PHYSICAL SCIENCE 20 (PRE-AP CHEMISTRY)

UNIT THREE

STOICHIOMETRY: CALCULATIONS WITH CHEMICAL FORMULAS

I CAN…

- **Balance equations** using an understanding of the law of conservation of mass.
- **Write** (and balance) **equations**, based on descriptions.
- **Classify reactions** as combustion, decomposition or synthesis.
- **Calculate formula weights** of elements, molecules or compounds.

I CAN…

- **Convert** between number of particles, mass or moles using conversion factors.
- **Determine the empirical formula** of a given compound.
- **Use stoichiometry** to determine mass of products, and required number of moles for a given reaction.

STOICHIOMETRY

- Chemical reactions are taking place around us all the time.
- Some are easy to see because of indicators like color change while others are happening inside us all the time without our knowledge.
- **Stoichiometry is the study of** chemical reactions, specifically how the **quantity of substances** are consumed or produced in relation to each other.

CHEMICAL EQUATIONS

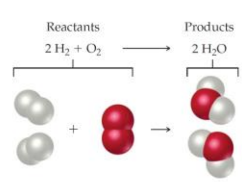
- We represent chemical reactions using a chemical equation.

$$CH_4 + O_2 \rightarrow CO_2 + 2H_2O$$

- We read the sign **+ as reacts** with, and the **→ as produces**.
- The substances on the left hand side of the → are considered to be **reactants**, while the **products** are shown on the right.

BALANCING CHEMICAL REACTIONS

- Atoms are neither created nor destroyed, this means the number of atoms on the reactant side must equal the number of atoms on the product side.
- To do balance reactions, **count the number of atoms and change by altering the coefficient** at the front.

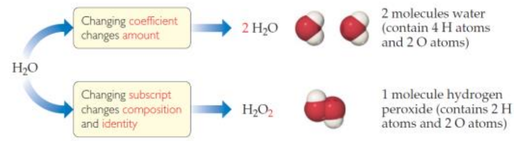


EXAMPLE: COUNTING ATOMS

- How many atoms of Mg, O and H are represented in the chemical formula 3 $Mg(OH)_2$?
- How many atoms of Al, C, H, and O are in the compound $Al(CH_3COO)_3$?

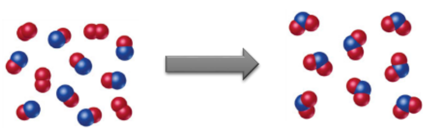
BALANCING EQUATIONS

- Once the reactants and products are known we can write an **unbalanced chemical reaction.**
- Changing the coefficient IS NOT THE SAME as changing a subscript. You can **ONLY change the coefficient**.



EXAMPLE: INTERPRETING CHEMICAL EQUATIONS

- The following diagram represents a chemical reaction in which the blue spheres are nitrogen, while the red are oxygen. (a) write the chemical formula for the reactants and products, (b) write a balanced chemical reaction, (c) is this diagram consistent with the law of conservation of mass?



INDICATING THE STATES

- Symbols indicating the physical state of the reactants and products are often shown.
- We use (g), (l), (s), and (aq) for gas, liquid, solid and aqueous (water) solution respectively.

$$CH_4(g) + O_2(g) \rightarrow CO_2(g) + 2H_2O(g)$$

- For reactions that involve the addition of heat, the symbol Delta (Δ) is used over the $\rightarrow$ symbol.

EXAMPLE: BALANCING

- **Balance the following equations:**
  - $Na(s) + \quad H_2O(l) \rightarrow \quad NaOH(aq) + \quad H_2(g)$
  - $Fe(s) + \quad O_2(g) \rightarrow \quad Fe_2O_3(s)$
  - $C_2H_2(g) + \quad O_2(g) \rightarrow \quad CO_2(g) + \quad H_2O(g)$
  - $Al(s) + \quad HCl(aq) \rightarrow \quad AlCl_3(aq) + \quad H_2(g)$

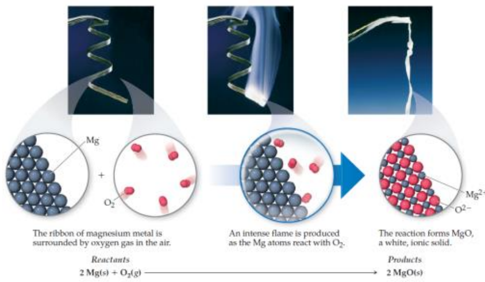
PATTERNS OF CHEMICAL REACTIVITY

- There are three* basic types of reactions to be covered in this unit: **combination** (synthesis), **decomposition** and **combustion**.
- Knowing patterns with reactivity allows us to **predict the products** of a reaction with knowing only the reactants.

