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Chapter 3
The Mole and Stoichiometry

Chemistry, 7th Edition
International Student Version
Brady/Jespersen/Hyslop

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Chapter in Context

- Use the mole and Avogadro's number as conversions between the molecular and laboratory scales of matter
- Perform calculations involving moles
- Calculate percent composition of a compound
- Determine empirical and molecular formulas
- Perform calculations involving mole of reactants and products in a reaction
- Determine limiting reactants and amounts of unreacted substance remaining
- Calculate percent yields for reactions

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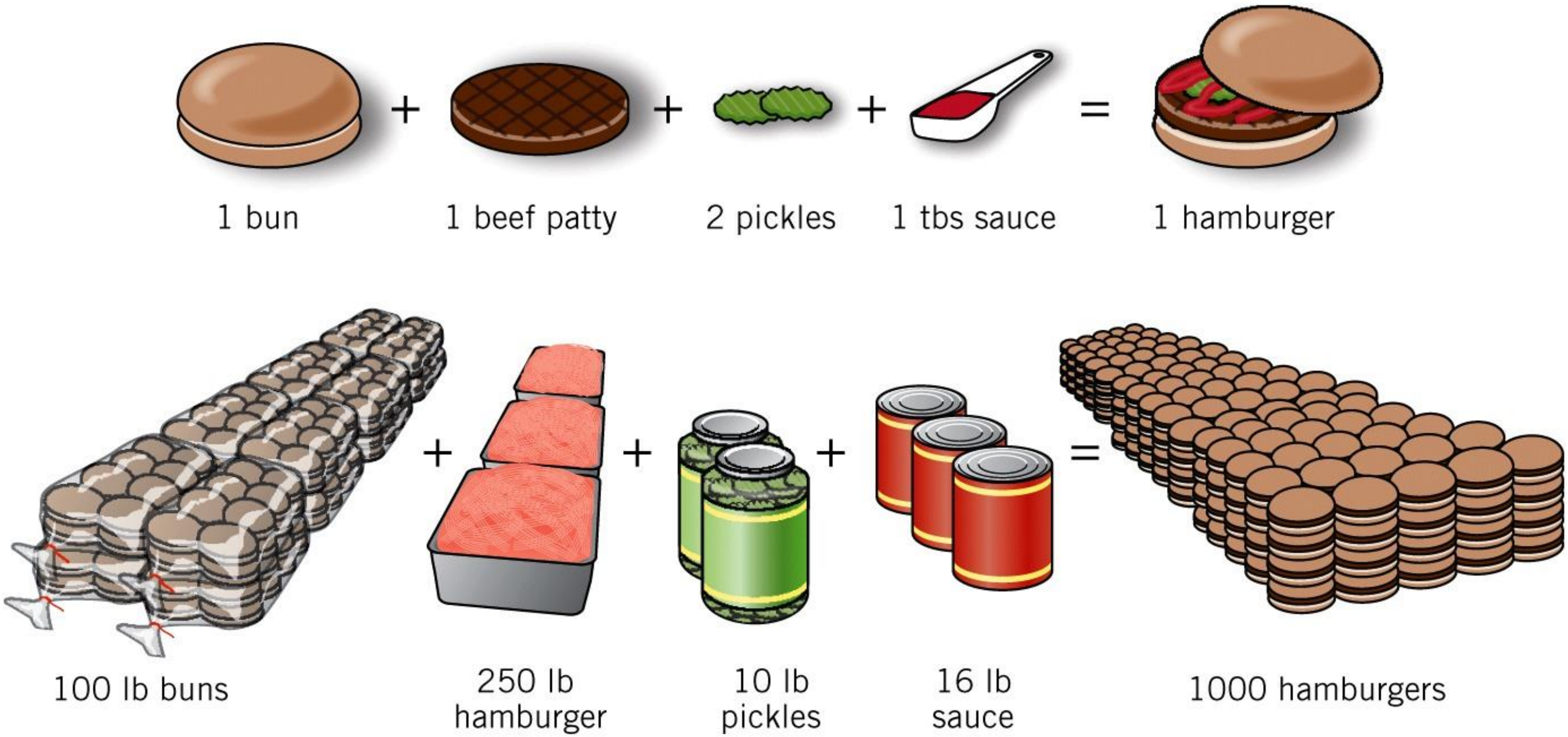
Using Mass to Count



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Defining The Mole

- Mole: A number equal to the number of atoms in exactly 12 grams of ^{12}C atoms

How many in 1 mole of ^{12}C ?

- Based on experimental evidence

1 mole of $^{12}C = 6.022 \times 10^{23}$ atoms ^{12}C

Avogadro's number = N_A

- Number of atoms, molecules or particles in one mole

- **1 mole of *X* = 6.022×10^{23} units of *X***
  - 1 mole Xe = 6.022×10^{23} Xe atoms
  - 1 mole $NO_2 = 6.022 \times 10^{23}$ NO_2 molecules

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Molecular to Laboratory Scale

- So far, we have looked at chemical formulas and reactions at a molecular scale
- It is known from experiments that:
  - Electrons, neutrons and protons have set masses
  - Atoms must also have characteristic masses
  - Atoms and molecules are extremely small
- Need a way to scale up chemical formulas and reactions to carry out experiments in laboratory
- **Mole** is our conversion factor

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Moles of Compounds

Atoms

- **Atomic Mass**
  - Mass of atom (from periodic table)

1 mole of atoms = gram atomic mass

= 6.022×10^{23} atoms

Molecules

- **Molecular Mass**
  - Sum of atomic masses of all atoms in compound's formula

1 mole of molecule X = gram molecular mass of X

= 6.022×10^{23} molecules

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Moles of Compounds

Ionic compounds

- **Formula Mass**
  - Sum of atomic masses of all atoms in ionic compound's formula

1 mole ionic compound *X* = gram formula mass of *X*

= 6.022×10^{23} formula units

General

Molar mass (MM)

- Mass of 1 mole of substance (element, molecule, or ionic compound) under consideration

1 mol of *X* = gram molar mass of *X*

= 6.022×10^{23} formula units

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SI Unit for Amount = Mole

1 mole of substance *X* = gram molar mass of *X*

- 1 mole S = 32.06 g S
- 1 mole NO_2 = 46.01 g NO_2

- Molar mass is our conversion factor between g and moles
- **1 mole of *X* = 6.022 × 10^{23} units of *X***
- N_A is our conversion factor between moles and molecules
  - 1 mole H_2O = 6.022 × 10^{23} molecules H_2O
  - 1 mole NaCl = 6.022 × 10^{23} formula units NaCl

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Your Turn!

What is the molar mass of C_2H_5COOH?

A. 148 g/mol

B. 62.5 g/mol

C. 73.0 g/mol

D. 112 g/mol

E. 74.0 g/mol

$$\left[3\,\cancel{\text{mol C}} \times \left(\frac{12.0\text{g C}}{\cancel{\text{mol C}}}\right)\right] + \left[6\,\cancel{\text{mol H}} \times \left(\frac{1.00\text{g H}}{\cancel{\text{mol H}}}\right)\right]$$

$$+ \left[2\,\cancel{\text{mol O}} \times \left(\frac{16.0\text{g O}}{\cancel{\text{mol O}}}\right)\right]$$

$$= \frac{74.0\text{ g } C_2H_5COOH}{\text{mol } C_2H_5COOH}$$

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Your Turn!

What is the formula mass of magnesium phosphate?

A. 262.9 g/mol

B. 150.9 g/mol

C. 333.6 g/mol

D. 119.3 g/mol

E. 166.9 g/mol

Formula is $Mg_3(PO_4)_2$

$$\left[3\ \text{mol Mg} \times \left(\frac{24.3\text{g Mg}}{\text{mol Mg}}\right)\right] + \left[2\ \text{mol P} \times \left(\frac{31.00\text{g P}}{\text{mol P}}\right)\right]$$

$$+ \left[8\ \text{mol O} \times \left(\frac{16.0\text{g O}}{\text{mol O}}\right)\right]$$

$$= \frac{262.9\ \text{g}\ Mg_3(PO_4)_2}{\text{mol}\ Mg_3(PO_4)_2}$$

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Learning Check: Using Molar Mass

Example: How many moles of iron (Fe) are in 15.34 g Fe?

- What do we want to determine?

15.34 g Fe = ? mol Fe

Start → (15.34 g Fe) End → (? mol Fe)

- What do we know?

1 mol Fe = 55.85 g Fe

- Set up ratio so that what you want is on top and what you start with is on the bottom

$$15.34\ \cancel{\text{g Fe}} \times \left(\frac{1\ \text{mol Fe}}{55.85\ \cancel{\text{g Fe}}}\right) = \mathbf{0.2747\ mol\ Fe}$$

Learning Check: Using Molar Mass

Example: If we need 0.168 mole $Ca_3(PO_4)_2$ for an experiment, how many grams do we need to weigh out?

- What do we want to determine?

$$0.168 \text{ mole } Ca_3(PO_4)_2 = ? \text{ g } Ca_3(PO_4)_2$$

Start → (0.168 mole) ... ← End (? g)

- Calculate MM of $Ca_3(PO_4)_2$

$3 \times$ mass Ca = 3×40.08 g = 120.24 g

$2 \times$ mass P = 2×30.97 g = 61.94 g

$8 \times$ mass O = 8×16.00 g = 128.00 g

$$1 \text{ mole } Ca_3(PO_4)_2 = 310.18 \text{ g } Ca_3(PO_4)_2$$

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Learning Check: Using Molar Mass

- Set up ratio so that what you want is on the top and what you start with is on the bottom

$$0.168\,\cancel{mol\;Ca_3(PO_4)_2} \times \left(\frac{310.18\;g\;Ca_3(PO_4)_2}{1\,\cancel{mol\;Ca_3(PO_4)_2}} \right)$$

= 52.11 g $Ca_3(PO_4)_2$

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Your Turn!

How many moles of CO_2 are there in 10.0 g?

A. 1.00 mol

B. 0.0227 mol

C. 4.401 mol

D. 44.01 mol

E. 0.227 mol

Molar mass of CO_2

$1 \times 12.01\ g = 12.01\ g\ C$

$2 \times 16.00\ g = 32.00\ g\ O$

$1\ mol\ CO_2 = 44.01\ g\ CO_2$

$$10.0\ \cancel{g\ CO_2}\left(\frac{1\ mol\ CO_2}{44.01\ \cancel{g\ CO_2}}\right)$$

= 0.227 mol CO_2

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Your Turn!

