CHEM 103
Stoichiometry

Lecture Notes
February 16, 2006
Prof. Sevian

1

Agenda

- A money analogy for moles
- Determining empirical formula from % composition of a compound
- The sandwich problem, the bicycle problem, and how they're related to chemical reactions
- Limiting reagent problems
- Combustion analysis

2

Announcements

- First exam is on Thursday, Feb 23.
- One-third of the class will be in an overflow room. I will announce who takes the exam where on Tuesday, and will also post on the course website.
- To be posted on the course website by Saturday:
  - Practice exam #1 (already there)
  - Answer key to practice exam #1
  - Study guide
- Bookstore says the ACS exam study guide (~$12) will be in by Friday.

3

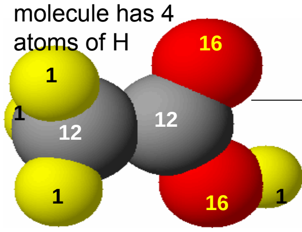
Moles like Money

Widget factory

Widget
save 12¢ per widget made

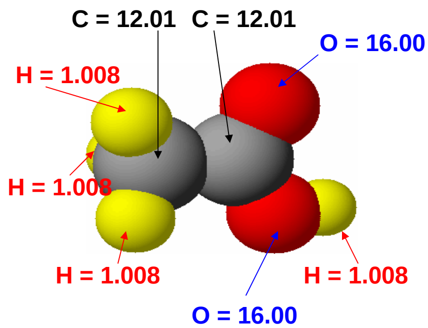
Factory makes 1,000,000 widgets per day. How much money do you save per day?

One acetic acid molecule has 4 atoms of H



One mole (6.022×10^{23} molecules) of acetic acid molecules. How many moles of H atoms are in it?

Scaling molecules to moles



Mass of one molecule of CH_3COOH is

60.05 amu

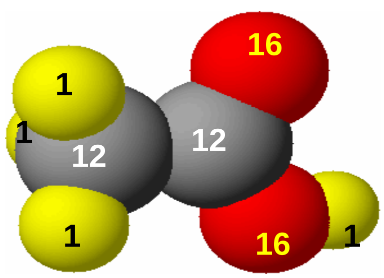
Mass of 1 mole of CH_3COOH molecules is

60.05 grams

Important note: Since there is always the same number of particles in a mole, when you determine the amu's of a unit, you are determining the mass in grams of a mole of that unit.

5

What does % composition mean?



Note: These are approximate atomic masses, for the purpose of demonstrating % composition. When actually calculating % composition, use the values from the Periodic Table.

<u>% Composition by Mass</u>

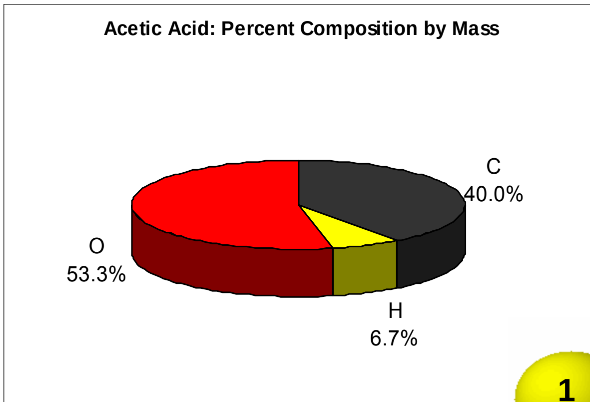
$$fraction\ \mathrm{C} = \frac{2 \times 12}{60} = 40.\%$$

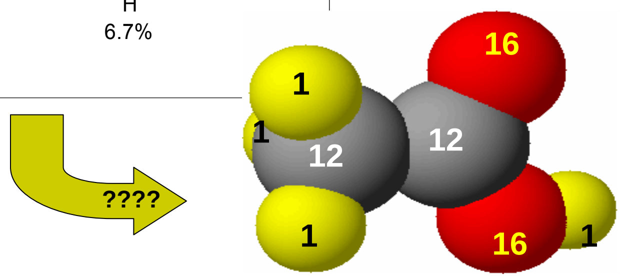
$$fraction\ \mathrm{H} = \frac{4 \times 1}{60} = 6.7\%$$

$$fraction\ \mathrm{O} = \frac{2 \times 16}{60} = 53\%$$

6

What does % composition mean?





