Chapter 3 Stoichiometry: Calculations with Chemical Formulas and Equations

3.1 Chemical Equations

- A ***chemical equation*** describes a chemical reaction.

Reactants (states) → Products (states)

$A(g) + B(l) \rightarrow C(s) + D(aq)$

$HC_2H_3O_2(aq) + NaHCO_3(s) \rightarrow NaC_2H_3O_2(aq) + H_2O(l) + CO_2(g)$

Balancing Chemical Equations

- *The number of atoms of each element must be the same on both sides of the arrow.* (***Balancing a chemical equation***)

$CH_4(g) + O_2(g) \rightarrow CO_2(g) + H_2O(l)$ **(Unbalanced.)**

$CH_4(g) + O_3(g) \rightarrow CO_2(g) + H_4O(l)$ **(Balanced?)**

Anatomy of a Chemical Equation

$CH_{4\,(g)} + 2\,O_{2\,(g)} \rightarrow CO_{2\,(g)} + 2\,H_2O_{(g)}$

Coefficients are inserted to balance the equation.

Subscripts and Coefficients Give Different Information

Subscripts tell the number of atoms of each element in a molecule.

Coefficients tell the number of molecules.

Balancing Chemical Equations

- *The process is trial and error.*
- General guidelines:
  1. Balance each element in the equation starting with the most complex formula.
  2. Balance polyatomic ions as a single unit if they appear on both sides of the equation.
  3. The coefficients ***must*** be whole numbers.
  4. Finally, check that you have the ***smallest*** whole number ratio of coefficients.

Problem 1

Balance the following equations:

$Mg(s) + \quad O_2(g) \rightarrow \quad MgO(s)$

$NH_3(g) + \quad O_2(g) \rightarrow \quad NO(g) \quad + \quad H_2O(g)$

$Al_2(SO_4)_3(aq) \quad + \quad Ba(NO_3)_2(aq) \rightarrow \quad Al(NO_3)_3(aq) \quad + \quad BaSO_4(s)$

Note: *In a balanced chemical equation at least one of the coefficients will be an odd number.*

Problem 2

Balance the following equations:

$Na_{(s)} \quad + \quad N_{2(g)} \rightarrow \quad Na_3N_{(s)}$

$Al_{(s)} \quad + \quad O_{2(g)} \rightarrow \quad Al_2O_{3(s)}$

$Cl_2O_7 \quad + \quad H_2O \rightarrow \quad HClO_4$

$PCl_5 \quad + \quad H_2O \rightarrow \quad H_3PO_4 \quad + \quad HCl$

3.2 Some Simple Patterns of Chemical Reactivity

Combination Reactions
Decomposition Reactions
Combustion Reactions

Combination Reactions – In this type of reaction two or more substances react to form one product.

Examples:

- $2\ Mg_{(s)} + O_{2\,(g)} \longrightarrow 2\ MgO_{(s)}$
- $N_{2\,(g)} + 3\ H_{2\,(g)} \longrightarrow 2\ NH_{3\,(g)}$
- $C_3H_{6\,(g)} + Br_{2\,(l)} \longrightarrow C_3H_6Br_{2\,(l)}$

1. metal + oxygen → metal oxide *(predictable)*

$2\ Mg_{(s)} + O_{2\,(g)} \longrightarrow 2\ MgO_{(s)}$

2. nonmetal + oxygen → nonmetal oxide *(unpredictable)*

$S(s) + O_2(g) \rightarrow SO_2(g)$

3. metal and a nonmetal → ionic compound (binary) (predictable)

$2\ Na(s) + Cl_2(g) \rightarrow 2\ NaCl(s)$

Problem 3

Aluminum reacts with bromine in a combination reaction. Predict the product and write the reaction.

Decomposition Reactions – In decomposition one substance breaks down into two or more substances.

Examples:

- $CaCO_{3\,(s)} \longrightarrow CaO_{(s)} + CO_{2\,(g)}$
- $2\ KClO_{3\,(s)} \longrightarrow 2\ KCl_{(s)} + O_{2\,(g)}$
- $2\ NaN_{3\,(s)} \longrightarrow 2\ Na_{(s)} + 3\ N_{2\,(g)}$ (Sodium Azide – airbags)

One reactant yields two or more products.