How many grams of platinum (Pt) are in 0.475 mole Pt?

A. 195 g

B. 0.0108 g

C. 0.000513 g

D. 0.00243 g

E. 92.7 g

Molar mass of Pt = 195.08 g/mol

$$0.475\ \text{mol Pt} \times \left(\frac{195.08\ \text{g Pt}}{1\ \text{mol Pt}}\right)$$

= 92.7 g Pt

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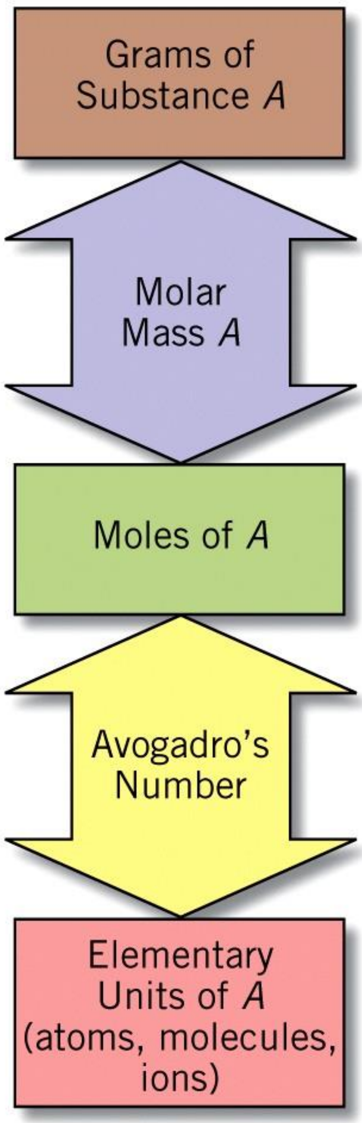
Using Moles in Calculations



- Start with either
  - Grams (Macroscopic)
  - Elementary units (Microscopic)
- Use molar mass to convert from grams to mole
- Use Avogadro's number to convert from moles to elementary units

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Macroscopic to Microscopic

How many silver atoms are in a 85.0 g silver bracelet?

- What do we want to determine?

85.0 g silver = ? atoms silver

- What do we know?

107.87 g Ag = 1 mol Ag

1 mol Ag = 6.022×10^{23} Ag atoms

g Ag ⟶ mol Ag ⟶ atoms Ag

$$85.0\ \text{g Ag} \times \left(\frac{1\ \text{mol Ag}}{107.87\ \text{g Ag}}\right) \times \left(\frac{6.022 \times 10^{23}\ \text{atoms Ag}}{1\ \text{mol Ag}}\right)$$

= 4.75×10^{23} Ag atoms

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Using Avogadro's Number

What is the mass, in grams, of one molecule of octane, C_8H_{18}?

Molecules octane $\longrightarrow$ mol octane $\longrightarrow$ g octane

1. Calculate molar mass of octane

Mass C = 8 × 12.01 g = 96.08 g

Mass H = 18 × 1.008 g = 18.14 g

1 mol octane = 114.22 g octane

2. Convert 1 molecule of octane to grams

$$\left(\frac{114.22\text{ g octane}}{1\text{ }\cancel{\text{mol octane}}}\right) \times \left(\frac{1\text{ }\cancel{\text{mol octane}}}{6.022 \times 10^{23}\text{ molecules octane}}\right)$$

= 1.897×10^{-22} g octane

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Learning Check: Mole Conversions

- Calculate the number of formula units of Na_2CO_3 in 1.29 moles of Na_2CO_3.

$$1.29\ \cancel{\text{mol } Na_2CO_3}\left(\frac{6.022\times 10^{23}\ \text{formula units } Na_2CO_3}{1\ \cancel{\text{mol } Na_2CO_3}}\right)$$

= 7.77 × 10^{23} particles Na_2CO_3

- How many moles of Na_2CO_3 are there in 1.15×10^5 formula units of Na_2CO_3 ?

$$1.15\times 10^{5}\ \cancel{\text{formula units } Na_2CO_3}\left(\frac{1\ \text{mol } Na_2CO_3}{6.022\times 10^{23}\ \cancel{\text{formula units } Na_2CO_3}}\right)$$

= 1.91×10^{-19} mol Na_2CO_3

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Your Turn!

How many atoms are in 1.00×10^{-9} g of U?

Molar mass U = 238.03 g/mole.

A. 6.02×10^{14} atoms

B. 4.20×10^{11} atoms

C. 2.53×10^{12} atoms

D. 3.95×10^{-31} atoms

E. 2.54×10^{21} atoms

$$\left(1.00 \times 10^{-9} \text{ g U}\right) \left(\frac{1 \text{ mol U}}{238.03 \text{ g U}}\right) \left(\frac{6.022 \times 10^{23} \text{ atoms U}}{1 \text{ mol U}}\right)$$

$= 2.53 \times 10^{12}$ atoms U

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Your Turn!

How much, in grams, do 8.85×10^{24} atoms of zinc weigh?

A. 3.49×10^{49} g

B. 961 g

C. 4.45 g

D. 5.33×10^{47} g

E. 1.47 g

$$8.85 \times 10^{24} \text{ atoms} \times \left(\frac{1 \text{ mol}}{6.022 \times 10^{23} \text{ atoms}} \right) \times \left(\frac{65.41 \text{ g Zn}}{1 \text{ mol}} \right)$$

= 961 g Zn

Your Turn!

Calculate the mass in grams of $FeCl_3$ in 1.53×10^{23} formula units. (molar mass = 162.204 g/mol)

A. 162.2 g

B. 0.254 g

C. 1.661×10^{-22} g

D. 41.2 g

E. 2.37×10^{-22}

$$1.53 \times 10^{23} \text{ units FeCl}_3 \left(\frac{1 \text{ mol FeCl}_3}{6.022 \times 10^{23} \text{ units FeCl}_3} \right) \times \left(\frac{162.2 \text{ g FeCl}_3}{1 \text{ mol FeCl}_3} \right)$$

= 41.2 g $FeCl_3$

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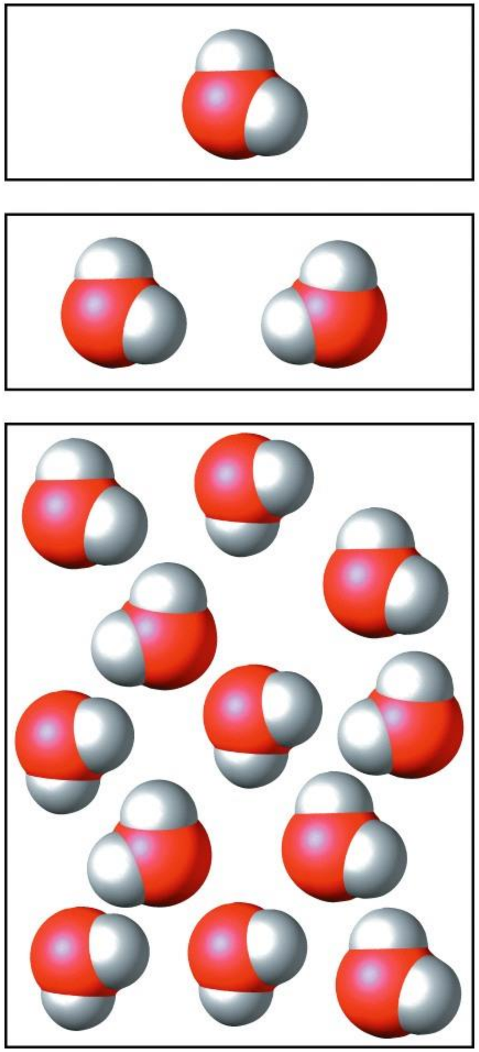
Mole-to-Mole Conversion Factors

- Can use chemical formula to relate amount of each atom to amount of compound
- In H_2O there are three relationships:
  - 2 mol H ⇔ 1 mol H_2O
  - 1 mol O ⇔ 1 mol H_2O
  - 2 mol H ⇔ 1 mol O
- Can also use these on atomic scale:
  - 2 atom H ⇔ 1 molecule H_2O
  - 1 atom O ⇔ 1 molecule H_2O
  - 2 atom H ⇔ 1 molecule O



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Stoichiometric Equivalencies

- Within chemical compounds, moles of atoms always combine in the same ratio as the individual atoms themselves
- Ratios of atoms in chemical formulas must be whole numbers
- These ratios allow us to convert between moles of each quantity

e.g., N_2O_5

2 mol N ⇔ 1 mol N_2O_5

5 mol O ⇔ 1 mol N_2O_5

2 mol N ⇔ 5 mol O

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Stoichiometric Equivalencies

Equivalency	Mole Ratio	Mole Ratio
2 mol N ⇔ 1 mol N_2O_5	$\frac{2 \text{ mol N}}{1 \text{ mol } N_2O_5}$	$\frac{1 \text{ mol } N_2O_5}{2 \text{ mol N}}$
5 mol O ⇔ 1 mol N_2O_5	$\frac{5 \text{ mol O}}{1 \text{ mol } N_2O_5}$	$\frac{1 \text{ mol } N_2O_5}{5 \text{ mol O}}$
2 mol N ⇔ 5 mol O	$\frac{5 \text{ mol O}}{2 \text{ mol N}}$	$\frac{2 \text{ mol N}}{5 \text{ mol O}}$

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Calculating the Amount of a Compound by Analyzing One Element

Calcium phosphate is widely found in natural minerals, bones, and some kidney stones. A sample is found to contain 0.864 moles of phosphorus. How many moles of $Ca_3(PO_4)_2$ are in that sample?

- What do we want to find?

$$0.864 \text{ mol P} = ? \text{ mol } Ca_3(PO_4)_2$$

- What do we know?

$$2 \text{ mol P} \Leftrightarrow 1 \text{ mol } Ca_3(PO_4)_2$$

- Solution

$$0.864 \cancel{\text{mol P}} \left(\frac{1 \text{ mol } Ca_3(PO_4)_2}{2 \cancel{\text{mol P}}} \right)$$

$$\mathbf{= 0.432 \text{ mol } Ca_3(PO_4)_2}$$

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Your Turn!