Composition of a Compound

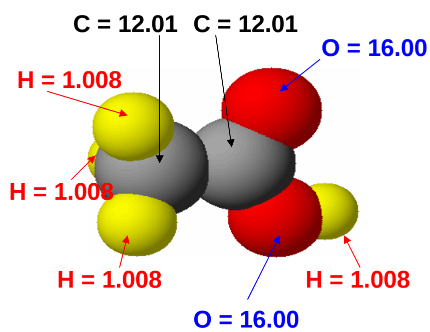
What is the composition by mass of acetic acid (CH_3COOH)?

$$\%C = \frac{24.02}{60.05} \times 100\% = 40.00\%$$

$$\%H = \frac{4.032g}{60.05g} \times 100\% = 6.714\%$$

$$\%O = \frac{32.00g}{60.05g} \times 100\% = 53.29\%$$

$$Check: 40.00 + 6.714 + 53.29 = 100.00\%$$



Recall from earlier:
Molar mass = 60.05 g/mol

8

Composition of a Hydrated Compound

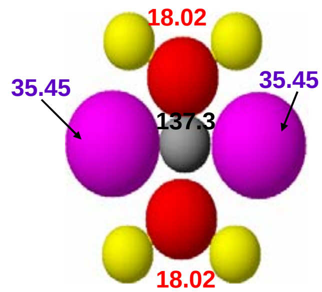
Heating barium chloride dihydrate ($BaCl_2{\bullet}2H_2O$) drives off the water, leaving the anhydrous compound ($BaCl_2$). The chemical reaction is

$$BaCl_2{\bullet}2H_2O\ (s) \rightarrow BaCl_2\ (s) + 2\ H_2O\ (g)$$

If you begin with a 10.0 g sample of the hydrated compound, what mass of water will be lost?

$$\%H_2O = \frac{2 \times 18.02}{244.2} \times 100\% = 7.379\%$$

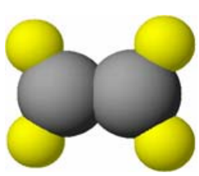
$$\begin{aligned}\text{mass of } H_2O \text{ in sample} &= 7.379\% \text{ of } 10.0\ g \\ &= 0.07379 \times 10.0g \\ &= 0.738g\end{aligned}$$



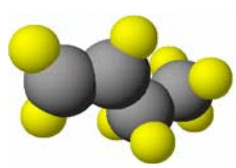
Formula weight = 244.2 g/mol

Chemical Compounds and Mass

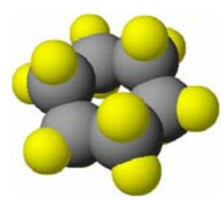
- Chemical formula to percent composition
  - Need to determine parts and whole
  - Use definition of percent
- Going the other direction
  - Percent composition alone is not enough information to determine molecular formula



C_2H_4



C_4H_8



C_6H_{12}

All three of these have 14.37% H and 85.63% C by mass

10

Empirical Formula

Lowest whole number ratio of elements in a chemical formula

Chemical formula	Empirical formula
C_2H_4	CH_2
C_4H_8	CH_2
C_6H_{12}	CH_2
$C_6H_{12}O_6$	
$Na_2C_2O_4$	
CH_3COOH	
H_2O_2	
H_2O	

11

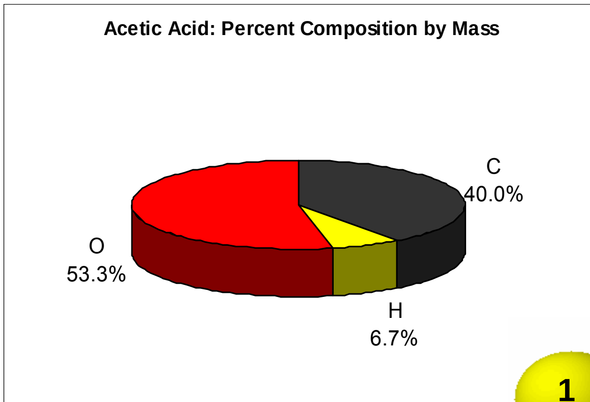
Chemical Compounds and Mass

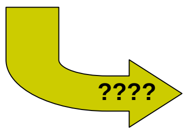
- Chemical formula to percent composition
  Ratio of moles → Percent by mass

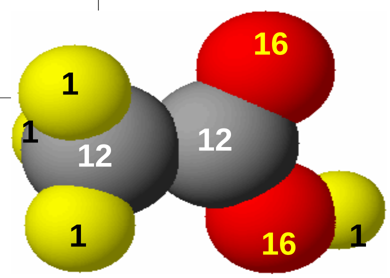
- Percent composition (or relative masses) to empirical formula
  Percent by mass → Ratio of moles

12

What does % composition mean?







% Composition to Empirical Formula

Analysis of a particular compound shows that it is composed of X% carbon, Y% hydrogen, and Z% oxygen.
What is the compound's empirical formula?