COMBINATION & DECOMPOSITION

- In combination reactions, **two or more reactants combine** to create a **single product**.

  $Mg(s) + O_2(g) \rightarrow 2MgO(s)$
- When magnesium reacts with oxygen, it loses electrons and forms Mg^{2+} while oxygen gains electrons to form O^{2-}. They 'bond' and form the compound MgO.
- All combination reactions follow the form A + B → C



DECOMPOSITION

- In a **decomposition reaction**, a single reactants breaks down into two or more other substances.

  $CaCO_3(s) \xrightarrow{\Delta} CaO(s) + CO_2(g)$
  - **Carbonates** (XCO_3) will break down into an oxide (XO) and carbon dioxide (CO_2)
  - **Chlorates** ($XClO_3$) will break down into a binary compound (XCl) and oxygen gas.
  - **Metal hydroxides** (MOH) will break down to an oxide (MO) and water.

EXAMPLE: PREDICTING PRODUCTS

- Write the balanced chemical equations for the following chemical descriptions:
  - the reaction between lithium metal and fluorine gas
  - a reaction that occurs when solid barium carbonate is heated.

COMBUSTION REACTIONS

- Combustion reactions are rapid reactions that involve a flame.
- Often the result of hydrocarbons (C_xH_y) burning in the presence of oxygen (O_2)
- All hydrocarbons produce CO_2 and H_2O.

  $C_xH_y(g) + O_2(g) \rightarrow CO_2(g) + H_2O(g)$

EXAMPLE: COMBUSTION

- Predict the products of the following reactions:
  - Ethane combusts when ignited in the presence of oxygen gas.
  - Propanol (an alcohol substituted propane) undergoes combustion when ignited in the presence of oxygen.

EXAMPLE: CLASSIFICATION

- A piece of silver will react chemically with oxygen when it is heated
- Liquid octane (C_8H_{18}) is burned completely in oxygen gas
- Chlorine gas is bubbled through a solution of sodium bromide
- Rubidium carbonate decomposes when heated above 100 C.
- Solid magnesium hydroxide breaks down when subjected to UV light
- Crystalline bismuth(III) oxide decomposes with heat
- Heptane is a flammable hydrocarbon above 30C.
- Crystalline aluminium chlorate is heated until it decomposes

EXAMPLE: PREDICTING

- Solid silver will react chemically with oxygen when it is heated
- Chlorine gas is bubbled through a solution of sodium bromide
- Solid magnesium hydroxide breaks down when put in UV light
- Heptane is a flammable hydrocarbon above 30C.

THE MOLE CONCEPT

THE MATHY PART BEGINS

FORMULA WEIGHTS

- Chemical formulas and chemical equations have a quantitative aspect, that is, they represent precise quantities.
- Similarly, the coefficients in a balanced chemical equation represent a quantity of reactants and products.
- How, if atoms are so small, can we perform a reaction with the correct number of atoms?

FORMULA AND MOLECULAR WEIGHT

- The formula weight of a substance is the sum of atomic weights of the atoms in the chemical formula of the substance.
- For example, the **formula weight of sulfuric acid** (H_2SO_4) is **98.1 amu:**

FW of H2SO4 = 2(AW of H) + (AW of S) + 4(AW of O)

= 2(1.0amu) + 32.1 amu + 4(16.0 amu)

= 98.1 amu

MOLECULAR WEIGHT

- If the chemical formula is that of an element, it is simply the value from the PT.
- If the chemical formula is a molecule it is called the molecular weight (it is calculated the same way).
  - What is the **MW of glucose?** ($C_6H_{12}O_6$)

EXAMPLE: FORMULA WEIGHTS

- Calculate the formula weight of:
  - Sucrose ($C_{12}H_{22}O_{11}$) [table sugar]
  - Calcium nitrate, $Ca(NO_3)_2$
  - Ruthenium(III) dihydrogen phosphate

PERCENTAGE COMPOSITION

- Chemists must sometimes calculate the percentage composition of a compound – how much **each element contributes to the mass** of the entire compound.
  - This test can be useful to determine if a white powder is sugar, salt or cocaine.

$$\%\ composition = \frac{(number\ of\ atoms\ of\ element)(atomic\ weight\ of\ element)}{formula\ weight\ of\ substance} \times 100\%$$

EXAMPLE: PERCENTAGE COMPOSITION

- Calculate the percentage of carbon, hydrogen and oxygen (by mass) in sucrose ($C_{12}H_{22}O_{11}$).