Calculate the number of moles of calcium in 2.53 moles of $Ca_3(PO_4)_2$

A. 2.53 mol Ca

B. 0.432 mol Ca

C. 3.00 mol Ca

D. 7.59 mol Ca

E. 0.843 mol Ca

2.53 moles of $Ca_3(PO_4)_2$ = ? mol Ca

3 mol Ca ⇔ 1 mol $Ca_3(PO_4)_2$

$$2.53\ \text{mol}\ Ca_3(PO_4)_2 \left(\frac{3\ \text{mol Ca}}{1\ \text{mol}\ Ca_3(PO_4)_2} \right)$$

= 7.59 mol Ca

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Your Turn!

A sample of sodium carbonate, Na_2CO_3, is found to contain 10.8 moles of sodium. How many moles of oxygen atoms (O) are present in the sample?

A. 10.8 mol O

B. 7.20 mol O

C. 5.40 mol O

D. 32.4 mol O

E. 16.2 mol O

10.8 moles of Na = ? mol O

2 mol Na ⇔ 3 mol O

$$10.8\,\cancel{\text{mol Na}}\left(\frac{3\,\text{mol O}}{2\,\cancel{\text{mol Na}}}\right) = \mathbf{16.2\ mol\ O}$$

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Mass-to-Mass Calculations

- Common laboratory calculation
- Need to know what mass of reagent *B* is necessary to completely react given mass of reagent *A* to form a compound
- Stoichiometry comes from chemical formula of compounds
  - Use the subscripts
- Summary of steps

mass *A* → moles *A* → moles *B* → mass *B*

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Mass-to-Mass Calculations

Chlorophyll, the green pigment in leaves, has the formula $C_{55}H_{72}MgN_4O_5$. If 0.0011 g of Mg is available to a plant for chlorophyll synthesis, how many grams of carbon will be required to completely use up the magnesium?

- Analysis

  0.0011 g Mg ⇔ ? g C

  0.0011 g Mg → mol Mg → mol C → g C

- Assembling the Tools

  24.305 g Mg = 1 mol Mg

  1 mol Mg ⇔ 55 mol C

  1 mol C = 12.011 g C

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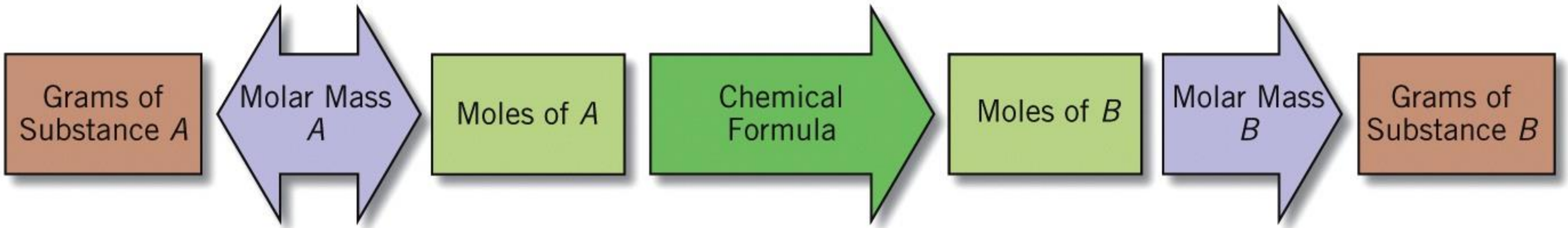
Ex. Mass-to-Mass Conversion



24.305 g Mg ⇔ 1 mol Mg

1 mol C ⇔ 12.011 g C

0.0011 g Mg → mol Mg → mol C → g C

1 mol Mg ⇔ 55 mol C

$$0.0011\,\cancel{g\ Mg} \times \left(\frac{1\,\cancel{mol\ Mg}}{24.305\,\cancel{g\ Mg}}\right) \times \left(\frac{55\,\cancel{mol\ C}}{1\,\cancel{mol\ Mg}}\right) \times \left(\frac{12.011\,g\ C}{1\,\cancel{mol\ C}}\right)$$

= 0.030 g C

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Your Turn!

How many g of iron are required to use up all of 25.6 g of oxygen atoms (O) to form Fe_2O_3?

A. 59.6 g

B. 29.8 g

C. 89.4 g

D. 134 g

E. 52.4 g

mass O → mol O → mol Fe → mass Fe

25.6 g O → ? g Fe

3 mol O ⇔ 2 mol Fe

$$25.6\ \cancel{\text{g O}} \times \left(\frac{1\ \cancel{\text{mol O}}}{16.0\ \cancel{\text{g O}}}\right) \times \left(\frac{2\ \cancel{\text{mol Fe}}}{3\ \cancel{\text{mol O}}}\right) \times \left(\frac{55.845\ \text{g Fe}}{1\ \cancel{\text{mol Fe}}}\right)$$

= 59.6 g Fe

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Your Turn!

Silver is often found in nature as the ore, argentite (Ag_2S). How many grams of pure silver can be obtained from a 836 g rock of argentite?

A. 7.75 g

B. 728 g

C. 364 g

D. 775 g

E. 418 g

mass Ag_2S → mol Ag_2S → mol Ag → mass Ag

836 g Ag_2S → ? g Ag

1 mol Ag_2S ⇔ 2 mol Ag

$$836\text{ g Ag}_2\text{S}\times\left(\frac{1\text{ mol Ag}_2\text{S}}{247.8\text{ g Ag}_2\text{S}}\right)\times\left(\frac{2\text{ mol Ag}}{1\text{ mol Ag}_2\text{S}}\right)\times\left(\frac{107.9\text{ g Ag}}{1\text{ mol Ag}}\right)$$

= 728 g Ag

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Percentage Composition

- Way to specify relative masses of each element in a compound
- List of percentage by mass of each element

Percentage by Mass

$$\% \text{ by mass of element} = \frac{\text{mass of element}}{\text{mass of sample}} \times 100\%$$

Example: Na_2CO_3 is

- 43.38% Na
- 11.33% C
- 45.29% O

- What is sum of the percentages? **100.00%**

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Example - Percent Composition

- Determine percentage composition based on chemical analysis of substance

Example: A sample of a liquid with a mass of 8.657 g was decomposed into its elements and gave 5.217 g of carbon, 0.9620 g of hydrogen, and 2.478 g of oxygen. What is the percentage composition of this compound?

Analysis:

- Calculate percentage by mass of each element in sample

Tools:

- Equation for percentage by mass
- Total mass = 8.657 g
- Mass of each element

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Ex. % Composition of Compound

For C: $\left(\frac{\text{g C}}{\text{g total}}\right)\times 100\% = \frac{5.217\text{ g C}}{8.657\text{ g}}\times 100\% = 60.26\%\text{ C}$

For H: $\left(\frac{\text{g H}}{\text{g total}}\right)\times 100\% = \frac{0.9620\text{ g H}}{8.657\text{ g}}\times 100\% = 11.11\%\text{ H}$

For O: $\left(\frac{\text{g O}}{\text{g total}}\right)\times 100\% = \frac{2.478\text{ g O}}{8.657\text{ g}}\times 100\% = 28.62\%\text{ O}$

Sum of percentages: 99.99%

- Percentage composition tells us mass of each element in 100.00 g of substance
- In 100.00 g of our liquid
  - 60.26 g C, 11.11 g H, and 28.62 g O

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Your Turn!

A sample was analyzed and found to contain 0.1417 g nitrogen and 0.4045 g oxygen. What is the percentage composition of this compound?

1. Calculate total mass of sample

Total sample mass = 0.1417 g + 0.4045 g = 0.5462 g

2. Calculate % Composition of N

$$\left(\frac{\text{g N}}{\text{g total}}\right)\times 100\% = \left(\frac{0.1417\text{ g N}}{0.5462\text{ g}}\right)\times 100\%$$ **= 25.94% N**

3. Calculate % Composition of O

$$\left(\frac{\text{g O}}{\text{g total}}\right)\times 100\% = \left(\frac{0.4045\text{ g O}}{0.5462\text{ g}}\right)\times 100\%$$ **= 74.06% O**

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Your Turn!

In a previous "You Turn!" slide, you found that an 836 g rock of argentite (Ag_2S) contained 728 g of silver. What are the percentages of silver and sulfur, by mass, in argentite?

A. 50.0% Ag, 50.0% S

B. 66.6% Ag, 33.4% S

C. 12.9% Ag, 87.1% S

D. 115% Ag, 108% S

E. 87.1% Ag, 12.9% S

Calculate % comp. of Ag:

$$\left(\frac{\text{g Ag}}{\text{g total}}\right)\times 100\%$$

$$=\left(\frac{728\text{ g Ag}}{836\text{ g}}\right)\times 100\%$$

= 87.1% Ag

Because the rest must be sulfur,
% S = 100 – 87.1 **= 12.9% S**

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Percent Compositions and Chemical Identity

Theoretical or Calculated Percentage Composition

- Calculated from molecular or ionic formula.
- Lets you distinguish between multiple compounds formed from the same two elements

- If experimental percent composition is known
  - Calculate theoretical percentage composition from proposed chemical formula
  - Compare with experimental composition

e.g., N and O form multiple compounds

- N_2O, NO, NO_2, N_2O_3, N_2O_4, and N_2O_5

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Example: Using Percent Composition

Are the mass percentages 30.54% N and 69.46% O consistent with the formula N_2O_4?

Procedure:

1. Assume one mole of compound
2. Subscripts tell how many moles of each element are present
   - 2 mol N and 4 mol O
3. Use molar masses of elements to determine mass of each element in 1 mole
   - Molar Mass of N_2O_4 = 92.14 g N_2O_4 / 1 mol
4. Calculate % by mass of each element

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Ex. Using Percent Composition (cont)

$$2 \text{ mol N} \times \frac{14.07 \text{ g N}}{1 \text{ mol N}} = 28.14 \text{ g N}$$

$$4 \text{ mol O} \times \frac{16.00 \text{ g O}}{1 \text{ mol O}} = 64.00 \text{ g O}$$

$$\%\text{N} = \frac{28.14 \text{ g N}}{92.14 \text{ g } N_2O_4} \times 100\% = \mathbf{30.54\% \text{ N in } N_2O_4}$$

$$\%\text{O} = \frac{64.00 \text{ g O}}{92.14 \text{ g } N_2O_4} \times 100\% = \mathbf{69.46\% \text{ O in } N_2O_4}$$

- The experimental values match the theoretical percentages for the formula N_2O_4.

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Your Turn!

If a sample containing only phosphorous and oxygen has percent composition 56.34% P and 43.66% O, is this P_4O_{10}?

