrow 4 \mathrm{CO}_{2}(\mathrm{~g})+6 \mathrm{H}_{2} \mathrm{O}(\mathrm{l})
\end{aligned}
$$

- Often polyatomic ions can be treated as single entities

Example: Balance the following skeletal eq. in aqueous solution:

$$
\mathrm{Co}\left(\mathrm{NO}_{3}\right)_{3}+\left(\mathrm{NH}_{4}\right)_{2} \mathrm{~S} \rightarrow \mathrm{Co}_{2} \mathrm{~S}_{3}+\mathrm{NH}_{4} \mathrm{NO}_{3}
$$

$\rightarrow$ balance Co and S :
$2 \mathrm{Co}\left(\mathrm{NO}_{3}\right)_{3}+3\left(\mathrm{NH}_{4}\right)_{2} \mathrm{~S} \rightarrow \mathrm{Co}_{2} \mathrm{~S}_{3}+\mathrm{NH}_{4} \mathrm{NO}_{3}$
$\rightarrow$ balance $\mathrm{NH}_{4}$ and $\mathrm{NO}_{3}$ :
$2 \mathrm{Co}\left(\mathrm{NO}_{3}\right)_{3}+3\left(\mathrm{NH}_{4}\right)_{2} \mathrm{~S} \rightarrow \mathrm{Co}_{2} \mathrm{~S}_{3}+6 \mathrm{NH}_{4} \mathrm{NO}_{3}$
$\rightarrow$ add physical state symbols:
$2 \mathrm{Co}\left(\mathrm{NO}_{3}\right)_{3}(\mathrm{aq})+3\left(\mathrm{NH}_{4}\right)_{2} \mathrm{~S}(\mathrm{aq}) \rightarrow \mathrm{Co}_{2} \mathrm{~S}_{3}(\mathrm{~s})+6 \mathrm{NH}_{4} \mathrm{NO}_{3}(\mathrm{aq})$

## Mole-to-Mole Conversions

- Conversion method
- The mole ratios are used as conversion factors
$(\mathbf{m o l}$ given $) \times($ mole ratio $)=(\mathbf{m o l}$ required $)$
Example: Determine the number of moles of water produced from $3.4 \mathrm{~mol} \mathrm{O}_{2}$.
$\rightarrow$ balanced equation: $\mathbf{2 H}_{\mathbf{2}}+\mathbf{O}_{\mathbf{2}} \rightarrow \mathbf{2 H}_{\mathbf{2}} \mathbf{O}$
$\rightarrow$ mole ratio (conversion factor): [2 $\mathbf{~ m o l ~} \mathbf{H}_{\mathbf{2}} \mathrm{O} / \mathbf{1} \mathbf{~ m o l ~ O} \mathbf{O}_{\mathbf{2}}$ ]
$3.4 \mathrm{~mol} \mathrm{O}_{2} \times\left(\frac{2 \mathrm{~mol} \mathrm{H}_{2} \mathrm{O}}{1 \mathrm{~mol} \mathrm{O}_{2}}\right)=6.8 \mathrm{~mol} \mathrm{H} \mathbf{2}_{2} \mathrm{O}$


## Mass-to-Mass Calculations

- Conversion method



### 3.4 Calculating Amounts of Reactants and Products

## Stoichiometric Equivalences

- Balanced chemical equations contain definite stoichiometric relations between reactants and products $\rightarrow$ stoichiometric mole ratios
Example: $\mathbf{2} \mathbf{H}_{\mathbf{2}}+\mathbf{O}_{\mathbf{2}} \boldsymbol{\rightarrow} \mathbf{2} \mathbf{H}_{\mathbf{2}} \mathbf{O}$ $2 \mathrm{~mol} \mathrm{H} 2 \Leftrightarrow 1 \mathrm{~mol} \mathrm{O} \mathbf{2}_{2}$ $2 \mathbf{~ m o l ~ H} \mathbf{2}^{\Leftrightarrow} \boldsymbol{2} \mathbf{~ m o l ~ H} \mathbf{2} \mathbf{O}$ $1 \mathbf{~ m o l ~} \mathrm{O}_{2} \Leftrightarrow 2 \mathrm{~mol} \mathrm{H} \mathbf{2}$ $1 \mathrm{~mol} \mathrm{O} / 2 \mathrm{~mol} \mathrm{H}$ $2 \mathrm{~mol} \mathrm{H} \mathbf{2} \mathrm{O} / 2 \mathrm{~mol} \mathrm{H}$ $2 \mathrm{~mol} \mathrm{H} \mathbf{2} \mathrm{O} / 1 \mathrm{~mol} \mathrm{O}_{2}$
stoichiometric equivalences
stoichiometric mole ratios
- Stoichiometric conversion factors are reaction specific
Example: Calculate the amount of $\mathbf{O}_{\mathbf{2}}$ needed to produce $3.5 \mathbf{~ m o l ~}_{\mathbf{H}}^{\mathbf{2}} \mathrm{O}$ by combustion of methane $\left(\mathrm{CH}_{4}\right)$.
$\rightarrow$ balanced equation:

$$
\mathrm{CH}_{4}+2 \mathrm{O}_{2} \rightarrow \mathrm{CO}_{2}+2 \mathrm{H}_{2} \mathrm{O}
$$