EXAMPLE: PERCENTAGE COMPOSITION

- Calculate the percentage of nitrogen, by mass, in calcium nitrate.

AVOGADRO'S NUMBER

6.02×10^{23}

How big is it?

THE MOLE

- When we buy eggs, we buy a dozen (12).
- When we buy shoes, they come in a pair (2).
- When we count atoms we use a mole which is based on 12 g of isotopically pure carbon-12. This number is precisely 6.0221421×10^{23}.
- We call this number (rounded to 6.02×10^{23}) Avogadro's number (N_A) in honor of the scientist (Amedeo Avogadro) who discovered it.

THE MOLE

- This number, sometimes written as 6.02×10^{23} mol^{-1} reminds us that any collection of objects that is 6.02×10^{23} is considered to be a mole.

$$1 \text{ mol } ^{12}\text{C atoms} = 6.02 \times 10^{23}\ ^{12}\text{C atoms}$$
$$1 \text{ mol } H_2O \text{ molecules} = 6.02 \times 10^{23}\ H_2O \text{ molecules}$$
$$1 \text{ mol } NO_3^- \text{ ions} = 6.02 \times 10^{23}\ NO_3^- \text{ ions}$$

EXAMPLE: THE MOLE

- Without using a calculator, arrange these samples in order of increasing carbon atoms:

a. 12g ^{12}C

b. 1.5 mol. of C_2H_2

c. 9×10^{23} molecules of CO_2

EXAMPLE: THE MOLE

- Calculate the number of H atoms in 0.350 mol of $C_6H_{12}O_6$.
- Determine the number of oxygen atoms in 0.125 mol of calcium nitrite

MOLAR MASS

- A dozen is the same number, 12, whether we have a dozen eggs or a dozen elephants.
- While the **number of atoms in a mole is the same, the mass is not.**
- Remember that one atom of carbon-12 is 12 amu, while one atom of magnesium-24 is 24 amu.
- Because one mole always contains the same number of atoms, this means that one mole of magnesium must weigh twice as much – 24g.

THE MOLE

- The **atomic weight of an element is atomic mass units is numerically equal** to the mass in grams of 1 mol of that element.
- Chlorine has an atomic weight of 35.5 amu → 1 mol of Cl has a mass of 35.5 g.
- Au has an atomic mass of 197 amu → 1 mol of Au has a mass of 197 g.
- **For other kinds of substances** (formula weight, molecular weight) the **relationship is the same.**

EXAMPLE: MOLAR MASS

- Determine the molar mass of the following:
  - A molecular of oxygen gas
  - The formula unit of sodium chloride
  - An ion of nitrate

DISCUSSION

A. Which has more mass, a mole of water (H_2O) or a mole of glucose ($C_6H_{12}O_6$)?

B. Which contains more molecules, a mole of water or a mole of glucose?

MOLE RELATIONSHIPS

TABLE 3.2 • Mole Relationships

Name of Substance	Formula	Formula Weight (amu)	Molar Mass (g/mol)	Number and Kind of Particles in One Mole
Atomic nitrogen	N	14.0	14.0	6.02×10^{23} N atoms
Molecular nitrogen	N_2	28.0	28.0	6.02×10^{23} N_2 molecules $2(6.02 \times 10^{23})$ N atoms
Silver	Ag	107.9	107.9	6.02×10^{23} Ag atoms
Silver ions	Ag^+	107.9*	107.9	6.02×10^{23} Ag^+ ions
Barium chloride	$BaCl_2$	208.2	208.2	6.02×10^{23} $BaCl_2$ formula units 6.02×10^{23} Ba^{2+} ions $2(6.02 \times 10^{23})$ Cl^- ions

EXAMPLE: MOLAR MASS

- Determine the molar mass of the following:

a. Heptanol

b. Lead(IV) acetate

c. Calcium chlorate

CONVERTING MASS AND MOLES

- Mol is a unit that is not ***directly measureable*** as it is impossible count atoms at the same time.
- Chemists instead determine the number of moles (or vice versa) by measuring the mass.
- 12 g of carbon-12 is exactly 12 grams, so 6 grams would 0.50 mol and 24 grams would be 2.0 mol.