- Metal hydrogen carbonates (*predictable*)
  - $Ni(HCO_3)_2(s) \rightarrow NiCO_3(s) + H_2O(l) + CO_2(g)$
- Metal carbonates (*predictable*)
  - $CaCO_3(s) \rightarrow CaO(s) + CO_2(g)$

Combustion Reactions

- These are generally rapid reactions that produce a flame.
- Most often involve hydrocarbons reacting with oxygen in the air.
- Examples:
  - $CH_{4\,(g)} + 2\ O_{2\,(g)} \longrightarrow CO_{2\,(g)} + 2\ H_2O_{(g)}$
  - $C_3H_{8\,(g)} + 5\ O_{2\,(g)} \longrightarrow 3\ CO_{2\,(g)} + 4\ H_2O_{(g)}$

Problem 4

Write and balance the equation for the combustion of:

a. C_6H_6

b. $C_6H_{12}O_6$

3.3 Formula Weight (FW)

A formula weight is the sum of the atomic weights for the atoms in a chemical formula.

So, the formula weight of calcium chloride, $CaCl_2$, would be:

$$\begin{array}{rl} Ca: & 1(40.1\text{ amu}) \\ \underline{+\ Cl:} & \underline{2(35.5\text{ amu})} \\ & 111.1\text{ amu} \end{array}$$

Formula weights are generally reported for ionic compounds.

Molecular Weight (MW)

A molecular weight is the sum of the atomic weights of the atoms in a molecule.

The MW of ethane (C_2H_6) would be:

$$\begin{array}{rl} C: & 2(12.0\text{ amu}) \\ +\ H: & 6(1.0\text{ amu}) \\ \hline & 30.0\text{ amu} \end{array}$$

Percent Composition

One can find the percentage of the mass of a compound that comes from each of the elements in the compound by using this equation:

$$\%\text{ element} = \frac{(\text{number of atoms})(\text{atomic weight})}{(\text{FW of the compound})} \times 100$$

So the percentage of carbon in ethane is:

$$\%C = \frac{(2)(12.0\text{ amu})}{(30.0\text{ amu})}$$

$$= \frac{24.0\text{ amu}}{30.0\text{ amu}} \times 100$$

$$= 80.0\%$$

Problem 5

Calculate the mass of each element in Iron (III) sulfate.

3.4 Avogadro's Number and the Mole

How do we count small things?

Two options (e.g. paper clips):

- a. One by one. (Too painful!!)
- b. Using the average weight.

Counting atoms by weighing

1. Atoms are too small to count individually. (So we have to count them by weighing)
2. Not all atoms are identical (remember isotopes…?).

Atomic mass unit (amu)

Atoms are tiny, so we use this 'amu' unit to work with their masses.

1 amu = 1.66×10^{-24}g

- 1 H atom weighs 1.008 amu.

- 1 C atom weighs 12.01 amu.

-1 Fe atom weighs 55.85 amu.

The Mole

1 dozen = 12

1 gross = 144

1 ream = 500

1 mole = 6.022*10^{23} (items) "Avogadro's number" Think of the mole as the chemist's "dozen".

In theory we could have a mole of whatever thing!!

1 mole of paper clips = 6.022*10^{23} paper clips

1 mole of tortillas = 6.022*10^{23} tortillas

1 mole of cars =6.022*10^{23} cars

1 mole of carbon atoms = 6.022*10^{23} C atoms

1 mole of H_2O = 6.022*10^{23} H_2O molecules

1 mole of NaCl = 6.022*10^{23} NaCl formula units

But just how big is Avogadro's Number (N_A)?

How much time would it take to travel a distance equal to 6.022 x 10^{23}mm moving at a rate of 100.0 km/hr (≈60 mi/hr)?

9.821 x 10^9 lifetimes (assuming 70 years)

The volume occupied by one mole of softballs would be about the size of the Earth.

Putting it all together:

- Masses of atoms are tiny:
  1 amu = 1.66*10^{-24}g
- N_A is very large!
  6.022 x 10^{23} items

What happens when we combine both?