A. Yes

B. No

$4 \text{ mol P} \Leftrightarrow 1 \text{ mol } P_4O_{10}$

$10 \text{ mol O} \Leftrightarrow 1 \text{ mol } P_4O_{10}$

$4 \text{ mol P} = 4 \times 30.97 \text{ g/mol P} = 123.9 \text{ g P}$

$10 \text{ mol O} = 10 \times 16.00 \text{ g/mol O} = \underline{160.0 \text{ g O}}$

$1 \text{ mol } P_4O_{10} = \mathbf{283.9\ g}\ P_4O_{10}$

$$\%\,P = \frac{123.9 \text{ g P}}{283.9 \text{ g } P_4O_{10}} \times 100\% = 43.64\%\ P$$

$$\%\,O = \frac{160.0 \text{ g O}}{283.9 \text{ g } P_4O_{10}} \times 100\% = 56.36\%\ O$$

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Determining Empirical and Molecular Formulas

- When making or isolating new compounds one must characterize them to determine structure and

Empirical Formula

  - Simplest ratio of atoms of each element in compound
  - Obtained from experimental analysis of compound

Molecular Formula

  - Exact composition of one molecule
  - Exact whole number ratio of atoms of each element in molecule

glucose **Empirical formula** CH_2O

Molecular formula $C_6H_{12}O_6$

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Three Ways to Calculate Empirical Formulas

1. From Masses of Elements

e.g., 2.448 g sample of which 1.771 g is Fe and 0.677 g is O.

2. From Percentage Composition

e.g., 43.64% P and 56.36% O

3. From Combustion Data

- Given masses of combustion products

e.g., The combustion of a 5.217 g sample of a compound of C, H, and O in pure oxygen gave 7.406 g CO_2 and 4.512 g of H_2O

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Strategy for Determining Empirical Formulas

1. Determine mass in g of each element
2. Convert mass in g to moles
3. Divide all quantities by smallest number of moles to get smallest ratio of moles
4. Convert any non-integers into integer numbers.
   - If number ends in decimal equivalent of fraction, multiply all quantities by the denominator of the fraction
   - Otherwise, round numbers to nearest integers

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1. Empirical Formula from Mass Data

When a 0.1156 g sample of a compound was analyzed, it was found to contain 0.04470 g of C, 0.01875 g of H, and 0.05215 g of N. Calculate the empirical formula of this compound.

Step 1: Calculate moles of each substance

$$0.04470\ \cancel{\text{g C}} \times \frac{1\ \text{mol C}}{12.011\ \cancel{\text{g C}}} = 3.722 \times 10^{-3}\ \text{mol C}$$

$$0.01875\ \cancel{\text{g H}} \times \frac{1\ \text{mol H}}{1.008\ \cancel{\text{g H}}} = 1.860 \times 10^{-2}\ \text{mol H}$$

$$0.05215\ \cancel{\text{g N}} \times \frac{1\ \text{mol N}}{14.0067\ \cancel{\text{g N}}} = 3.723 \times 10^{-3}\ \text{mol N}$$

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1. Empirical Formula from Mass Data

Step 2: Select the smallest number of moles

- Smallest is 3.722×10^{-3} mole

Mole ratio   Integer ratio

- $C = \dfrac{3.722 \times 10^{-3} \text{ mol C}}{3.722 \times 10^{-3} \text{ mol C}} = 1.000 = 1$
- $H = \dfrac{1.860 \times 10^{-2} \text{ mol H}}{3.722 \times 10^{-3} \text{ mol C}} = 4.997 = 5$
- $N = \dfrac{3.723 \times 10^{-3} \text{ mol N}}{3.722 \times 10^{-3} \text{ mol C}} = 1.000 = 1$

Step 3: Divide all number of moles by the smallest one

Empirical formula = CH_5N

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Empirical Formula from Mass Data

One of the compounds of iron and oxygen, "black iron oxide," occurs naturally in the mineral magnetite. When a 2.448 g sample was analyzed it was found to have 1.771 g of Fe and 0.677 g of O. Calculate the empirical formula of this compound.

Assembling the tools:

1 mol Fe = 55.845 g Fe 1 mol O = 16.00 g O

1. Find the moles of each element, then find the ratio of the moles of the elements.
2. Calculate moles of each substance

$$1.771\ \text{g Fe} \times \frac{1\ \text{mol Fe}}{55.485\ \text{g Fe}} = 0.03182\ \text{mol Fe}$$

$$0.677\ \text{g O} \times \frac{1\ \text{mol O}}{16.00\ \text{g O}} = 0.0423\ \text{mol O}$$

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1. Empirical Formula from Mass Data

2. Divide both by smallest number mol to get smallest whole number ratio.

$$\frac{0.03171 \text{ mol Fe}}{0.03171 \text{ mol Fe}} = 1.000 \text{ Fe} \times 3 = 3.000 \text{ Fe}$$

$$\frac{0.0423 \text{ mol O}}{0.03171 \text{ mol Fe}} = 1.33 \text{ O} \times 3 = 3.99 \text{ O}$$

Or

$$Fe_{\frac{0.03171}{0.03171}}O_{\frac{0.0423}{0.03171}} = Fe_{1.00}O_{1.33}$$

$$Fe_{(1.00\times3)}O_{(1.33\times3)} = Fe_3O_{3.99}$$

Empirical Formula = Fe_3O_4

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2. Empirical Formula from Percentage Composition

- New compounds are characterized by elemental analysis, from which the percentage composition can be obtained
- Use percentage composition data to calculate empirical formula
- Must convert percentage composition to grams
- Assume 100.00 g sample
  - Convenient
  - Sum of percentage composition = 100%
  - Sum of masses of each element = 100 g

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2. Empirical Formula from Percentage Composition

Calculate the empirical formula of a compound whose percentage composition data is 43.64% P and 56.36% O. If the molar mass is determined to be 283.9 g/mol, what is the molecular formula?

Step 1: Assume 100 g of compound

- 43.64 g P　　　　1 mol P = 30.97 g
- 56.36 g O　　　　1 mol O = 16.00 g

$$43.64\ \text{g P} \times \frac{1\ \text{mol P}}{30.97\ \text{g P}} = 1.409\ \text{mol P}$$

$$56.36\ \text{g O} \times \frac{1\ \text{mol O}}{16.00\ \text{g O}} = 3.523\ \text{mol O}$$

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2. Empirical Formula from Percentage Composition

Step 2: Divide by smallest number of moles

$$\frac{1.409\ \text{mol P}}{1.409\ \text{mol P}} = 1.000 \quad \times 2 = 2$$

$$\frac{3.523\ \text{mol O}}{1.409\ \text{mol P}} = 2.500 \quad \times 2 = 5$$

Step 3: Multiple to get integers

$$1.000 \times 2 = 2$$
$$2.500 \times 2 = 5$$

Empirical formula = P_2O_5

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3. Empirical Formulas from Indirect Analysis:

- In practice, compounds are not broken down into elements, but are changed into other compounds whose formula is known

Combustion Analysis

- Compounds containing carbon, hydrogen, and oxygen, can be burned completely in pure oxygen gas
  - Only carbon dioxide and water are produced

e.g., Combustion of methanol (CH_3OH)

$$2CH_3OH + 3O_2 \longrightarrow 2CO_2 + 4H_2O$$

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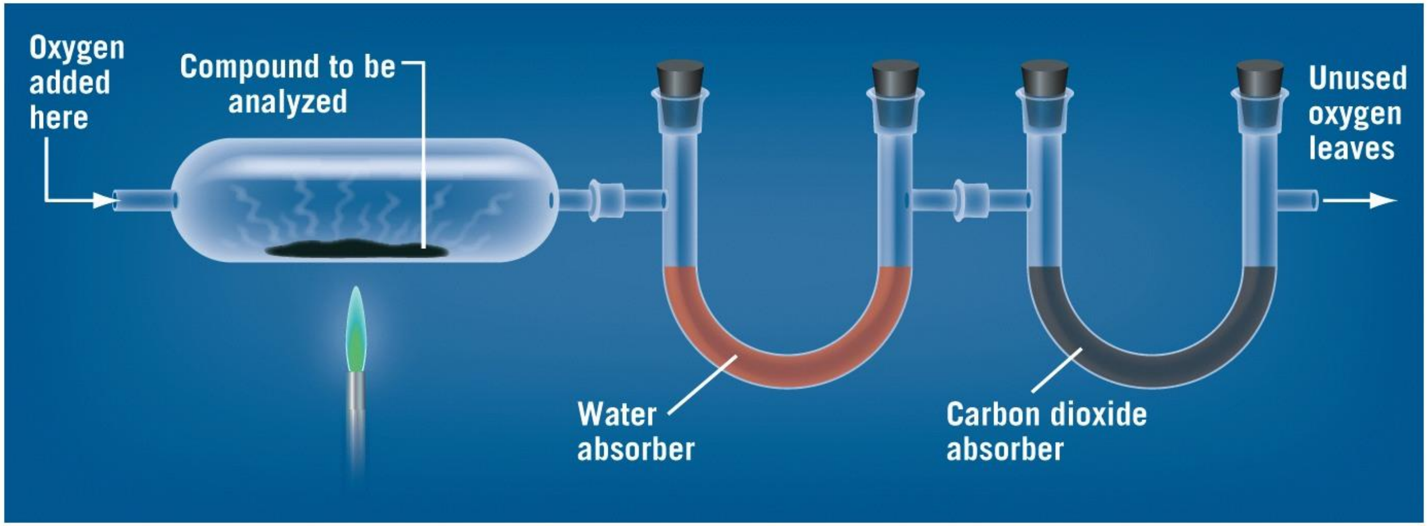
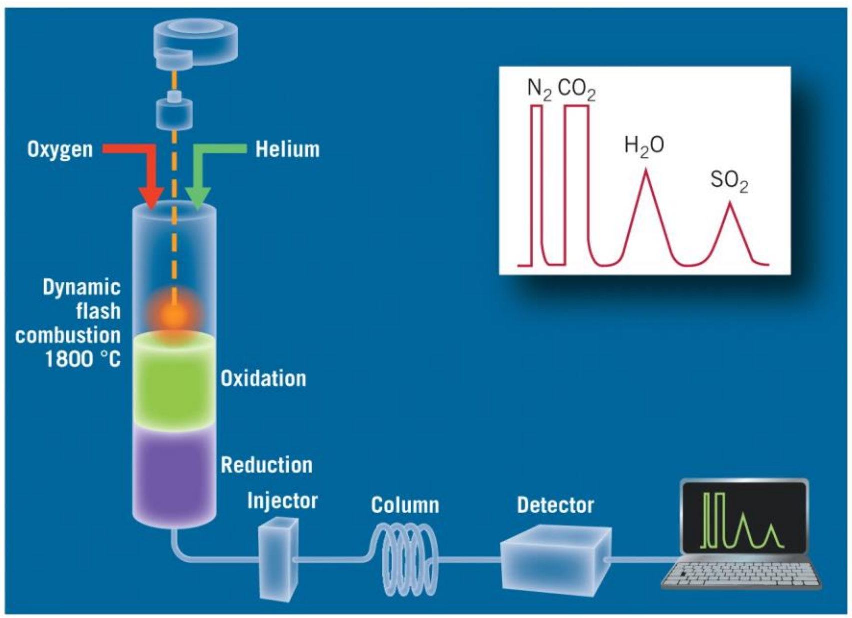
Combustion Analysis