$\rightarrow$ mole ratio (conversion factor):
$2 \mathbf{~ m o l ~ O} \mathbf{2}^{\Leftrightarrow} \mathbf{2} \mathbf{~ m o l ~ H} \mathbf{2}$
[ $2 \mathbf{~ m o l ~ O} \mathbf{O}_{2} / \mathbf{2} \mathbf{~ m o l ~ H} \mathrm{H}_{2} \mathrm{O}$ ]
$3.5 \mathrm{~mol} \mathrm{H}_{2} \mathrm{O} \times\left(\frac{2 \mathrm{~mol} \mathrm{O}_{2}}{2 \mathrm{molH}_{2} \mathrm{O}}\right)=3.5 \mathrm{~mol} \mathrm{O}{ }_{2}$

Example: Calculate the mass of oxygen needed to completely burn $\mathbf{5 . 4} \mathbf{~ k g}$ of butane $\left(\mathrm{C}_{4} \mathrm{H}_{10}\right)$.
$\rightarrow$ balanced equation:
$2 \mathrm{C}_{4} \mathrm{H}_{10}+\mathbf{1 3 O}_{2} \rightarrow \mathbf{8 C O}+\mathbf{1 0 H}_{2} \mathrm{O}$
$\rightarrow$ mole ratio: $\left[\mathbf{1 3} \mathbf{~ m o l ~ O} \mathbf{O}_{2} / \mathbf{2} \mathbf{~ m o l ~ C} \mathbf{4}_{\mathbf{4}} \mathrm{H}_{\mathbf{1 0}}\right.$ ]
$\rightarrow$ molar masses:

$$
\begin{gathered}
\mathrm{C}_{4} \mathrm{H}_{10} \rightarrow 58.1 \mathrm{~g} / \mathrm{mol} \quad \mathrm{O}_{2} \rightarrow 32.0 \mathrm{~g} / \mathrm{mol} \\
5.4 \mathrm{~kg} \mathrm{C}_{4} \mathrm{H}_{10} \times\left(\frac{10^{3} \mathrm{~g} \mathrm{C}_{4} \mathrm{H}_{10}}{1 \mathrm{~kg} \mathrm{C}_{4} \mathrm{H}_{10}}\right) \times\left(\frac{1 \mathrm{~mol} \mathrm{C}_{4} \mathrm{H}_{10}}{58.1 \mathrm{~g} \mathrm{C}_{4} \mathrm{H}_{10}}\right) \times \\
\left(\frac{13 \mathrm{~mol} \mathrm{O}_{2}}{2 \mathrm{~mol} \mathrm{C}_{4} \mathrm{H}_{10}}\right) \times\left(\frac{32.0 \mathrm{~g} \mathrm{O}_{2}}{1 \mathrm{molO}_{2}}\right)=1.9 \times 10^{4} \mathrm{~g} \mathrm{O}_{2}=19 \mathrm{~kg} \mathrm{O}_{2}
\end{gathered}
$$

## Reaction Yield

- Theoretical yield - the maximum amount of product that can be expected from a given amount of reactant
- Actual yield - the actual amount of product isolated in a reaction

Actual Yield $\leq$ Theoretical Yield

- Percentage yield:
$\%$ Yield $=\frac{\text { Actual Yield }}{\text { Theoretical Yield }} \times 100 \%$

Example: Calculate the theoretical yield of carbon dioxide produced by the combustion of 25.0 g propane $\left(\mathrm{C}_{3} \mathrm{H}_{8}\right)$ in excess oxygen.
$\rightarrow$ balanced equation:

$$
\mathrm{C}_{3} \mathrm{H}_{8}+5 \mathrm{O}_{2} \rightarrow 3 \mathrm{CO}_{2}+4 \mathrm{H}_{2} \mathrm{O}
$$