And the trick is…

1 H atom weighs 1.008 amu.
1 mol of H atoms weighs 1.008 grams!

1 C atom weighs 12.01 amu.
1 mol of C atoms weighs 12.01 grams!

1 Fe atom weighs 55.85 amu.
1 mol of Fe atoms weighs… ?

Get the picture??

Molar masses of compounds

Molecular Weight = 12.01 amu + 4(1.008 amu) = 16.04 **amu/molecule**

Molar Mass =12.01 g + 4(1.008 g) = 16.04 **g/mol**

New Conversion Factors

1 mole = 6.022*10^{23} particles

Molar mass = #g/1 mole (*Depending on the material*)

We now can relate the following:

#atoms ⇔ #moles ⇔ #grams

Problem 6

How many moles of cobalt are there in 10.5 g Co? (Co: 58.93 g/mol)

Problem 7

What is the mass of 3.06*10^{20} carbon atoms?

Problem 8
How many atoms of helium are there in 25.0 g He?

Problem 9
How many moles of SO_3 are there in 10.0g of SO_3?

Problem 10
How many oxygen atoms are there in 25.0mg of $C_6H_{12}O_6$ (glucose)?

3.5 Finding Empirical Formulas

The ***empirical formula*** of a compound is the simplest whole number ratio of atoms of each element in a molecule. Formula units for ionic compounds are equal to their empirical formulas

One can calculate the empirical formula from the percent composition.

1. Convert masses to moles (if you are given mass %, assume 100 grams of sample).
2. Find the mole ratio – divide by the lowest number of moles.
3. Make sure it is a whole number ratio.

Example 1
Determine the empirical formula of acetic anhydride if its percent composition is:
47% carbon, 47% oxygen, and 6.0% hydrogen.

Assume 100 g of sample: 47 g C, 47 g O, and 6.0 g H.
Convert the grams to moles

$$47\text{g C} \times \frac{1\text{ mol C}}{12.01\text{g}} = 3.92\text{ mol C} \qquad 47\text{ g O} \times \frac{1\text{ mol O}}{16.00\text{ g}} = 2.94\text{ mol O} \qquad 6.0\text{ g H} \times \frac{1\text{ mol H}}{1.008\text{ g}} = 5.95\text{ mol H}$$

Note: Keep an extra digit…

Divide each by the smallest number of moles. (For this example, 2.9 is the smallest.)

$$3.91\text{ mol C} \div 2.94 = 1.33 \qquad 5.95\text{ mol H} \div 2.94 = 2.0 \qquad 2.94\text{ mol O} \div 2.94 = 1$$

If any of the ratios is not a whole number, multiply all the ratios by a factor to make it a whole number.

$$3.91\text{ mol C} \div 2.94 = 1.33 \text{ x } 3 = 4 \qquad 5.95\text{ mol H} \div 2.94 = 2.0 \text{ x } 3 = 6 \qquad 2.9\text{ mol O} \div 2.9 = 1 \text{ x } 3 = 3$$

Use the ratios as the subscripts in the empirical formula: $C_4H_6O_3$

Example 2

The compound *para*-aminobenzoic acid (you may have seen it listed as PABA on your bottle of sunscreen) is composed of carbon (61.31%), hydrogen (5.14%), nitrogen (10.21%), and oxygen (23.33%). Find the empirical formula of PABA.

Assuming 100.00 g of *para*-aminobenzoic acid,

C: $61.31\ g \times \frac{1\ mol}{12.01\ g} = 5.105\ mol\ C$

H: $5.14\ g \times \frac{1\ mol}{1.01\ g} = 5.09\ mol\ H$

N: $10.21\ g \times \frac{1\ mol}{14.01\ g} = 0.7288\ mol\ N$

O: $23.33\ g \times \frac{1\ mol}{16.00\ g} = 1.456\ mol\ O$

Calculate the mole ratio by dividing by the smallest number of moles:

C: $\frac{5.105\ mol}{0.7288\ mol} = 7.005 \approx 7$

H: $\frac{5.09\ mol}{0.7288\ mol} = 6.984 \approx 7$

N: $\frac{0.7288\ mol}{0.7288\ mol} = 1.000$

O: $\frac{1.458\ mol}{0.7288\ mol} = 2.001 \approx 2$

These are the subscripts for the empirical formula: $C_7H_7NO_2$

Molecular Formulas from Empirical Formulas

- Is always a multiple of the empirical formula.
- Divide the molar mass known for the compound(given in the problem) by the molar mass calculated for the empirical formula. Then round your answer to the nearest whole number.