M A S S (*grams*) ⇒ M O L E S (*mol*)

$$\left.\begin{array}{l} \dfrac{\text{X } grams}{100\ grams}\text{ are carbon} \\[2ex] \dfrac{\text{Y } grams}{100\ grams}\text{ are hydrogen} \\[2ex] \dfrac{\text{Z } grams}{100\ grams}\text{ are oxygen} \end{array}\right\} \Rightarrow \left\langle \begin{array}{l} \text{specific whole number ratio of} \\ moles\ \text{C} : moles\ \text{H} : moles\ \text{O} \\ \text{is a : b : c} \\ \text{empirical formula is } \text{C}_a\text{H}_b\text{O}_c \end{array}\right.$$

14

M A S S (*grams*) ⇒ M O L E S (*mol*)

% Composition to Empirical Formula

Analysis of a particular compound shows that it is composed of 73.14% carbon, 7.37% hydrogen, and the remainder is oxygen. What is the compound's empirical formula?

$$\left.\begin{aligned} \frac{73.14\ g\ \mathrm{C}}{} \times \frac{1\ mol\ \mathrm{C}}{12.01\ g} &= 6.089\ mol\ \mathrm{C} \\ \frac{7.37\ g\ \mathrm{H}}{} \times \frac{1\ mol\ \mathrm{H}}{1.008\ g} &= 7.31\ mol\ \mathrm{H} \\ \frac{19.49\ g\ \mathrm{O}}{} \times \frac{1\ mol\ \mathrm{O}}{16.00\ g} &= 1.218\ mol\ \mathrm{O} \end{aligned}\right\} \Rightarrow \left\langle \begin{aligned} &\text{specific whole number ratio of} \\ &moles\ \mathrm{C} : moles\ \mathrm{H} : moles\ \mathrm{O} \\ &\text{is } 6.089 : 7.31 : 1.218 \\ &= \frac{6.089}{6.089} : \frac{7.31}{6.089} : \frac{1.218}{6.089} \\ &= 1 : 1.200 : 0.2000 \\ &= 1\times 5 : 1.200\times 5 : 0.2000\times 5 \\ &= 5 : 6 : 1 \\ &\text{so, empirical formula is } C_5H_6O_1 \end{aligned}\right.$$

Variations on Determining Empirical Formula

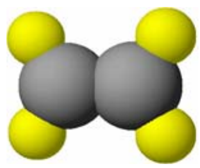
- Start with % composition of elements in a compound
- Start with masses of elements in a compound
- Start with % or masses of parts of a hydrated compound (*e.g.*, determine *n* in $CuSO_4 \cdot nH_2O$, given mass of $CuSO_4$ and mass of H_2O lost when compound is heated)

How to get to Molecular Formula

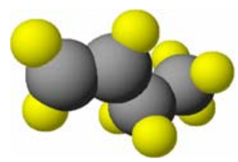
- A hydrocarbon has 85.63% carbon by mass. What is its empirical formula?

CH_2

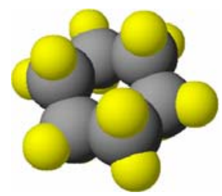
- What else do you need to know to determine molecular formula?



C_2H_4



C_4H_8

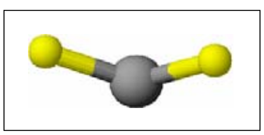


C_6H_{12}

(All three have 14.37% H and 85.63% C by mass)

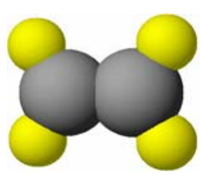
17

How many empirical formulas?

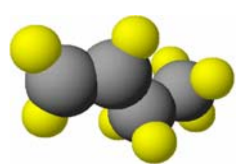


Empirical Unit CH_2

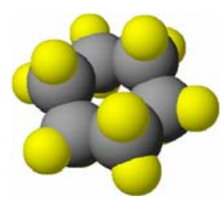
Mass is 12.01 + 2(1.008) = 14.03 g/mol



C_2H_4



C_4H_8



C_6H_{12}

$2 \times (CH_2)$	**$4 \times (CH_2)$**	**$6 \times (CH_2)$**
$= 2 \times (14.03)$	**$= 4 \times (14.03)$**	**$= 6 \times (14.03)$**
= **28.06 g/mol**	= **56.12 g/mol**	= **84.18 g/mol**

18

Chemical Equations

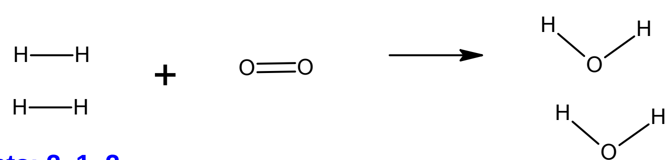
- Represent a chemical change of matter
- Reactants (starting materials) on left
- Products (ending materials) on right