MOLE CONVERSION W, D.A.

- Calculate the number of moles of titanium(IV) chloride in 50.0 gram sample.

EXAMPLE: MOLE CONVERSION

How many moles of sodium hydrogen carbonate (sodium bicarbonate) are in a sample that weights 508 g?

EXAMPLE: MOLE CONVERSION

- Calculate the mass, in grams of 0.422 mol of copper(II) bromide.

EXAMPLE

- Determine the mass of 0.500 mol of ammonium iodate.

MOLE RELATIONSHIP

- The mol relates to mass, and particles and this relationship can be used to move from mass, to mole to particles or the inverse.
  - Dimensional analysis makes this process easier!

$$\text{Cu atoms} = (3\ \cancel{\text{g Cu}})\left(\frac{1\ \cancel{\text{mol Cu}}}{63.5\ \cancel{\text{g Cu}}}\right)\left(\frac{6.02 \times 10^{23}\ \text{Cu atoms}}{1\ \cancel{\text{mol Cu}}}\right)$$
$$= 3 \times 10^{22}\ \text{Cu atoms}$$

EXAMPLE: CONVERSIONS

- What number would you use to convert:

a. Moles of methane to grams of methane

b. Number of molecules of methane to moles of methane?

Grams ⟷ (Use molar mass) ⟷ Moles ⟷ (Use Avogadro's number) ⟷ Formula units

EXAMPLE: CONVERSIONS

- How many glucose molecules are in 5.23 g of $C_6H_{12}O_6$?
- How many oxygen atoms are in this sample?

EMPIRICAL FORMULAS

- Recall that the **empirical formula** is the number of atoms of each element in a substance.
- The formula H_2O tells us that there is 2 hydrogen atoms for each oxygen atom.
- By using the mole we can determine the empirical formula of unknown substances.

EMPIRICAL FORMULA

- Mercury and Chlorine form a compound that is 73.9% Hg and 26.1% Cl (by mass).
- By assuming a sample size of 100g, 73.9g is Hg and 26.1g is Cl.
- Using the atomic weights of each element we can determine the number of moles.

$$(73.9\ \cancel{\text{g Hg}})\left(\frac{1\ \text{mol Hg}}{200.6\ \cancel{\text{g Hg}}}\right) = 0.368\ \text{mol Hg}$$

$$(26.1\ \cancel{\text{g Cl}})\left(\frac{1\ \text{mol Cl}}{35.5\ \cancel{\text{g Cl}}}\right) = 0.735\ \text{mol Cl}$$

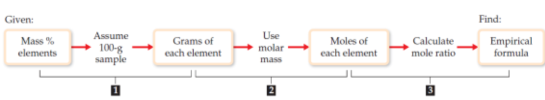
EMPIRICAL FORMULA

- The formula $Hg_{0.368}Cl_{0.735}$ doesn't quite look right (remember that formulas have to be **whole number ratios**.
- Obtain whole number ratio's by **dividing by same term** (usually the element with the lowest ratio).
- Round when necessary (1.98 – 2.02). This is caused by experimental errors and limitation with experimental errors.

$$\frac{\text{moles of Cl}}{\text{moles of Hg}} = \frac{0.735\ \text{mol Cl}}{0.368\ \text{mol Hg}} = \frac{1.99\ \text{mol Cl}}{1\ \text{mol Hg}}$$

EXAMPLE: EMPIRICAL FORMULA

- Ascorbic acid (vitamin C) contains 40.92% C, 4.58% H, and 54.50% O by mass. What is the empirical formula of ascorbic acid?



EXAMPLE: EMPIRICAL FORMULA

- A 5.325-g sample of methyl benzoate, a compound used in the manufacture of perfumes, contains 3.758 g of carbon, 0.316 g of hydrogen, and 1.251 g of oxygen. What is the empirical formula of this substance?