Example

Determine the molecular formula of benzopyrene if it has a molar mass of 252 g and an empirical formula of C_5H_3

Determine the empirical formula (if it is not given).

May need to calculate it as previously C_5H_3

Determine the molar mass of the empirical formula: C_5H_3

5 C = 60.05 g, 3 H = 3.024 g

C_5H_3 = 63.07 g

Divide the given molar mass of the compound by the molar mass of the empirical formula.

Round to the nearest whole number: $\frac{252g}{63.07g} = 4$

Multiply the empirical formula by the calculated factor to give the molecular formula: $(C_5H_3)_4 = C_{20}H_{12}$

Combustion Analysis

Compounds containing C, H and O are routinely analyzed through combustion in a chamber like this.

- C is determined from the mass of CO_2 produced.
- H is determined from the mass of H_2O produced.
- O is determined by difference after the C and H have been determined.

Example

Isopropyl alcohol, sold as rubbing alcohol, is composed of C, H and O. Combustion of 0.255 g of isopropyl alcohol produces 0.516 g of CO_2 and 0.306 g of H_2O. Determine the empirical formula of isopropyl alcohol.

- From the mass of CO_2 we calculate the mass of C, and from the mass of H_2O we calculate the mass of H. The difference with the total mass of the sample will give us the mass of O.

$$grams\ of\ C = (0.561\ g\ CO_2)\left(\frac{1 mol CO_2}{44.0\ g\ CO_2}\right)\left(\frac{1\ mol\ C}{1\ mol\ CO_2}\right)\left(\frac{12.0\ g\ C}{1\ mol\ C}\right) = 0.153\ g\ C$$

$$grams\ of\ H = (0.306\ g\ H_2O)\left(\frac{1 mol H_2O}{18.0\ g\ H_2O}\right)\left(\frac{2\ mol\ H}{1\ mol\ H_2O}\right)\left(\frac{1.01\ g\ H}{1\ mol\ H}\right) = 0.0343\ g\ H$$

$$Mass\ of\ O = mass\ of\ sample - (mass\ of\ C + mass\ of\ H)$$

$$Mass\ of\ O = 0.255\ g - (0.153\ g + 0.0343\ g)$$

- The empirical formula of isopropyl alcohol is:

$$moles\ of\ C = (0.153\ g\ C)\left(\frac{1\ mol\ C}{12.0\ g\ C}\right) = 0.0128\ mol\ C$$

$$moles\ of\ H = (0.0343\ g\ H)\left(\frac{1\ mol\ H}{1.01\ g\ H}\right) = 0.0340\ mol\ H$$

$$moles\ of\ O = (0.068\ g\ O)\left(\frac{1\ mol\ O}{16.0\ g\ O}\right) = 0.0043\ mol\ O$$

$$C: \left(\frac{0.128}{0.0043}\right) = 3.0 \qquad H: \left(\frac{0.340}{0.0043}\right) = 7.9 \qquad O: \left(\frac{0.0043}{0.0043}\right) = 1$$

C_3H_8O

3.6 Quantitative Information from Balanced Equations

The coefficients in a balanced equation give the *relative* numbers of molecules.

A ***balanced*** chemical equation is like a *recipe*.

Cheesecake recipe: 3 blocks cream cheese + 5 eggs + 1 cup sugar → 1 cake

Given that the balanced equation is: 3 blocks cream cheese + 5 eggs + 1 cup sugar → 1 cake

How many eggs are required to bake 2 cakes?

- What we want: How many eggs
- What we are given: 2 cakes

2 cakes x (conversion factor) = ? eggs

The conversion factor, 5 eggs / 1 cake, comes directly from the balanced equation.