$\rightarrow$ mass-to-mass conversion:

$$
\begin{aligned}
& 25.0 \mathrm{~g} \mathrm{C}_{3} \mathrm{H}_{8} \times\left(\frac{1 \mathrm{~mol} \mathrm{C}_{3} \mathrm{H}_{8}}{44.09 \mathrm{~g} \mathrm{C}_{3} \mathrm{H}_{8}}\right) \times\left(\frac{3 \mathrm{~mol} \mathrm{CO}_{2}}{1 \mathrm{~mol} \mathrm{C}_{3} \mathrm{H}_{8}}\right) \times \\
& \times\left(\frac{44.01 \mathrm{~g} \mathrm{CO}_{2}}{1 \mathrm{~mol} \mathrm{CO}_{2}}\right)=74.9 \mathrm{~g} \mathrm{CO}_{2} \rightarrow \text { Theor. Yield }
\end{aligned}
$$

## Limiting Reactants

- Reactants present in equivalent amounts
- All reactants are consumed at the same time
- Nonequivalent amounts of reactants
- One reactant, called limiting reactant, is consumed before the others
- The other reactants are in excess
- Limiting reactant
- The reaction stops when the limiting reactant is consumed
- Limits the maximum amount of product achievable (limits the theoretical yield)
- Stoichiometric calculations based on the limiting reactant give the lowest amount of product compared to calculations based on the other reactants
- Reasons for the difference between actual and theoretical yield
- incomplete reaction
- loss of product
- side reactions


Example: Calculate the percentage yield of carbon dioxide, if the combustion of $\mathbf{2 5 . 0} \mathbf{~ g}$ propane in excess oxygen yields $\mathbf{4 8 . 5} \mathbf{g}$ carbon dioxide.
$\rightarrow$ theoretical yield (from prev. problem): $\mathbf{7 4 . 9} \mathbf{g ~ C O}_{\mathbf{2}}$ $\rightarrow$ side reaction (consumes some of the propane):

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

$\rightarrow$ actual yield: $\mathbf{4 8 . 5} \mathrm{g} \mathrm{CO}_{\mathbf{2}}$
$\rightarrow$ percentage yield:

$$
\% \text { Yield }=\frac{48.5 \mathrm{~g} \mathrm{CO}_{2}}{74.9 \mathrm{~g} \mathrm{CO}_{2}} \times 100 \%=64.8 \%
$$

Example: Identify the limiting reactant in the reaction of $\mathbf{5 . 0} \mathbf{~ m o l ~ H}_{\mathbf{2}}$ with $\mathbf{3 . 0} \mathbf{~ m o l ~} \mathrm{N}_{2}$, and determine the theoretical yield of $\mathrm{NH}_{3}$ in this reaction.
$\rightarrow$ balanced equation: $\quad \mathbf{3 H}_{\mathbf{2}}+\mathbf{N}_{\mathbf{2}} \rightarrow \mathbf{\mathbf { N H } _ { \mathbf { 3 } }}$
$\rightarrow$ calculate the theoretical yield based on each of the reactants and chose the smaller result:
$3.0 \mathrm{~mol} \mathrm{~N}_{2} \times\left(\frac{2 \mathrm{~mol} \mathrm{NH}_{3}}{1 \mathrm{~mol}_{2}}\right)=6.0 \mathrm{~mol} \mathrm{NH}_{3}$
$\begin{aligned} & \text { 5.0 } \mathrm{mol} \mathrm{H}_{2} \times\left(\frac{2 \mathrm{~mol} \mathrm{NH}_{3}}{3 \mathrm{molH}_{2}}\right)=\sqrt{3.3 \mathrm{~mol} \mathrm{NH}_{3} \rightarrow \text { Theor. Yield }} \\ & \Rightarrow \mathbf{H}_{2} \text { is the limiting reactant }\end{aligned}$ smaller amount

Example: Calculate the theoretical yield of $\mathrm{HNO}_{3}$ in the reaction of $\mathbf{2 8} \mathrm{g} \mathrm{NO}_{2}$ and $\mathbf{1 8} \mathrm{g} \mathrm{H}_{\mathbf{2}} \mathrm{O}$ by the chemical equation:

$$
3 \mathrm{NO}_{2}(\mathrm{~g})+\mathrm{H}_{2} \mathrm{O}(\mathrm{l}) \rightarrow 2 \mathrm{HNO}_{3}(\mathrm{l})+\mathrm{NO}(\mathrm{~g}) .
$$