EMPIRICAL FORMULA TO MOLECULAR FORMULA

- Recall that empirical formula's are the reduced whole number multiples of molecular formula.
- To determine a molecular formula from an empirical formula divide the molecular mass by the empirical formula weight.

$$\text{Whole-number multiple} = \frac{\text{molecular weight}}{\text{empirical formula weight}}$$

EMP. FORMULA TO MOLE. FORMULA

- Previously we determined the empirical formula of vitamin C to be $C_3H_4O_3$ which has a mass of 88.0 amu.
- The experimentally determined molecular weight is 176 amu.

$$\text{Whole-number multiple} = \frac{\text{molecular weight}}{\text{empirical formula weight}} = \frac{176\ \text{amu}}{88.0\ \text{amu}} = 2$$

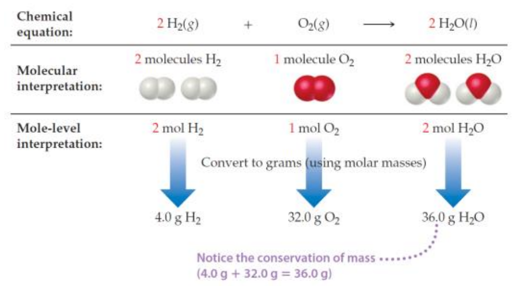
- The **molecular formula** for ascorbic acid is $\mathbf{C_6H_8O_6}$

BALANCED REACTIONS

- The coefficients in a balanced chemical reaction indicate the number of moles AND the number of particles (formula units or molecules).

2 $H_2(g)$ + **1**$O_2(g) \rightarrow$ **2**$H_2O(l)$

$2\ H_2(g)$	+	$O_2(g)$	$\longrightarrow$	$2\ H_2O(l)$
2 molecules		1 molecule		2 molecules
$2(6.02 \times 10^{23}$ molecules)		$1(6.02 \times 10^{23}$ molecules)		$2(6.02 \times 10^{23}$ molecules)
2 mol		1 mol		2 mol



STOICHIOMETRIC QUANTITIES

2 $H_2(g)$ + **1**$O_2(g) \rightarrow$ **2**$H_2O(l)$

2 mol $H_2 \approx$ 1 mol $O_2 \approx$ 2 mol H_2O

- The quantities represented above are considered to be **stoichiometrically equivalent**.
- This means that a given value can be converted to the next.

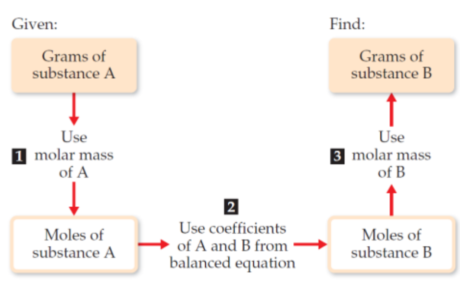
EXAMPLE: STOICHIOMETRIC CONVERSION

$2\ H_2(g) + 1O_2(g) \rightarrow 2H_2O(l)$

- Using the reaction shown above determine the number of moles of water produced when 1.57 moles of hydrogen reacts with excess oxygen.
- How many moles of oxygen and hydrogen are required to produce 3.58 moles of water?

STOICHIOMETRY WITH MASS

- As we are able to **convert mass to moles** we are able to use the stoichiometric process a given value of mass instead of moles.
- This is more practical as there is no direct method to determine moles in the lab, it is usually the result of mass measurement.



EXAMPLE: MASS – MASS STOICHIOMETRY

- Calculate the mass of carbon dioxide produced when 5.00-g of butane is burnt with excess oxygen.

EXAMPLE: MASS – MASS STOICHIOMETRY

- Determine how many grams of water are produced in the oxidation of 1.00 g of glucose, $C_6H_{12}O_6$.

EXAMPLE: MASS – MASS STOICHIOMETRY

- The decomposition of potassium chlorate is used to create oxygen for some reactions. Determine the mass of oxygen produced if 4.50 g of potassium chlorate breaks down.

EXAMPLE: MASS – MASS STOICHIOMETRY

- Propane is used for many cooking appliance and in home heating. Determine the mass of oxygen gas required to combust 3.00 gram of propane.