2 cakes x (5 eggs / 1 cake) = 10 eggs

The coefficients from a balanced equation can be put in the form of **mole ratios** (conversion factors for factor-label calculations). Example: P_4 (s) + $6Cl_2$ (g) → $4PCl_3$ (s)

$$\frac{1molP_4}{6molCl_2}\ or\ \frac{6molCl_2}{1molP_4}\ or\ \frac{6molCl_2}{4molPCl_3}\ or\ \frac{4molPCl_3}{1molP_4}, etc.$$

Problem 11

How many moles of P_4 are needed to react with 1.50 moles of Cl_2? P_4 (s) + $6Cl_2$ (g) → $4PCl_3$ (s)

Problem 12

How many moles of PCl_3 can be formed starting with 5.oo moles of P_4? P_4 (s) + $6Cl_2$ (g) → $4PCl_3$ (s)

Problem 13

How many moles of Cl_2 are needed to produce 7.00 moles of PCl_3? P_4 (s) + $6Cl_2$ (g) → $4PCl_3$ (s)

Stoichiometry

The process of using a chemical equation to calculate the relative masses of reactants and products involved in a reaction is called **stoichiometry**.

$$\text{g X} \underset{\text{MM of X}}{\Leftrightarrow} \text{mol X} \underset{\text{bal. eq.}}{\Leftrightarrow} \text{mol Y} \underset{\text{MM of Y}}{\Leftrightarrow} \text{g Y}$$

The balanced equation tells us the ratio of moles of compounds that react and/or are produced.

Example 1

Given the equation:

$$Na_3PO_{4(aq)} + Cu(NO_3)_{2(aq)} \rightarrow Cu_3(PO_4)_{2(s)} + NaNO_{3(aq)}$$

Q. If 30.0 g Na_3PO_4 reacts with enough $Cu(NO_3)_2$, what mass of copper (II) phosphate will be formed?

1. We need to balance the equation!

$$\mathbf{2}\ Na_3PO_{4(aq)} + \mathbf{3}\ Cu(NO_3)_{2(aq)} \rightarrow Cu_3(PO_4)_{2(s)} + \mathbf{6}\ NaNO_{3(aq)}$$

2. We need the molar mass of the compounds involved:
   - MM Na_3PO_4 = 3(22.99) + 30.97 + 4(16.00) = 163.94 g/mol
   - MM $Cu_3(PO_4)_2$ = 3(63.55) + 2(30.97) + 8(16.00) = 380.59 g/mol

3. $\text{g X} \underset{\text{MM of X}}{\Leftrightarrow} \text{mol X} \underset{\text{bal. eq.}}{\Leftrightarrow} \text{mol Y} \underset{\text{MM of Y}}{\Leftrightarrow} \text{g Y}$

$$30.0 gNa_3PO_4\left(\frac{1molNa_3PO_4}{163.94gNa_3PO_4}\right)\left(\frac{1molCu_3PO_4}{2molNa_3PO_4}\right)\left(\frac{380.59gCu_3PO_4}{1molCu_3PO_4}\right) = 34.8gCu_3PO_4$$

Example 2

Given the equation:

$$B\ (s) + O_2\ (g) \rightarrow B_2O_3\ (s)$$

Q. When 3.00 moles of Boron reacts with enough O_2, what mass of B_2O_3 is formed?

We need to balance the equation!

$$\mathbf{4}\ B\ (s) + \mathbf{3}\ O_2\ (g) \rightarrow \mathbf{2}\ B_2O_3\ (s)$$

$$3.00molB\left(\frac{2molB_2O_3}{4molB}\right)\left(\frac{69.62gB_2O_3}{1molB_2O_3}\right) = 104gB_2O_3$$

Problem 14

What mass of P_4O_{10} is needed to react with 25.0 g of H_2O?

$$P_4O_{10} + H_2O \rightarrow H_3PO_4$$

Problem 15

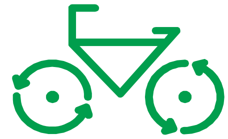
What mass of H_2O is needed to produce 50.0g of H_3PO_4 in the same reaction?