Classic



Modern CHN analysis

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3. Empirical Formulas from Indirect Analysis:

- Carbon dioxide and water are separated and weighed separately
  - All C ends up as CO_2
  - All H ends up as H_2O
  - Mass of C can be derived from amount of CO_2
    - mass $CO_2 \rightarrow$ mol $CO_2 \rightarrow$ mol C $\rightarrow$ mass C
  - Mass of H can be derived from amount of H_2O
    - mass $H_2O \rightarrow$ mol $H_2O \rightarrow$ mol H $\rightarrow$ mass H
  - Mass of oxygen is obtained by difference
    - mass O = mass sample – (mass C + mass H)

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Ex. Indirect or Combustion Analysis

The combustion of a 5.217 g sample of a compound of C, H, and O in pure oxygen gave 7.406 g CO_2 and 4.512 g of H_2O. Calculate the empirical formula of the compound.

	C	H	H_2O	CO_2
MM (g/mol)	12.011	1.008	18.015	44.01

1. Calculate mass of C from mass of CO_2.

mass CO_2 → mole CO_2 → mole C → mass C

$$7.406\ \text{g CO}_2 \left(\frac{1\ \text{mol CO}_2}{44.01\ \text{g CO}_2}\right)\left(\frac{1\ \text{mol C}}{1\ \text{mol CO}_2}\right)\left(\frac{12.011\ \text{g C}}{1\ \text{mol C}}\right)$$

= 2.021 g C

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Ex. Indirect or Combustion Analysis

The combustion of a 5.217 g sample of a compound of C, H, and O gave 7.406 g CO_2 and 4.512 g of H_2O. Calculate the empirical formula of the compound.

2. Calculate mass of H from mass of H_2O.

mass H_2O → mol H_2O → mol H → mass H

$$4.512\ \text{g H}_2\text{O}\left(\frac{1\ \text{mol H}_2\text{O}}{18.015\ \text{g H}_2\text{O}}\right)\left(\frac{2\ \text{mol H}}{1\ \text{mol H}_2\text{O}}\right)\left(\frac{1.008\ \text{g H}}{1\ \text{mol H}}\right)$$

= 0.5049 g H

3. Calculate mass of O from difference.

5.217 g sample – 2.021 g C – 0.5049 g H **= 2.691 g O**

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Ex. Indirect or Combustion Analysis

	C	H	O
At. mass	12.011	1.008	15.999
g	2.021	0.5049	2.691

4. Calculate mol of each element

$$\text{mol C} = \frac{\text{g C}}{\text{MM C}} = \frac{2.021\ \cancel{\text{g}}}{12.011\ \cancel{\text{g}}/\text{mol}} = 0.1683\ \text{mol C}$$

$$\text{mol H} = \frac{\text{g H}}{\text{MM H}} = \frac{0.5049\ \cancel{\text{g}}}{1.008\ \cancel{\text{g}}/\text{mol}} = 0.5009\ \text{mol H}$$

$$\text{mol O} = \frac{\text{g O}}{\text{MM O}} = \frac{2.691\ \cancel{\text{g}}}{15.999\ \cancel{\text{g}}/\text{mol}} = 0.1682\ \text{mol O}$$

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Ex. Indirect or Combustion Analysis

- Preliminary empirical formula
  - $C_{0.1683}H_{0.5009}O_{0.1682}$

5. Calculate mol ratio of each element

$$C_{\frac{0.1683}{0.1682}}H_{\frac{0.5009}{0.1682}}O_{\frac{0.1682}{0.1682}} = C_{1.00}H_{2.97}O_{1.00}$$

- Because all values are close to integers, round to

Empirical Formula = CH_3O

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Your Turn!

The combustion of a 13.660 g sample of a compound of C, H, and S in pure oxygen gave 19.352 g CO_2 and 11.882 g of H_2O. Calculate the empirical formula of the compound.

A. $C_4H_{12}S$

B. CH_3S

C. C_2H_6S

D. $C_2H_6S_3$

E. CH_3S_2

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Your Turn! Solution

1. Calculate mass of C from mass of CO_2.

mass CO_2 → mole CO_2 → mole C → mass C

$$19.352\ \text{g CO}_2 \left(\frac{1\ \text{mol CO}_2}{44.01\ \text{g CO}_2}\right)\left(\frac{1\ \text{mol C}}{1\ \text{mol CO}_2}\right)\left(\frac{12.011\ \text{g C}}{1\ \text{mol C}}\right)$$

= 5.281 g C

2. Calculate mass of H from mass of H_2O.

mass H_2O → mol H_2O → mol H → mass H

$$11.882\ \text{g H}_2\text{O} \left(\frac{1\ \text{mol H}_2\text{O}}{18.015\ \text{g H}_2\text{O}}\right)\left(\frac{2\ \text{mol H}}{1\ \text{mol H}_2\text{O}}\right)\left(\frac{1.008\ \text{g H}}{1\ \text{mol H}}\right)$$

= 1.330 g H

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Your Turn! Solution Continued

3. Calculate mass of S from difference.

13.66 g sample – 5.281 g C – 1.330 g H **= 7.049 g S**

$$\text{mol C} = \frac{\text{g C}}{\text{MM C}} = \frac{5.281\,\cancel{\text{g}}}{12.011\,\cancel{\text{g}}/\text{mol}}$$ = 0.4497 mol C

$$\text{mol H} = \frac{\text{g H}}{\text{MM H}} = \frac{1.330\,\cancel{\text{g}}}{1.008\,\cancel{\text{g}}/\text{mol}}$$ = 1.319 mol H

$$\text{mol S} = \frac{\text{g S}}{\text{MM S}} = \frac{7.049\,\cancel{\text{g}}}{32.065\,\cancel{\text{g}}/\text{mol}}$$ = 0.2198 mol S

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Your Turn! Solution Continued

- Preliminary empirical formula
  - $C_{0.4497}H_{1.319}O_{0.2198}$

5. Calculate mol ratio of each element

$$C_{\frac{0.4497}{0.2198}}H_{\frac{1.319}{0.2198}}O_{\frac{0.2198}{0.2198}} = C_{2.03}H_{6.00}O_{1.00}$$

- Because all values are close to integers, round to

Empirical Formula = C_2H_6S

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Determining Molecular Formulas

- **Empirical formula**
  - Accepted formula unit for ionic compounds
- **Molecular formula**
  - Preferred for molecular compounds
- In some cases molecular and empirical formulas are the same
- When they are different, the subscripts of molecular formula are integer multiples of those in empirical formula
  - If empirical formula is A_xB_y
  - Molecular formula will be $A_{n \times x}B_{n \times y}$

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Determining Molecular Formula

- Need molecular mass and empirical formula
- Calculate ratio of molecular mass to mass predicted by empirical formula and round to nearest integer

$$n = \frac{\text{molecular mass}}{\text{empirical formula mass}}$$

Example: Glucose

Molecular mass is 180.16 g/mol

Empirical formula = CH_2O

Empirical formula mass = 30.03 g/mol

$$n = \frac{180.16\ \text{g}}{30.03\ \text{g}} = 6$$

Molecular formula = $C_6H_{12}O_6$

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Learning Check

The empirical formula of a compound containing phosphorous and oxygen was found to be P_2O_5. If the molar mass is determined to be 283.9 g/mol, what is the molecular formula?

$$n = \frac{\text{molecular mass}}{\text{empirical mass}}$$

Step 1: Calculate empirical mass

$$\begin{aligned}\text{empirical mass } P_2O_5 &= (2 \times \text{mass P}) + (5 \times \text{mass O}) \\ &= (2 \times 30.97\text{ g/mol}) + (5 \times 16.00\text{ g/mol}) \\ &= (61.94 + 80.00)\text{ g/mol} \\ &= 141.94\text{ g/mol } P_2O_5\end{aligned}$$

Step 2: Calculate ratio of molecular to empirical mass

$$n = \frac{283.9\text{ g/mol}}{141.94\text{ g/mol}} = 2$$

Molecular formula = P_4O_{10}

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Your Turn!

The empirical formula of hydrazine is NH_2, and its molecular mass is 32.0. What is its molecular formula?

Atomic Mass: N = 14.007; H = 1.008; O = 15.999

A. NH_2

B. N_2H_4

C. N_3H_6

D. N_4H_8

E. $N_{1.5}H_3$

Molar mass of NH_2 =

$(1 \times 14.01)\text{ g} + (2 \times 1.008)\text{ g} = 16.017\text{ g}$

$n = (32.0/16.02) = 2$

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Balanced Chemical Equations

- Useful tool for problem solving
  - Prediction of reactants and products
  - All atoms present in reactants must also be present among products
  - Coefficients are multipliers that are used to balance equations
- Two step process
  1. Write unbalanced equation
     - Given products and reactants
     - Organize with plus signs and arrow
  2. Adjust coefficients to get equal numbers of each kind of atom on both sides of arrow

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Guidelines for Balancing Equations

1. Start balancing with the most complicated formula first
   - Elements, particularly H_2 and O_2, should be left until the end
2. Balance atoms that appear in only two formulas: one as a reactant and the other as a product
   - Leave elements that appear in three or more formulas until later
3. Balance as a group those polyatomic ions that appear unchanged on both sides of the arrow

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Balancing Equations

- Use the inspection method

Step 1. Write unbalanced equation

$Zn(s) + HCl(aq) \rightarrow ZnCl_2(aq) + H_2(g)$ **unbalanced**

Step 2. Adjust coefficients to balance numbers of each kind of atom on both sides of arrow.

- Since $ZnCl_2$ has two Cl on the product side, 2HCl on reactant side is needed to balance the equation.