Reactants → Products

- What goes in must come out, just connected (bonded) differently

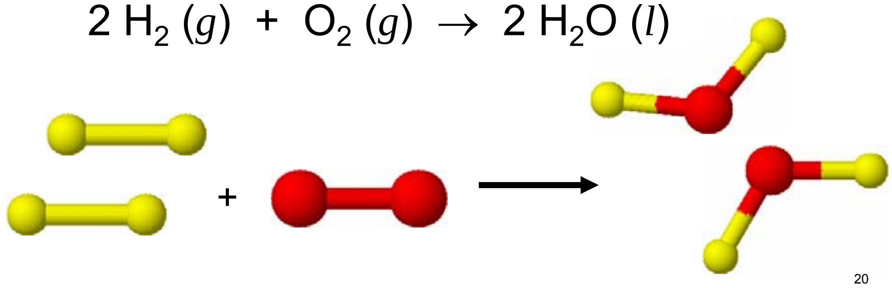
19

Formation of Water



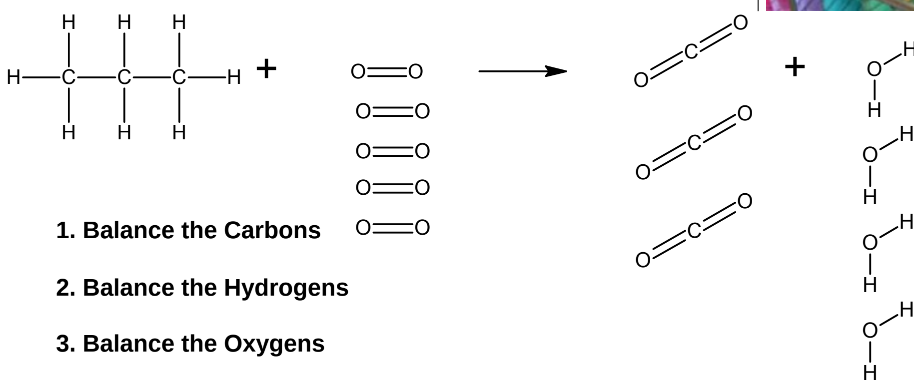
Coefficients: 2, 1, 2

$$2\ H_2\ (g)\ +\ O_2\ (g)\ \rightarrow\ 2\ H_2O\ (l)$$



20

Combustion of propane



1. Balance the Carbons

2. Balance the Hydrogens

3. Balance the Oxygens

4. Is it balanced?

Balanced chemical equation:

$C_3H_8 + 5\ O_2 \rightarrow 3\ CO_2 + 4\ H_2O$

21

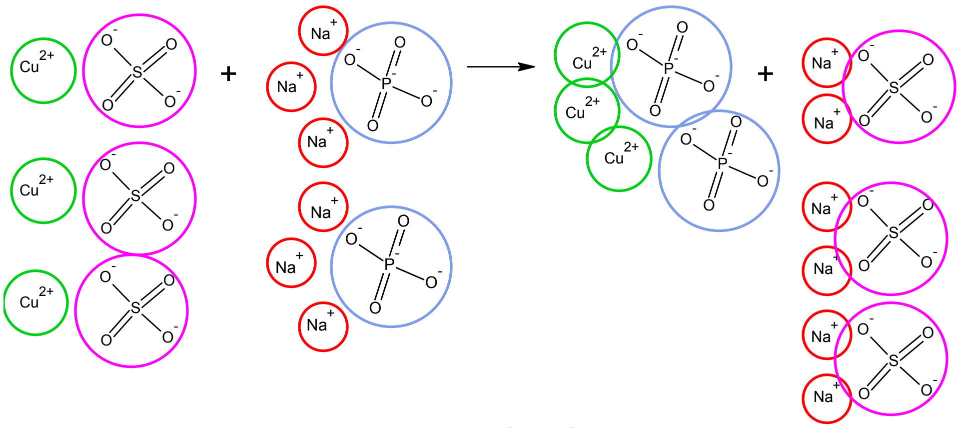
Combustion Reactions

- Flame-producing reaction of a chemical with oxygen to produce oxides
  - $4\ Fe\ (s) + 3\ O_2\ (g) \rightarrow 2\ Fe_2O_3\ (s)$
  - $2\ Mg\ (s) + O_2\ (g) \rightarrow 2\ MgO\ (s)$
- Hydrocarbons (C and H) burn to produce CO_2 and H_2O (the oxides of C and H), if enough oxygen is present
  - $CH_4\ (g) + 2\ O_2\ (g) \rightarrow CO_2\ (g) + 2\ H_2O\ (l)$
  - $2\ C_2H_6\ (g) + 7\ O_2\ (g) \rightarrow 4\ CO_2\ (g) + 6\ H_2O\ (l)$
- Organic compounds (containing C, H, N and O) burn to produce CO_2, H_2O and N_2, if enough oxygen is present
  - $2\ C_8H_{14}N_4O_2\ (s) + 21\ O_2\ (g) \rightarrow 16\ CO_2\ (g) + 14\ H_2O\ (l) + 4\ N_2\ (g)$