P_4O_{10} + **6** H_2O $\rightarrow$ **4** H_3PO_4

3.7 Limiting Reactant

Say you are going to 'react' bicycle frames with bicycle wheels to 'form' bicycles

- If you have 20 bicycle frames and 42 wheels



Which 'reactant' is in excess?
Which 'reactant' is limiting?
Which 'reactant' is completely 'consumed' in this reaction?
How many of the excess reactants are left over.

How Many Cookies Can I Make?

You can make cookies until you run out of one of the ingredients.
Once this family runs out of sugar, they will stop making cookies (at least any cookies you would want to eat).

Limiting Reactants

The limiting reactant is the reactant present in the smallest stoichiometric amount.
In other words, it's the reactant you'll run out of first.

There are two ways to find the limiting reactant:

1. Converting the mass or moles of all reactants to mass of one (any) of the products; the one that yields the least amount is the LR.

Example 1

If we have the reaction:

$$MnO_2(s) + 4\,HCl(aq) \rightarrow Cl_2(g) + MnCl_2(g) + 2\,H_2O(l)$$

a. When 10.2 g MnO_2 react with 18.3 g HCl, which one is the limiting reactant?
b. What mass of chlorine gas can be produced?
c. How many molecules of water can be produced?
(*<u>Read the whole problem so you can simplify your work.</u>)

$$MnO_2(s) + 4\,HCl(aq) \rightarrow Cl_2(g) + MnCl_2(g) + 2\,H_2O(l)$$

a. When 10.2 g MnO_2 react with 18.3 g HCl, which one is the limiting reactant?

$$10.2gMnO_2 \frac{1molMnO_2}{86.94gMnO_2}\frac{1molCl_2}{1molMnO_2} = 0.117molCl_2$$

$$18.3gHCl \frac{1molHCl}{36.46gHCl}\frac{1molCl_2}{4molHCl} = 0.125molCl_2$$

$MnO_2(s)$ is the limiting reactant.

b. What mass of chlorine gas can be produced?
(Notice we already know what is the maximum amount of chlorine produced – in moles – from point a.)

The maximum amount will be the one produced by the limiting reactant.

$$0.117molCl_2 \frac{70.90gCl_2}{1molCl_2} = 8.30gCl_2$$

c. How many molecules of water can be produced?
(*Notice how everything is related to the LR.)

$$10.2gMnO_2\left(\frac{1molMnO_2}{86.94gMnO_2}\right)\left(\frac{2molH_2O}{1molMnO_2}\right)\left(\frac{6.022*10^{23}moleculesH_2O}{1molH_2O}\right) = 1.41*10^{23}moleculesH_2O$$

Remember, there are two ways to find the limiting reactant:
2. Compare the mass (or number of moles) of reactants that we *actually have*, to those that we would need in *theory* for the reaction.

Example 2
Determine the number of moles of carbon dioxide produced when 3.2 moles oxygen reacts with 4.0 moles of carbon monoxide.

Write the balanced equation:
$2\ CO + O_2 \rightarrow 2\ CO_2$

The amounts of reactants we actually have are: 3.2 moles O_2 and 4.0 moles CO.
Now we calculate what we would need in theory:

$$3.2 \text{ moles } O_2 \text{ x } \frac{2 \text{ moles CO}}{1 \text{ mole } O_2} = 6.4 \text{ moles CO}$$

Since the calculated moles of CO (6.4 moles) needed to react with all the oxygen is greater than the given 4.0 moles of CO we can say that CO is the **limiting reactant.**

Finally, use the limiting reactant (CO in this case) to determine the moles of product:

$$4.0 \text{ moles CO x } \frac{2 \text{ moles } CO_2}{2 \text{ mole CO}} = 4.0 \text{ moles } CO_2$$

Example 3
If you combine 10.0 g P_4 and 10.0 g Cl_2, what mass of PCl_3 can be formed? What mass of the excess reactant remains?
$P_4\ (s) + Cl_2\ (g) \rightarrow PCl_3\ (s)$

1. Balance the Eq.
$P_4\ (s) + \mathbf{6}\ Cl_2\ (g) \rightarrow \mathbf{4}\ PCl_3\ (s)$

2. Find the moles of each reactant.

$$10.0 \text{ g } Cl_2 \left(\frac{1 \text{ mol } Cl_2}{70.90 \text{ g } Cl_2}\right) = 0.14\mathbf{1}0 \text{ mol } Cl_2$$

$$10.0 \text{ g } P_4 \left(\frac{1 \text{ mol } P_4}{123.88 \text{ g } P_4}\right) = 0.080\mathbf{7}2 \text{ mol } P_4$$