$\rightarrow$ Calculate the theoretical yield based on each of the reactants and chose the smaller result:

$$
\begin{aligned}
& 18 \mathrm{~g} \mathrm{H}_{2} \mathrm{O} \times\left(\frac{1 \mathrm{~mol} \mathrm{H}_{2} \mathrm{O}}{18.0 \mathrm{~g} \mathrm{H}_{2} \mathrm{O}}\right) \times\left(\frac{2 \mathrm{~mol} \mathrm{HNO}_{3}}{1 \mathrm{~mol} \mathrm{H}_{2} \mathrm{O}}\right) \times \\
& \times\left(\frac{63.0 \mathrm{~g} \mathrm{HNO}_{3}}{1 \mathrm{~mol} \mathrm{HNO}_{3}}\right)=130 \mathrm{~g} \mathrm{HNO}_{3}
\end{aligned}
$$

### 3.5 Solution Stoichiometry

- Solutions - homogeneous mixtures
- Solvent and solute(s)
-Solution concentration


## Molarity (M)

- Measure of the solute concentration $M=\left(\frac{\text { amount of solute (mol) }}{\text { volume of solution (L) }}\right) \quad$ or $\quad M=\frac{n}{V}$ - Units - molar (M) $\quad \mathbf{1} \mathbf{~ m}=\mathbf{1} \mathbf{~ m o l} / \mathrm{L}$


## Example:

Calculate the molarity of a solution prepared by dissolving 5.33 g NaOH in water using a $100.0 \mathbf{m L}$ volumetric flask.
$\Rightarrow$ convert the mass to moles:
$5.33 \mathrm{~g} \mathrm{NaOH} \times\left(\frac{1 \mathrm{~mol} \mathrm{NaOH}}{40.00 \mathrm{~g} \mathrm{NaOH}}\right)=0.133 \mathrm{~mol} \mathrm{NaOH}$
$\Rightarrow$ convert volume to liters: $100.0 \mathrm{~mL}=\mathbf{0 . 1 0 0 0} \mathrm{L}$
$\Rightarrow$ divide moles by solution volume:

$28 \mathrm{~g} \mathrm{NO}_{2} \times\left(\frac{1 \mathrm{molNO}_{2}}{46.0 \mathrm{~g} \mathrm{NO}_{2}}\right) \times\left(\frac{2 \mathrm{~mol} \mathrm{HNO}_{3}}{3 \mathrm{molNO}_{2}}\right) \times$ $\times\left(\frac{63.0 \mathrm{~g} \mathrm{HNO}_{3}}{1 \mathrm{~mol} \mathrm{HNO}_{3}}\right)=26 \mathrm{~g} \mathrm{HNO}_{3} \rightarrow$ Theor. Yield
smaller amount
$\Rightarrow$ The smaller amount of product results from the calculation based on $\mathrm{NO}_{2}$
$\Rightarrow \mathbf{N O}_{\mathbf{2}}$ is the limiting reactant and $26 \mathbf{g ~ H N O} 3$ is the theoretical yield

- Preparation of solutions with known molarity
- Transfer a known mass of solute in a volumetric flask
- Dissolve in small amount of water
- Add water to the mark

- Molarity as a conversion factor Example:

Calculate the mass of NaOH in $\mathbf{2 . 5 0} \mathbf{L}$ of $1.33 \mathbf{M ~ N a O H}$ solution.
$2.50 \mathrm{E}\left(\frac{1.33 \mathrm{~mol} \mathrm{NaOH}}{1 \mathrm{~L}}\right)\left(\frac{40.00 \mathrm{~g} \mathrm{NaOH}}{1 \mathrm{~mol} \mathrm{NaOH}}\right)=133 \mathrm{~g} \mathrm{NaOH}$

## Example:

Calculate the volume of $\mathbf{1 . 3 3} \mathbf{~ m ~ N a O H}$ solution that contains $\mathbf{5 . 0 0} \mathbf{~ m o l ~ N a O H}$.
$5.00 \mathrm{~mol} \mathrm{NaOH} \times\left(\frac{1 \mathrm{~L}}{1.33 \mathrm{~mol} \mathrm{NaOH}}\right)=3.76 \mathrm{~L}$

## Dilution

- Reducing the concentration of the solute by adding more solvent
- Stock solutions - concentrated solutions used to store reagents
- Dilution Procedure
- Use a pipette to measure a small volume of the concentrated solution and transfer it to a volumetric flask
- Add solvent to fill the volumetric flask to the mark
- Dilution calculations
- dilution doesn't change the total \# of moles of solute in the solution
$n=M \times V \quad n_{d}=n_{c} \quad M_{d} \times V_{d}=M_{c} \times V_{c}$
Example:
Calculate the molarity of a solution prepared by dilution of $\mathbf{5 . 0 0} \mathbf{~ m L ~} \mathbf{2 . 0} \mathbf{~ M ~ H C l}$ stock solution to $\mathbf{1 0 0 . 0} \mathbf{~ m L}$.