22

When the balancing units are ions, not atoms

$CuSO_4$ + Na_3PO_4 → $Cu_3(PO_4)_2$ + Na_2SO_4



3 $CuSO_4$ + 2 Na_3PO_4 → $Cu_3(PO_4)_2$ + 3 Na_2SO_4

Stoichiometry

- "Counting atoms"
- Quantitative part of chemistry
- Foundation is conservation of matter
- Must use balanced chemical equations
- Reaction coefficients (also called stoichiometric coefficients) tell you how many units of a chemical are required, compared to units of other chemicals in the reaction
- We can't measure units in the laboratory (we measure mass, volume, *etc.*)

An Example from Real Life

Chocolate chip cookie recipe calls for:

- 3 eggs
- 1 cup brown sugar
- 2 cups flour
- Some other stuff

Produces: 64 cookies

What if you want to make 48 cookies?

But in the laboratory you cannot count atoms or molecules or ionic units…

25

Simple Stoichiometry

What mass of carbon dioxide gas is produced when 227 grams of propane (C_3H_8) combust completely?

Balanced chemical equation:

$$C_3H_8 + 5\,O_2 \rightarrow 3\,CO_2 + 4\,H_2O$$

1 mol C_3H_8 for every 3 mol CO_2

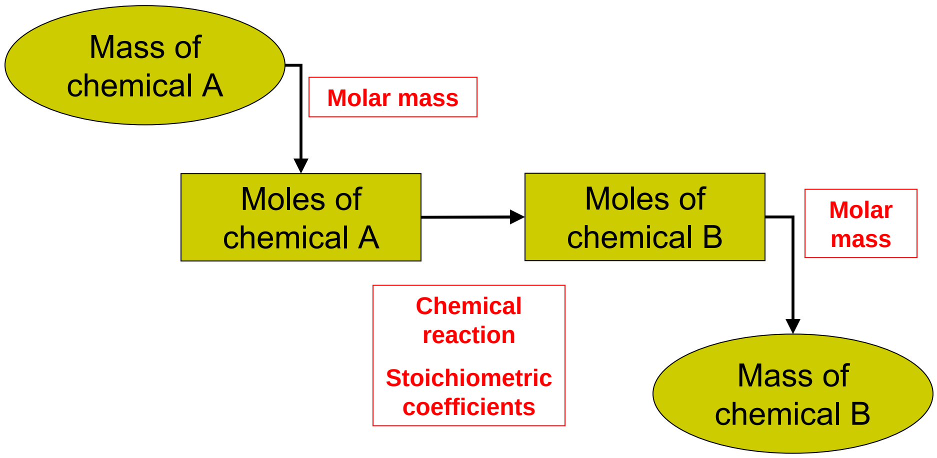
Start | End

227 g C_3H_8	1 mol C_3H_8	3 mol CO_2	44.01 g CO_2	=	~~679.76 g CO_2~~
	44.09 g C_3H_8	1 mol C_3H_8	1 mol CO_2		

680. g CO_2

26

General Strategy for Simple Stoichiometry Problems



27

Types of Stoichiometry Problems

- Simple stoichiometry: Mass of one chemical (reactant or product) is specified. Find out mass of another chemical required or produced in the reaction (assuming just enough of each reactant is present). Must use a balanced chemical equation.
- Chemical analysis: Known and unknown chemicals or quantities given. Figure out unknown chemicals or quantities.
- Limiting reagent: Masses of two different reactants are specified. One of the reactants limits the reaction (it gets used up first). Figure out the maximum mass of a product that could be formed if all of the limiting reactant is used up. Must use a balanced chemical equation.

28

A Simple Stoichiometry Problem

If solutions containing calcium chloride and silver nitrate are combined, white silver chloride crystals precipitate out of the mixture, and the remaining solution contains calcium nitrate.

(a) Write the balanced chemical equation for this reaction.

(b) If 0.252 g of calcium chloride were present in the original calcium chloride solution, how many grams of silver chloride should be formed (assuming there is enough silver nitrate)?

29

Writing the Chemical Equation

If solutions containing calcium chloride and silver nitrate are combined, white silver chloride crystals precipitate out of the mixture, and the remaining solution contains calcium nitrate.

(a) Write the balanced chemical equation for this reaction.

Reactants → **Products**

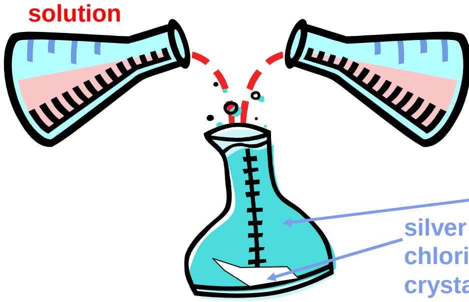
30

Writing the Chemical Equation

If solutions containing calcium chloride and silver nitrate are combined, white silver chloride crystals precipitate out of the mixture, and the remaining solution contains calcium nitrate.