LIMITING REACTANT

- Suppose you are making several sandwiches using one slice of cheese and two slices of bread, the recipe is written below:

$$2\ Bd + Ch \rightarrow Bd_2Ch$$

- If you have 10 slices of bread and 7 slices of cheese – how many sandwiches can you make, is there something left over?
- This occurs for chemical reactions, some are **limited** in the amount of product formed due to a **reactant**!

DISCUSSION

- If 20.00 g of a compound reacts completely with 30.00 grams of another compound in a combination reaction, how many grams of product are formed?
- Why can't this understanding be applied *all* reactions?

LIMITING REACTANTS

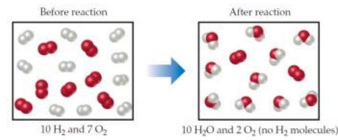
- Consider a mixture of hydrogen and oxygen.
  - 10 mol of H_2
  - 7 mol O_2

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

$$\text{Moles } O_2 = (10\ \cancel{\text{mol } H_2})\left(\frac{1\ \text{mol } O_2}{2\ \cancel{\text{mol } H_2}}\right) = 5\ \text{mol } O_2$$

LIMITING REACTANT

- For this reaction all the hydrogen would be consumed, this prevents any more water being product. The hydrogen gas is considered to be a limiting reactant.
- This reaction only requires 5 moles of O_2, therefore 2 would be left over, in excess. The oxygen gas is considered to be the excess reactant.



EXAMPLE: LIMITING REACTANT

- The most important commercial process for converting nitrogen from the air into a nitrogen compound is based on the reaction between nitrogen and hydrogen to form ammonia (NH_3). Determine the mass of ammonia formed if 3.0 mol of nitrogen and 6.0 mol of hydrogen is available.

EXAMPLE: LIMITING REACTANT

- When 1.50 mol of Al and 3.00 mol of chlorine gas combine in the reaction 2 Al(s) + $3Cl_2$(g) → $2AlCl_3$(s), (a) which is the limiting reactant? (b) how many moles of $AlCl_3$ are formed? (c) how many moles of excess reactant remain at the end of the reaction?

EXAMPLE: LIMITING REACTANT

- The reaction: $2H_2(g) + O_2(g) \rightarrow 2H_2O(g)$ is used to produce electricity in a hydrogen fuel cell. Suppose a fuel cell contains 150 g of H_2(g) and 1500 g of O_2(g) (each measured to 2 sig fig). How many grams of water can form?

EXAMPLE: LIMITING REACTANT

- When a 2.00-g strip of zinc metal is placed in an aqueous solution containing 2.50-g of silver nitrate the reaction is

Zn(s) + 2 $AgNO_3$(aq) → Zn(NO3)$_2$(aq) + 2 Ag(s)

(a) Which reactant is the limiting reagent?

(b) how many grams of Ag form?

(c) how many grams of $Zn(NO_3)_2$ form?

(d) how many grams of the excess reactant are left at the end of the reaction?

THEORETICAL YIELD

- The quantity of product calculated to form (using the previously learned method) is considered to be the **theoretical yield.**
- The amount of product collected is the **actual yield**.
- The closer to the theoretical yield the actual yield is the **fewer the experimental errors**.

THEORETICAL YIELD

- The actual yield can be greater then 100% if there are impurities, otherwise it will be less than 100% as the reaction has not gone to completion.

$$\text{Percent yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100\%$$

EXAMPLE: THEORETICAL YIELD

- Adipic acid, $H_2C_6H_8O_4$, used to produce nylon, is made commercially by a reaction between cyclohexane (C_6H_{12}) and O_2.

$$C_6H_{12}(l) + 5O_2(g) \rightarrow 2H_2C_6H_8O_4(l) + 2\ H_2O(g)$$

(a) Assume you carry out this reaction with 25.0 g of cyclohexane and that cyclohexane is the limiting reactant. What is the theoretical yield of adipic acid?

(b) If you obtain 33.5 g of adipic acid, what is the percent yield for the reaction?

EXAMPLE: THEORETICAL YIELD

- Imagine you are working on ways to improve the process by which iron ore containing iron(III) oxides is converted into iron according to the following formula

$$Fe_2O_3(s) + 3CO(g) \rightarrow 2Fe(s) + 3CO_2(g)$$

a. If you started with 150. g of Fe_2O_3 as the limiting reactant, what is the theoretical yield of Fe?

b. If your actual yield is 87.9 g, what is the percent yield?