$Zn(s) + \mathbf{2}HCl(aq) \longrightarrow ZnCl_2(aq) + H_2(g)$

- One Zn each side
- Two H each side
- Two Cl each side

Balanced!

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Learning Check: Balancing Equations

$AgNO_3(aq) + Na_3PO_4(aq) \rightarrow Ag_3PO_4(s) + NaNO_3(aq)$

- Count atoms

Reactants	Products
1 Ag	3 Ag
3 Na	1 Na

- Adjust coefficients of both $AgNO_3$+ $NaNO_3$ to three.

$3AgNO_3(aq) + Na_3PO_4(aq) \rightarrow Ag_3PO_4(s) + 3NaNO_3(aq)$

- Now check polyatomic ions

3 NO_3^-	3 NO_3^-
1 PO_4^{3-}	1 PO_4^{3-}

- Equation is balanced

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Balance by Inspection

$\_\_C_3H_8(g) + \_\_O_2(g) \rightarrow \_\_CO_2(g) + \_\_H_2O(l)$

Assume 1 in front of C_3H_8

3 C | 1 C × 3

8 H | 2 H × 4

$1C_3H_8(g) + \_\_O_2(g) \rightarrow 3CO_2(g) + 4H_2O(l)$

2 O × 5 = 10 | O = (3 × 2) + 4 = 10

8 H | H = 2 × 4 = 8

$1C_3H_8(g) + 5O_2(g) \rightarrow 3CO_2(g) + 4H_2O(l)$

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Your Turn!

Balance each of the following equations.
What are the coefficients in front of each compound?

$\underline{1}$ $Ba(OH)_2(aq)$ + $\underline{1}$ $Na_2SO_4(aq) \rightarrow$ $\underline{1}$ $BaSO_4(s)$ + $\underline{2}$ $NaOH(aq)$

$\underline{2}$ $KClO_3(s) \rightarrow$ $\underline{2}$ $KCl(s)$ + $\underline{3}$ $O_2(g)$

$\underline{2}$ $H_3PO_4(aq)$ + $\underline{3}$ $Ba(OH)_2(aq) \rightarrow$ $\underline{1}$ $Ba_3(PO_4)_2(s)$ + $\underline{6}$ $H_2O(l)$

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Using Balanced Equations: Reaction Stoichiometry

- **Balanced equation**
  - Critical link between substances involved in chemical reactions
  - Gives relationship between amounts of reactants used and amounts of products formed
- **Numeric coefficient tells us**
  - The mole ratios for reactions
  - How many individual particles are needed in reaction on microscopic level
  - How many moles are necessary on macroscopic level

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Stoichiometric Ratios

- Consider the reaction

$$N_2 + 3H_2 \rightarrow 2NH_3$$

- Could also be read as:

"When 1 mole of nitrogen reacts with 3 moles of hydrogen, 2 moles of ammonia are formed."

- **Molar relationships**
  - 1 mole $N_2 \Leftrightarrow$ 2 mole NH_3
  - 3 mole $H_2 \Leftrightarrow$ 2 mole NH_3
  - 1 mole $N_2 \Leftrightarrow$ 3 mole H_2

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Stoichiometric Ratios

- Consider the reaction

$$N_2 + 3H_2 \rightarrow 2NH_3$$

- Could be read as:

"When 1 molecule of nitrogen reacts with 3 molecules of hydrogen, 2 molecules of ammonia are formed."

- **Molecular relationships**
- 1 molecule $N_2 \Leftrightarrow$ 2 molecule NH_3
- 3 molecule $H_2 \Leftrightarrow$ 2 molecule NH_3
- 1 molecule $N_2 \Leftrightarrow$ 3 molecule H_2

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Stoichiometry

- Mass balance of all formulas involved in chemical reactions

Stoichiometric Calculations

- Conversions from one set of units to another using dimensional analysis
- Need to know:
  1. Equalities to make conversion factors
  2. Steps to go from starting units to desired units

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Using Stoichiometric Ratios

Example: For the reaction $N_2 + 3\ H_2 \rightarrow 2NH_3$, how many moles of N_2 are used when 2.3 moles of NH_3 are produced?

- Assembling the tools
  - 2 moles NH_3 = 1 mole N_2
  - 2.3 mole NH_3 = ? moles N_2

$$2.3\ \cancel{\text{mol NH}_3}\left(\frac{1\ \text{mol N}_2}{2\ \cancel{\text{mol NH}_3}}\right) = 1.2\ \text{mol N}_2$$

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Your Turn!

If 0.575 mole of CO_2 is produced by the combustion of propane, C_3H_8, how many moles of oxygen are consumed? The balanced equation is

$$C_3H_8(g) + 5O_2(g) \rightarrow 3CO_2(g) + 4H_2O(g)$$

A. 0.575 mole

B. 2.88 mole

C. 0.192 mole

D. 0.958 mole

E. 0.345 mole

Assembling the tools

- 0.575 mole CO_2 = ? moles O_2
- 3 moles CO_2 = 5 mole O_2

$$0.575\ \cancel{\text{mol CO}_2}\left(\frac{5\ \text{mol O}_2}{3\ \cancel{\text{mol CO}_2}}\right) = 0.958\ \text{mol O}_2$$

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Your Turn!

How many moles of hydrochloric acid are required to completely react with 1.43 moles of iron(II) chloride according to the reaction below?

$$14HCl + Na_2Cr_2O_7 + 6FeCl_2 \rightarrow 2CrCl_3 + 7H_2O + 6FeCl_3 + 2NaCl$$

A. 20.0 mole

B. 1.43 mole

C. 0.613 mole

D. 3.34 mole

E. 8.58 mole

Assembling the tools

- 1.43 mole $FeCl_2$ = ? moles HCl
- 6 moles $FeCl_2$ = 14 mole HCl

$$1.43\,\cancel{\text{mol FeCl}_2}\left(\frac{14\text{ mol HCl}}{6\,\cancel{\text{mol FeCl}_2}}\right)$$

= 3.34 mol HCl

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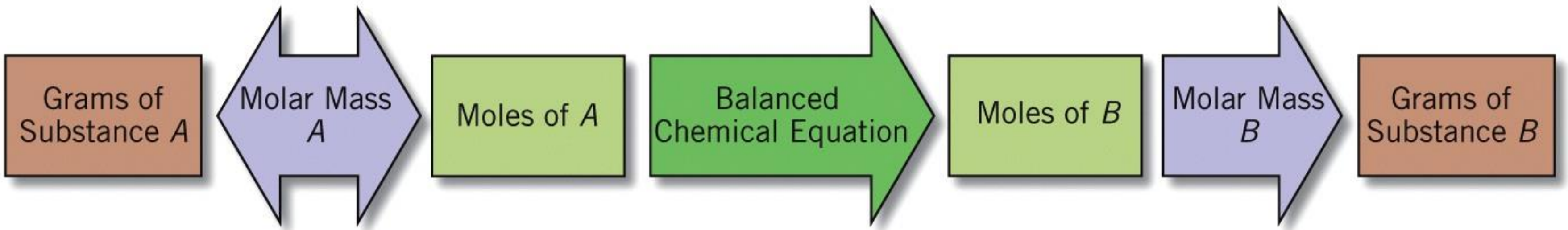
Mass-to-Mass Conversions

- Most common stoichiometric conversions that chemists use involve converting mass of one substance to mass of another.



- Use molar mass *A* to convert grams *A* to moles *A*
- Use chemical equations to relate moles *A* to moles *B*
- Use molar mass *B* to convert to moles *B* to grams *B*

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Stoichiometry Calculations Using a Balanced Chemical Equation

Example: What mass of O_2 will react with 96.1 g of propane (C_3H_8) gas, to form gaseous carbon dioxide and water?

Strategy

1. Write the balanced equation

$$C_3H_8(g) + 5O_2(g) \rightarrow 3CO_2(g) + 4H_2O(g)$$

2. Assemble the tools

$$96.1\ g\ C_3H_8 \rightarrow moles\ C_3H_8 \rightarrow moles\ O_2 \rightarrow g\ O_2$$

$$1\ mol\ C_3H_8 = 44.1\ g\ C_3H_8$$

$$1\ mol\ O_2 = 32.00\ g\ O_2$$

$$1\ mol\ C_3H_8 = 5\ mol\ O_2$$

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Stoichiometry Calculations Using a Balanced Chemical Equation

Example: What mass of O_2 will react with 96.1 g of propane in a complete combustion?

$$C_3H_8(g) + 5O_2(g) \rightarrow 3CO_2(g) + 4H_2O(g)$$

3. Assemble conversions so units cancel correctly

$$96.1 \text{ g } C_3H_8 \times \frac{1 \text{ mol } C_3H_8}{44.1 \text{ g } C_3H_8} \times \frac{5 \text{ mol } O_2}{1 \text{ mol } C_3H_8} \times \frac{32.0 \text{ g } O_2}{1 \text{ mol } O_2}$$

= 349 g of O_2 are needed

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Your Turn!

How many grams of Al_2O_3 are produced when 41.5 g Al react?

$$2Al(s) + Fe_2O_3(s) \rightarrow Al_2O_3(s) + 2Fe(l)$$

A. 78.4 g

B. 157 g

C. 314 g

D. 22.0 g

E. 11.0 g

$$41.5\ \text{g Al}\left(\frac{1\ \text{mol Al}}{26.98\ \text{g Al}}\right)\left(\frac{1\ \text{mol } Al_2O_3}{2\ \text{mol Al}}\right)\left(\frac{101.96\ \text{g } Al_2O_3}{1\ \text{mol } Al_2O_3}\right)$$

$= 78.4\ \text{g } Al_2O_3$

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Your Turn!