(a) **Write the balanced chemical equation for this reaction.**

Reactants → Products



31

UMass Boston, Chem 103, Spring 2006

Writing the Chemical Equation

If solutions containing calcium chloride and silver nitrate are combined, white silver chloride crystals precipitate out of the mixture, and the remaining solution contains calcium nitrate.

(a) **Write the balanced chemical equation for this reaction.**

Reactants → Products

calcium chloride solution + silver nitrate solution ⟶ silver chloride crystals + calcium nitrate solution

$$CaCl_2\,(aq) + AgNO_3\,(aq) \longrightarrow AgCl\,(s) + Ca(NO_3)_2\,(aq)$$

32

Balancing the Chemical Equation

(a) Write the balanced chemical equation for this reaction.

What are the units that remain constant on both sides of the arrow? That is, what goes in and comes out unchanged?

$$CaCl_2 + 2\,AgNO_3 \longrightarrow 2\,AgCl + Ca(NO_3)_2$$

33

The Stoichiometry Part

(b) If 0.252 g of calcium chloride were present in the original calcium chloride solution, how many grams of silver chloride should be formed?

$$CaCl_2 + 2\,AgNO_3 \longrightarrow 2\,AgCl + Ca(NO_3)_2$$

1 mol $CaCl_2$ for every 2 mol AgCl

Start | End

0.252 g $CaCl_2$	1 mol $CaCl_2$	2 mol AgCl	143.4 g AgCl	=	0.651 g AgCl
	110.98 g $CaCl_2$	1 mol $CaCl_2$	1 mol AgCl		

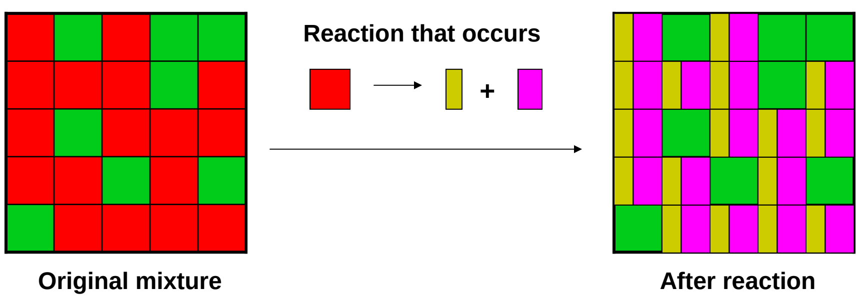
34

Quantitative Analysis

- Determine the composition of a mixture
  - React one substance in the mixture according to a known reaction.
  - Measure results of reaction.
  - Use stoichiometry to determine how much of original substance was present.
- Determine the empirical formula of an unknown chemical
  - React the substance and measure amounts of different chemical products.
  - Use stoichiometry to determine moles of elements present in original sample.
  - Find empirical formula from ratio of moles.

35

Composition of a Mixture



- Products of the reaction must be known
- If you can measure the mass of one of the products, then you can use stoichiometry to determine how much of the original reactant was present
- Examples: product is a gas or precipitate

Example: Gravimetric Analysis

A mixture of unknown percentage composition of white $BaCl_2 \bullet 2H_2O$ crystals and white $Na_2SO_4 \bullet 10H_2O$ crystals is provided. How could you determine the percent composition of the mixture?

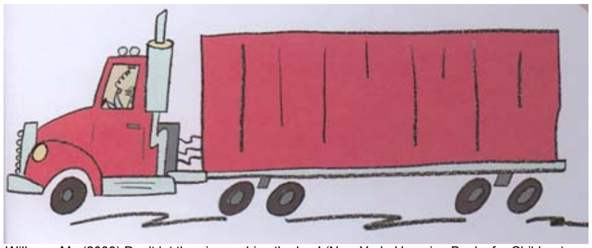
1. How could you get a reaction to occur?
2. What reaction would occur?
3. What would you need to measure?
4. How would you measure it?
5. What information could you calculate by knowing that?
6. What additional information might you need?

37

Limiting Reactants

- If you use an excess of one reactant, it is more likely that all of the other reactant will be used up in the chemical reaction.
- The reactant that is in excess will be present in the final products, since it didn't all get used up.

38



Willems, Mo (2003) Don't let the pigeon drive the bus! (New York: Hyperion Books for Children).