3. Using the balanced eq., find the LR:
a. By converting the moles of reactants to moles of one of the products (we have just one option here: PCl_3)

$$0.14\mathbf{1}0 \text{ mol } Cl_2 \left(\frac{4 \text{ mol } PCl_3}{6 \text{ mol } Cl_2}\right) = 0.094\mathbf{0}0 \text{ mol } PCl_3 \quad \textbf{LR}$$

$$0.080\mathbf{7}2 \text{ mol } P_4 \left(\frac{4 \text{ mol } PCl_3}{1 \text{ mol } P_4}\right) = 0.32\mathbf{2}8 \text{ mol } PCl_3$$

b. By comparing what we actually have with the theoretical amount needed.

$$0.080\mathbf{7}2 \text{ mol } P_4 \frac{6 \text{ mol } Cl_2}{1 \text{ mol } P_4} = 0.484 \text{ mol } Cl_2 \text{ (Needed)}$$

Since we already calculated we have only 0.14**1**0 mol of Cl_2, this is the **LR** (Same as above.)

4. Once the LR has been identified, use its number of moles to calculate the amount of product obtained, and the amount of the other reactants that is used.

$$0.1410 \text{ mol } Cl_2 \left(\frac{4 \text{ mol } PCl_3}{6 \text{ mol } Cl_2}\right)\left(\frac{137.32\text{g } PCl_3}{1 \text{ mol } PCl_3}\right) = 12.9 \text{ g } PCl_3 \text{ (form)}$$

$$0.1410 \text{ mol } Cl_2 \left(\frac{1 \text{ mol } P_4}{6 \text{ mol } Cl_2}\right)\left(\frac{123.88\text{g } P_4}{1 \text{ mol } P_4}\right) = 2.911 \text{ g } P_4 \text{ (reacted)}$$

To find what is left of the reactant in excess:

$$\underset{\text{(start)}}{10.0 \text{ g } P_4} - \underset{\text{(reacted)}}{2.911 \text{ g } P_4} = 7.088 \text{ g } P_4 \rightarrow \underset{\text{(left)}}{7.1 \text{ g } P_4}$$

Example 3 (Alternate Method)
Use a table of amounts in moles *<u>after determining the LR</u>*:

Substance	P_4	+	$6\ Cl_2$	→	$4\ PCl_3$
Initial	0.08072 mol		0.1410 mol		0 mol
Change	$-x$		$-6x$		$+4x$
Final	$0.08072 - x$		$0.1410 - 6x$		$4x$

Since Cl_2 is the LR, completely used up, final Cl_2 = 0. Therefore:
$0.1410 - 6x = 0$; $x = 0.1410/6 = 0.0235$ mol Cl_2.

PCl_3 formed = $4x = 4(0.0235 \text{ mol}) = 0.0940$ mol PCl_3
P_4 left = $0.08072 - x = 0.08072 \text{ mol} - 0.0235 \text{ mol} = 0.0940$ mol P_4

With the molar masses we can convert these results in moles to grams.

Problem 16
If 100. g of butane (C_4H_{10}) is burned in 390. g oxygen gas, what mass of CO_2 is produced? What mass of the excess reactant is left over? Use a table of amounts to answer.

Theoretical Yield

The theoretical yield is the maximum amount of product that can be made.

- In other words it's the amount of product possible as calculated through the stoichiometry problem.

This is different from the actual yield, which is the amount one actually produces and measures.

One finds the percent yield by comparing the amount actually obtained (actual yield) to the amount it was possible to make (theoretical yield).

$$\text{Percent Yield} = \frac{\text{Actual Yield}}{\text{Theoretical Yield}} \times 100$$

Percent Yield

$$92\% \text{ yield means } \frac{92 \text{ g actual}}{100 \text{ g theoretical}}$$

Problem 17
If a synthesis has an 87% yield, what theoretical yield is needed to produce 75 g of product?