How many grams of sodium dichromate are required to produce 24.7 g iron(III) chloride from the following reaction?

$$14HCl + Na_2Cr_2O_7 + 6FeCl_2 \rightarrow 2CrCl_3 + 7H_2O + 6FeCl_3 + 2NaCl$$

A. 6.64 g $Na_2Cr_2O_7$

B. 0.152 g $Na_2Cr_2O_7$

C. 8.51 g $Na_2Cr_2O_7$

D. 39.9 g $Na_2Cr_2O_7$

E. 8.04 g $Na_2Cr_2O_7$

$$24.7\ \text{g FeCl}_3 \times \left(\frac{1\ \text{mol FeCl}_3}{162.2\ \text{g FeCl}_3}\right) \times \left(\frac{1\ \text{mol Na}_2\text{Cr}_2\text{O}_7}{6\ \text{mol FeCl}_3}\right) \times \left(\frac{262.0\ \text{g Na}_2\text{Cr}_2\text{O}_7}{1\ \text{mol Na}_2\text{Cr}_2\text{O}_7}\right)$$

$$= 6.64\ \text{g Na}_2\text{Cr}_2\text{O}_7$$

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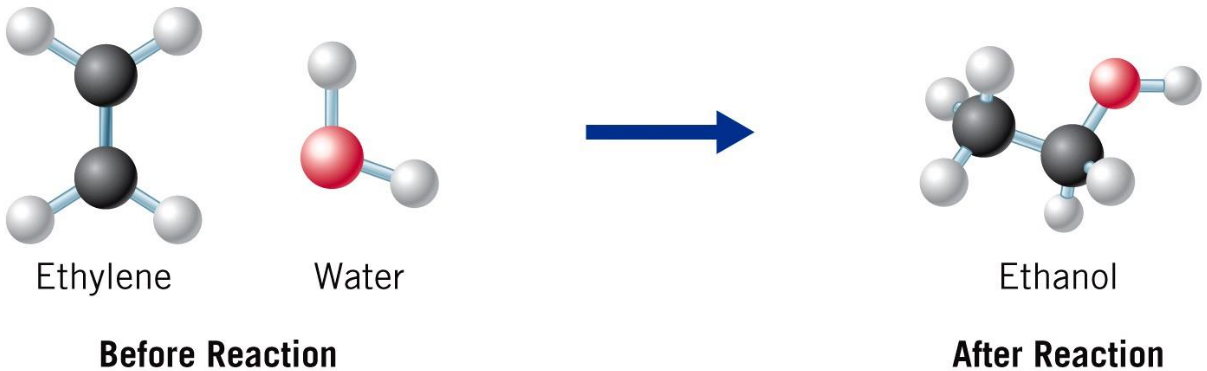
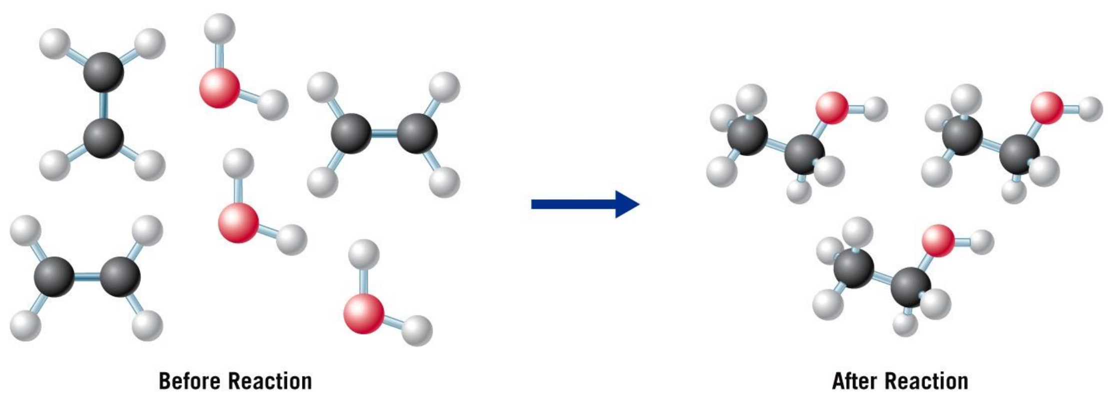
Molecular Level of Reactions

- Consider industrial synthesis of ethanol

$$C_2H_4 + H_2O \longrightarrow C_2H_5OH$$



- 3 molecules ethylene + 3 molecules water react to form 3 molecules ethanol



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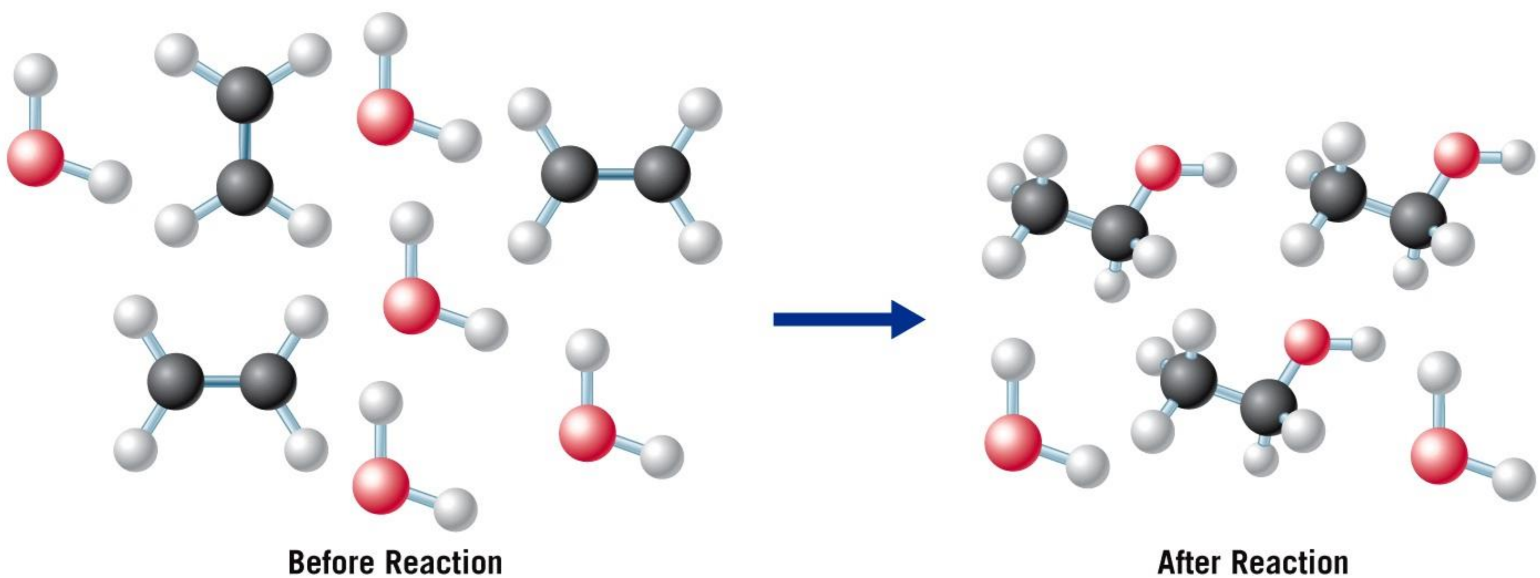
Molecular Level of Reactions

- What happens if these proportions are not met?
  - 3 molecules ethylene + 5 molecules of water



  - All ethylene will be consumed and some water will be left over

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Limiting Reactant

- Reactant that is completely used up in the reaction
- Present in lower number of moles
- It determines the amount of product produced
- For this reaction the limiting reactant is ethylene

Excess reactant

- Reactant that has some amount left over at end
- Present in higher number of moles
- For this reaction it is water

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Limiting Reactant Calculations

1. Write the balanced equation
2. Identify the limiting reagent
   - Calculate amount of reactant *B* needed to react with reactant *B*

mass reactant *A* have ⟶ **mol reactant *A*** ⟶ **mol reactant *B*** ⟶ **Mass reactant *B* need**

   - Compare amount of *B* you need with amount of *B* you actually have.
     - If need **more** *B* than you have, then *B* is limiting
     - If need **less** *B* than you have, then *A* is limiting

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Limiting Reactant Calculations

3. Calculate mass of desired product, using amount of **limiting reactant** and mole ratios.

mass limiting reactant → **mol limiting reactant** → **mol product** → **mass product**

Ex. Limiting Reactant Calculation

How many grams of NO can form when 30.0 g NH_3 and 40.0 g O_2 react according to:

$$4NH_3 + 5O_2 \longrightarrow 4NO + 6H_2O$$

Solution: Step 1

mass NH_3 → mole NH_3 → mole O_2 → mass O_2

Assembling the tools

- 1 mol NH_3 = 17.03 g
- 1 mol O_2 = 32.00 g
- 4 mol NH_3 ⇔ 5 mol O_2

Only have 40.0 g O_2, O_2 limiting reactant

$$30.0\ \text{g NH}_3 \times \frac{1\ \text{mol NH}_3}{17.03\ \text{g NH}_3} \times \frac{5\ \text{mol O}_2}{4\ \text{mol NH}_3} \times \frac{32.00\ \text{g O}_2}{1\ \text{mol O}_2}$$

= 70.5 g O_2 needed

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Ex. Limiting Reactant Calculation

How many grams of NO can form when 30.0 g NH_3 and 40.0 g O_2 react according to:

$$4\ NH_3 + 5\ O_2 \longrightarrow 4\ NO + 6\ H_2O$$

Solution: Step 2

mass O_2 → mole O_2 → mole NO → mass NO

Assembling the tools

Can only form 30.0 g NO

- 1 mol O_2 = 32.00 g
- 1 mol NO = 30.01 g
- 5 mol O_2 ⇔ 4 mol NO

$$40.0\ \text{g}\ O_2 \times \frac{1\ \text{mol}\ O_2}{32.00\ \text{g}\ O_2} \times \frac{4\ \text{mol NO}}{5\ \text{mol}\ O_2} \times \frac{30.01\ \text{g NO}}{1\ \text{mol NO}}$$

= 30.0 g NO formed

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Your Turn!

If 18.1 g NH_3 is reacted with 90.4 g CuO, what is the maximum amount of Cu metal that can be formed?

$$2NH_3(g) + 3CuO(s) \rightarrow N_2(g) + 3Cu(s) + 3H_2O(g)$$

(MM) (17.03) (79.55) (28.01) (63.55)(18.02)
(g/mol)

$$18.1\,g\,NH_3 \times \frac{1\,mol\,NH_3}{17.03\,g\,NH_3} \times \frac{3\,mol\,CuO}{2\,mol\,NH_3} \times \frac{79.55\,g\,CuO}{1\,mol\,CuO}$$

A. 127 g
B. 103 g
C. 72.2 g
D. 108 g
E. 56.5 g

127 g CuO needed
Only have 90.4 g so CuO limiting

$$90.4\,g\,CuO \times \frac{1\,mol\,CuO}{79.55\,g\,CuO} \times \frac{3\,mol\,Cu}{3\,mol\,CuO} \times \frac{63.546\,g\,Cu}{1\,mol\,Cu}$$

= 72.2 g Cu can be formed

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Your Turn!