An analogy to illustrate limiting reactants

To build a semi tractor-trailer requires:

18 wheels + 5 axles + 4 cylinders + 1 pigeon → 1 semi

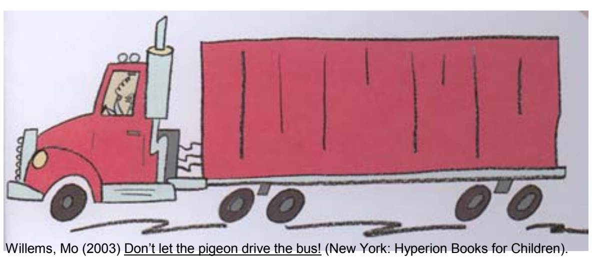
Let's say you have in stock:

- 198 wheels × **(1 semi)/(18 wheels) = 11 semis possible**
- 100 axles × **(1 semi)/(5 axles) = 20 semis possible**
- 100 cylinders × **(1 semi)/(4 cylinders) = 25 semis possible**
- 18 pigeons × **(1 semi)/(1 pigeon) = 18 semis possible**

Maximum quantity of semis you could produce is 11

How many semis could you produce?

LIMITING REACTANT



Willems, Mo (2003) Don't let the pigeon drive the bus! (New York: Hyperion Books for Children).

An analogy to illustrate limiting reactants

18 wheels + 5 axles + 4 cylinders + 1 pigeon → 1 semi

After you build 11 semis, what remains of the 198 wheels, 100 axles, 100 cylinders, and 18 pigeons?

	18 wheels	5 axles	4 cylinders	1 pigeon	→	1 semi
Initial	198	100	100	18		0
Change	-198	-(11×5)	-(11×4)	-(11×1)		+11
Final	0	45	56	7		11

What was actually in the barium chloride + sodium sulfate mixture

$BaCl_2\ (aq)\ +\ Na_2SO_4\ (aq)\ \rightarrow\ 2\ NaCl\ (aq)\ +\ BaSO_4\ (s)$

$$5.00g\ \mathrm{BaCl_2 \bullet 2H_2O} \times \frac{1\,mol\ \mathrm{BaCl_2 \bullet 2H_2O}}{244.2g\ \mathrm{BaCl_2 \bullet 2H_2O}} \times \frac{1\,mol\ \mathrm{BaCl_2}}{1\,mol\ \mathrm{BaCl_2 \bullet 2H_2O}} = 0.0205\,mol\ \mathrm{BaCl_2}$$

$$5.00g\ \mathrm{Na_2SO_4 \bullet 10H_2O} \times \frac{1\,mol\ \mathrm{Na_2SO_4 \bullet 10H_2O}}{322.3g\ \mathrm{Na_2SO_4 \bullet 10H_2O}} \times \frac{1\,mol\ \mathrm{Na_2SO_4}}{1\,mol\ \mathrm{Na_2SO_4 \bullet 10H_2O}} = 0.0155\,mol\ \mathrm{Na_2SO_4}$$

moles	**$BaCl_2$**	**Na_2SO_4**	$\rightarrow$	**2 NaCl**	**$BaSO_4$**
Initial	**0.0205**	**0.0155**		**0**	**0**
Change	**-0.0155**	**-0.0155**		**+2(0.0155)**	**+0.0155**
Final	**0.0050**	**0**		**0.0310**	**0.0155**

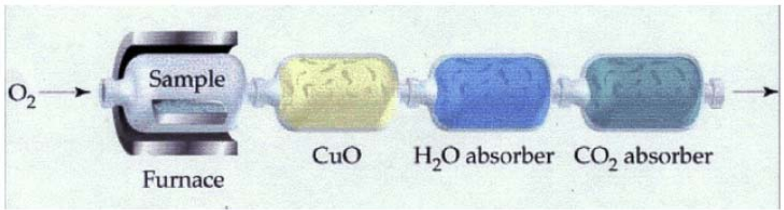
41

Chemical Analysis

1. Unknown quantity of a known substance
   - Two known chemicals react to exactly the point of completion
   - Quantity of one of them is known
   - Determine quantity that must have been present of the other one
   - Example: titration
2. Known quantity of an unknown substance
   - A specific amount of an unknown substance reacts
   - Known products are formed, and their quantities are measured
   - Determine empirical formula of the unknown reactant from this information
   - Examples: gravimetric analysis, combustion analysis

42

Combustion Analysis



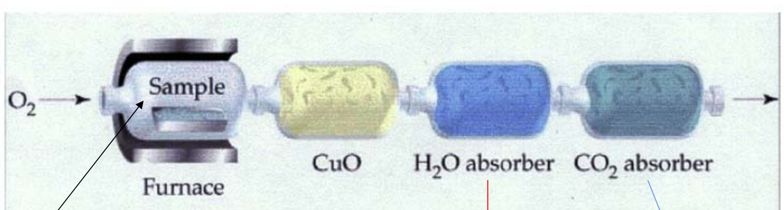
Unbalanced reaction is

Sample (containing C, H, and O) + O_2 → H_2O + CO_2

- **Excess O_2 used, so that all of the sample reacts**
- **CuO ensures that any carbon monoxide converts to carbon dioxide**
- **Water absorber is usually $Mg(ClO_4)_2$**
- **Carbon dioxide is usually collected by sodium hydroxide on asbestos**