$$
M_{d}=\frac{M_{c} \times V_{c}}{V_{d}}=\frac{2.0 \mathrm{M} \times 5.00 \mathrm{~mL}}{100.0 \mathrm{~mL}}=0.10 \mathrm{M}
$$

## Example:

What volume of $\mathbf{0 . 0 8 3 6} \mathbf{~ m ~ H}_{2} \mathbf{S O}_{4}$ solution will react completely with $\mathbf{1 6 . 4} \mathbf{~ m L ~} \mathbf{0 . 2 5 5} \mathbf{~ m ~ K O H}$.
$\Rightarrow$ balanced equation:

$$
2 \mathrm{KOH}_{(\mathrm{aq})}+\mathrm{H}_{2} \mathrm{SO}_{4}(\mathrm{aq}) \rightarrow \mathrm{K}_{2} \mathrm{SO}_{4}(\mathrm{aq})+2 \mathrm{H}_{2} \mathrm{O}_{(\mathrm{l})}
$$

$\Rightarrow$ mole ratio: $\left[1 \mathbf{~ m o l ~ H}_{2} \mathrm{SO}_{4} / \mathbf{2} \mathbf{~ m o l ~ K O H}\right]$
$16.4 \times 10^{-3} \mathrm{~L} \times\left(\frac{0.255 \mathrm{~mol} \mathrm{KOH}}{1 \mathrm{~L}}\right) \times\left(\frac{1 \mathrm{~mol} \mathrm{H}_{2} \mathrm{SO}_{4}}{2 \mathrm{~mol} \mathrm{KOH}}\right)$ $\times\left(\frac{1 \mathrm{~L}}{\mathbf{0 . 0 8 3 6 ~ \mathrm { mol } \mathrm { H }} \mathbf{2 O}_{4}}\right)=25.0 \times 10^{-3} \mathrm{~L}=25.0 \mathrm{~mL}$
$\Rightarrow$ calculation based on HCl :
$2.0 \mathrm{~L} \times\left(\frac{0.15 \mathrm{~mol} \mathrm{HCt}}{1 \mathrm{~L}}\right) \times\left(\frac{1 \mathrm{~mol} \mathrm{H}_{2}}{2 \mathrm{~mol} \mathrm{HCl}^{2}}\right) \times\left(\frac{2.02 \mathrm{~g} \mathrm{H}_{2}}{1 \mathrm{~mol} \mathrm{H}_{2}}\right)$
$=0.30 \mathrm{~g} \mathrm{H}_{2}$
$\Rightarrow$ calculation based on $\mathbf{Z n}$ :
$2.5 \mathrm{~g} \mathrm{Zn} \times\left(\frac{1 \mathrm{~mol} \mathrm{Zn}}{65.4 \mathrm{~g} \mathrm{Zn}}\right) \times\left(\frac{1 \mathrm{~mol} \mathrm{H}_{2}}{1 \mathrm{~mol} \mathrm{Zn}}\right) \times\left(\frac{2.02 \mathrm{~g} \mathrm{H}_{2}}{1 \mathrm{~mol} \mathrm{H}_{2}}\right)$
$=0.077 \mathrm{~g} \mathrm{H}_{2} \leftarrow$ smaller amount
$\Rightarrow$ The calculation based on Zn yields less product so $\mathbf{Z n}$ is the limiting reactant

## Limiting reactant problems in solution

## Example:

What mass of $\mathbf{H}_{2}$ gas can be produced by the reaction of $\mathbf{2 . 5} \mathbf{g ~ Z n}$ with $2.0 \mathrm{~L} \mathbf{0 . 1 5} \mathbf{~ m ~ H C l}$ solution. The other product is $\mathrm{ZnCl}_{2}(\mathrm{aq})$.
$\Rightarrow$ balanced equation:

$$
\mathrm{Zn}(\mathrm{~s})+2 \mathrm{HCl}_{(\mathrm{aq})} \rightarrow \mathrm{ZnCl}_{2}(\mathrm{aq})+\mathbf{H}_{2}(\mathrm{~g})
$$

$\Rightarrow$ mole ratios: [ $1 \mathbf{~ m o l ~} \mathrm{H}_{2} / \mathbf{2} \mathbf{~ m o l ~ H C l}$ ]
[ $1 \mathbf{~ m o l ~ H} \mathbf{H}_{2} / \mathbf{~ m o l ~ Z n ]}$
$\Rightarrow$ Calculate the mass of $\mathrm{H}_{2}$ produced based on both reactants and choose the smaller amount