If 8.51 g C_2H_5SH reacts with 22.4 g O_2, what is the maximum amount of sulfur dioxide that can form?

$$2C_2H_5SH(\ell) + 9O_2(g) \rightarrow 4CO_2(g) + 6H_2O(g) + 2SO_2(g)$$

(62.13) (32.00) (44.01) (18.02) (64.06)

A. 19.7 g

B. 4.38 g

C. 39.5 g

D. 9.97 g

E. 8.77 g

$$8.51\,\text{g}\,C_2H_5SH \times \frac{1\,\text{mol}\,C_2H_5SH}{62.13\,\text{g}\,C_2H_5SH} \times \frac{9\,\text{mol}\,O_2}{2\,\text{mol}\,C_2H_5SH} \times \frac{32.00\,\text{g}\,O_2}{1\,\text{mol}\,O_2}$$

19.7 g O_2 needed

Have 22.4 g so C_2H_5SH is limiting

$$8.51\,\text{g}\,C_2H_5SH \times \frac{1\,\text{mol}\,C_2H_5SH}{62.13\,\text{g}\,C_2H_5SH} \times \frac{2\,\text{mol}\,SO_2}{2\,\text{mol}\,C_2H_5SH} \times \frac{64.06\,\text{g}\,SO_2}{1\,\text{mol}\,SO_2}$$

= 8.77 g SO_2 can form

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Reaction Yield

- In many experiments, the amount of product is less than expected
- Losses occur for several reasons
  - Mechanical issues – sticks to glassware
  - Evaporation of volatile (low boiling) products.
  - Some solid remains in solution
  - Competing reactions and formation of by-products.
    - **Main reaction:**
      - $2\ P(s) + 3\ Cl_2(g) \rightarrow 2\ PCl_3(l)$
    - **Competing reaction:**
      - $PCl_3(l) + Cl_2(g) \rightarrow PCl_5(s)$ By-product

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Theoretical vs. Actual Yield

- **Theoretical Yield**
  - Amount of product that must be obtained if no losses occur
  - Amount of product formed if all of limiting reagent is consumed
- **Actual Yield**
  - Amount of product that is actually isolated at end of reaction
  - Amount obtained experimentally
  - How much is obtained in mass units or in moles

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Percentage Yield

Useful to calculate percentage yield

Percentage yield

- Relates the actual yield to the theoretical yield
- It is calculated as:

$$\text{percentage yield} = \left(\frac{\text{actual yield}}{\text{theoretical yield}}\right) \times 100\%$$

Example: If a cookie recipe predicts a yield of 36 cookies and yet only 24 are obtained, what is the percentage yield?

$$\text{percentage yield} = \left(\frac{24}{36}\right) \times 100\% = 67\%$$

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Ex. Percentage Yield Calculation

When 18.1 g NH_3 and 90.4 g CuO are reacted, the theoretical yield is 72.2 g Cu. The actual yield is 58.3 g Cu. What is the percent yield?

$$2NH_3(g) + 3CuO(s) \rightarrow N_2(g) + 3Cu(s) + 3H_2O(g)$$

$$\text{percentage yield} = \frac{58.3 \text{ g Cu}}{72.2 \text{ g Cu}} \times 100\% \quad \mathbf{= 80.7\%}$$

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Learning Check: Percentage Yield

A chemist set up a synthesis of solid phosphorus trichloride by mixing 12.0 g of solid phosphorus with 35.0 g chlorine gas and obtained 42.4 g of solid phosphorus trichloride. Calculate the percentage yield of this compound.

Analysis:

Write balanced equation

$$P(s) + Cl_2(g) \longrightarrow PCl_3(s)$$

Determine Limiting Reagent → Determine Theoretical Yield → Calculate Percentage Yield

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Learning Check: Percentage Yield

Assembling the Tools:

- 1 mol P = 30.97 g P
- 1 mol Cl_2 = 70.90 g Cl_2
- 3 mol Cl_2 ⇔ 2 mol P

Solution

1. Determine Limiting Reactant

$$12.0\ \text{g P} \times \frac{1\ \text{mol P}}{30.97\ \text{g P}} \times \frac{3\ \text{mol Cl}_2}{2\ \text{mol P}} \times \frac{70.90\ \text{g Cl}_2}{1\ \text{mol Cl}_2} = 41.2\ \text{g Cl}_2$$

- But you only have 35.0 g Cl_2, so Cl_2 is limiting reactant

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Learning Check: Percentage Yield

Solution

2. Determine Theoretical Yield

$$35.0\ \text{g Cl}_2 \times \frac{1\ \text{mol Cl}_2}{70.90\ \text{g Cl}_2} \times \frac{2\ \text{mol PCl}_3}{3\ \text{mol Cl}_2} \times \frac{137.32\ \text{g PCl}_3}{1\ \text{mol PCl}_3}$$

$= 45.2\ \text{g PCl}_3$

3. Determine Percentage Yield

- Actual yield = 42.4 g

$$\text{percentage yield} = \left(\frac{42.4\ \text{g PCl}_3}{45.2\ \text{g PCl}_3}\right) \times 100\%$$

= 93.8 %

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Your Turn!

When 6.40 g of CH_3OH was mixed with 10.2 g of O_2 and ignited, 6.12 g of CO_2 was obtained. What was the percentage yield of CO_2?

$$2CH_3OH + 3O_2 \longrightarrow 2CO_2 + 4H_2O$$

MM(g/mol) (32.04) (32.00) (44.01) (18.02)

A. 6.12%

B. 8.79%

C. 100%

D. 142%

E. 69.6%

$$6.40\ \text{g}\ CH_3OH \times \frac{1\ \text{mol}\ CH_3OH}{32.04\ \text{g}\ CH_3OH} \times \frac{3\ \text{mol}\ CO_2}{2\ \text{mol}\ CH_3OH} \times \frac{32.00\ \text{g}\ O_2}{1\ \text{mol}\ O_2}$$

= 9.59 g O_2 needed; CH_3OH limiting

$$6.40\ \text{g}\ CH_3OH \times \frac{1\ \text{mol}\ CH_3OH}{32.04\ \text{g}\ CH_3OH} \times \frac{2\ \text{mol}\ CO_2}{2\ \text{mol}\ CH_3OH} \times \frac{44.01\ \text{g}\ CO_2}{1\ \text{mol}\ CO_2}$$

= 8.79 g CO_2 in theory

$$\frac{6.12\ \text{g}\ CO_2\ \text{actual}}{8.79\ \text{g}\ CO_2\ \text{theory}} \times 100\ \% = 69.6\%$$

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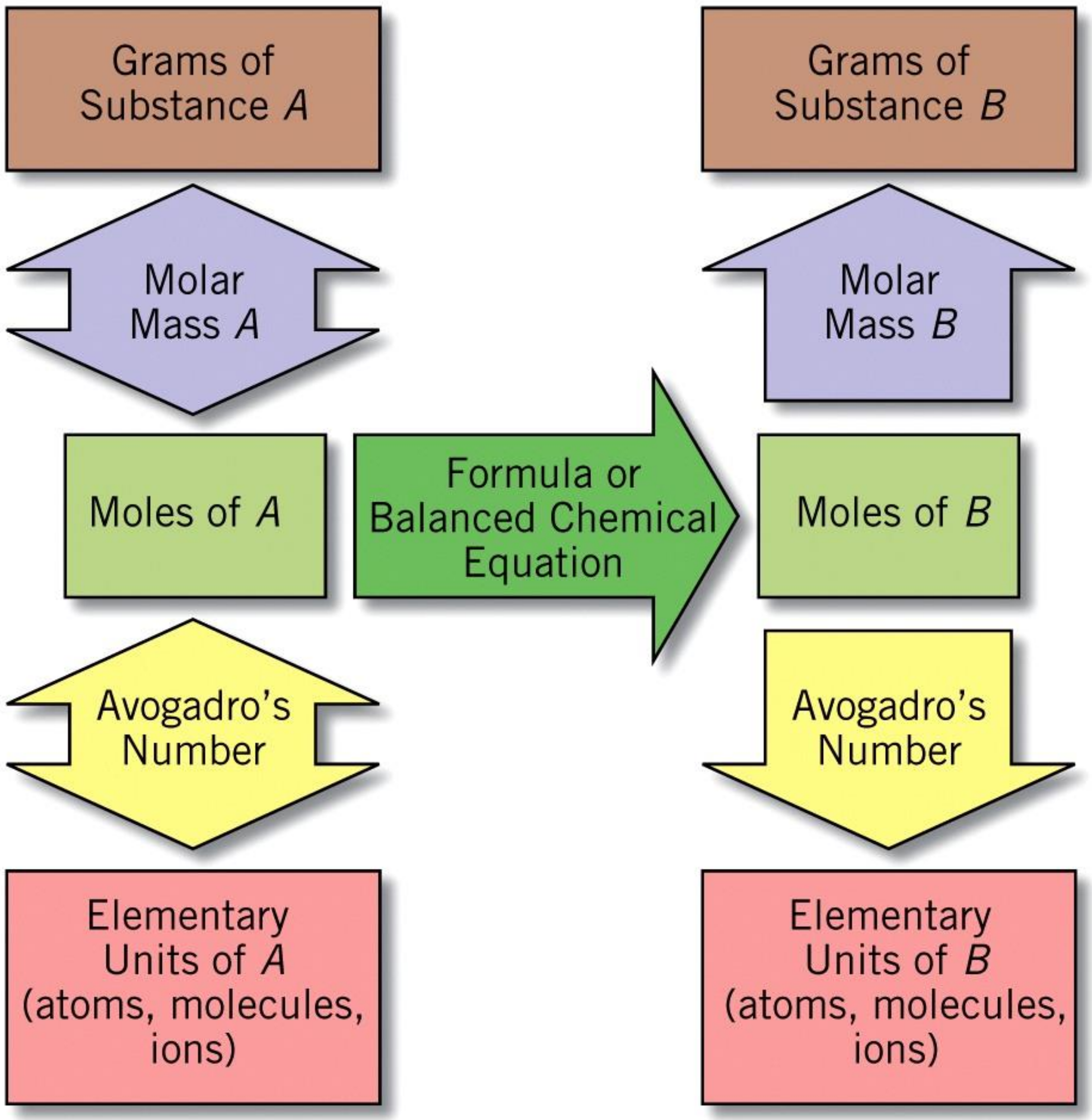
Stoichiometry Summary



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