Picture from http://itl.chem.ufl.edu/2045_s00/lectures/lec_4.html

Combustion Analysis



Known mass of sample reacts

Mass of H_2O is measured

Mass of CO_2 is measured

Mass of H_2O → Moles of H_2O → Moles of H atoms present in original sample

Mass of CO_2 → Moles of CO_2 → Moles of C atoms present in original sample

(Mass of original sample) – (Mass of H atoms + Mass of C atoms)

= Mass of O atoms, if present in original sample

→ Moles of O atoms present in original sample

Combustion Analysis Example

The combustion of 0.5320 g butane (in a lighter) produces 1.6114 g of carbon dioxide and 0.8247 g of water.

(a) What is the empirical formula for butane?

(b) A different analytical procedure indicated that 9.153×10^{-3} moles of butane were present in the original sample of butane. What is the molecular formula for butane?

Chemical reaction is

butane + $O_2 \rightarrow CO_2 + H_2O$

45

Combustion Analysis Example

The combustion of 0.5320 g butane (in a lighter) produces 1.6114 g of carbon dioxide and 0.8247 g of water.

(a) What is the empirical formula for butane?

Strategy:

- **Empirical formula means ratio of moles**
- **Need to know moles of C, moles of H (and possibly moles of O)**
- **Get moles of C from mass of CO_2**
- **Get moles of H from mass of H_2O**
- **Get moles of O (if any) by determining if C and H account for entire mass of butane**
- **Determine empirical formula of butane from ratio of moles C:H(:O)**

46

Combustion Analysis Example

The combustion of 0.5320 g butane (in a lighter) produces 1.6114 g of carbon dioxide and 0.8247 g of water.

(a) What is the empirical formula for butane?

Start → End

1.6114 g CO_2	**1 mol CO_2**	**1 mol C**	=	**0.036614 mol C**
	44.011 g CO_2	**1 mol CO_2**		

Start → End

0.8247 g H_2O	**1 mol H_2O**	**2 mol H**	=	**0.09153 mol H**
	18.02 g H_2O	**1 mol H_2O**		

47

Combustion Analysis Example

The combustion of 0.5320 g butane (in a lighter) produces 0.4028 g of carbon dioxide and 0.8243 g of water.

(a) What is the empirical formula for butane?

Is there any O in butane?

0.036614 mol C	**12.011 g C**	=	**0.43973 g C**
	1 mol C		
0.09153 mol H	**1.008 g H**	=	**0.09226 g H**
	1 mol H		

Sum is 0.5320 g

48

Combustion Analysis Example

The combustion of 0.5320 g butane (in a lighter) produces 0.4028 g of carbon dioxide and 0.8243 g of water.

(a) What is the empirical formula for butane?

Ratio of Moles C : Moles H

$$\frac{0.036614 \text{ mol C}}{0.036614} : \frac{0.09153 \text{ mol H}}{0.036614} = 1 : 2.5 = 2 : 5$$

Empirical formula is C_2H_5

49

Combustion Analysis Example

The combustion of 0.5320 g butane (in a lighter) produces 1.6114 g of carbon dioxide and 0.8247 g of water.

(b) A different analytical procedure indicated that 9.153×10^{-3} moles of butane were present in the original sample of butane. What is the molecular formula for butane?

Strategy:

- **Start with empirical formula from part (a)**
- **Use mass and moles to calculate molar mass of butane**
- **Find out how many empirical units are in butane**
- **Molecular formula of butane is same factor $\times$ empirical formula**

50

Combustion Analysis Example

The combustion of 0.5320 g butane (in a lighter) produces 1.6114 g of carbon dioxide and 0.8247 g of water.

(b) A different analytical procedure indicated that 9.153×10^{-3} moles of butane were present in the original sample of butane. What is the molecular formula for butane?

Molar mass is measured in g/mol

$$\text{Molar mass of butane} = \frac{0.5320 \text{ g butane}}{9.153 \times 10^{-3} \text{ moles of butane}} = 58.12 \text{ g/mol}$$

51

Combustion Analysis Example

The combustion of 0.5320 g butane (in a lighter) produces 1.6114 g of carbon dioxide and 0.8247 g of water.

(b) A different analytical procedure indicated that 9.153×10^{-3} moles of butane were present in the original sample of butane. What is the molecular formula for butane?

	Empirical	Molecular
Formula	C_2H_5	C_4H_{10}
Molar mass	**29.06 g/mol**	**58.12 g/mol**

×2

×2

52