Chapter 3 - Moles, Atoms, Mass Percents and Stoichiometry

<u>5 - Stoichiometry – Limiting and Excess Reagent</u>

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Introduction - Limiting Reagent

Reactions can start with one reactant or two or more reactants. To make sure that the reaction works, without wasting chemicals, one has to calculate exactly how much of each reactant is needed. This is done by the stoichiometric you have already learned. In cases where this is not done, there might be a reactant that is left over (excess reagent) and a reactant that is completely used up (limiting reagent). As soon as a reactant is consumed, the reaction will stop.

We will learn here how to calculate which of the reactants is limiting reagent and how much, if any, reactant is left over.

- Any problem giving the starting amount for more than one reactant is a limiting reactant/reagent problem.
- The limiting reagent (LR) is entirely consumed when a reaction goes to completion.
- **All amounts produced and reacted are determined by the limiting reactant.**

Setting up Calculations

1) How do we know it's a limiting reagent problem? When two or more reactant quantities are given then it is a limiting reagent (LR) problem.

2) How can we determine the limiting reactant?

This requires double (or triple depending on number of reactants) calculations of the stoichiometry.

a) Use each given amount to calculate the amount of product produced.

b) The limiting reactant will produce the *lesser* or *least* amount of product.

3) Depending on type of calculations, if calculating percent yield: use the lower of the two quantities to calculate percent yield.

4) To calculate excess reagent, the simple way is to go in reverse. See example for calculations.

Solved Problem: Calculating mols of limiting reagent and product

Magnesium metal is used to prepare zirconium metal, which is used to make the container for nuclear fuel (the nuclear fuel rods):

$$ZrCl_4(g) + 2Mg(s) \rightarrow 2MgCl_2(s) + Zr(s)$$

How many moles of zirconium metal can be produced from a reaction mixture containing 0.20 mol $ZrCl_4$ and 0.50 mol Mg?

$ZrCl_4(g)$	$+ 2Mg(s)$	$\rightarrow 2MgCl_2(s) + Zr(s)$
0.20 mol	0.50 mol	**? mol**

$$0.20\ \text{mol ZrCl}_4 \times \frac{1\ \text{mol Zr}}{1\ \text{mol ZrCl}_4} = 0.20\ \text{mol Zr}$$

Limiting reagent

$$0.50\ \text{mol Mg} \times \frac{1\ \text{mol Zr}}{2\ \text{mol Mg}} = 0.25\ \text{mol Zr}$$

Since $ZrCl_4$ gives the lesser amount of Zr,
$ZrCl_4$ is the limiting reactant.

0.20 mol Zr will be produced.

Solved Problem: Calculating theoretical yield, limiting and excess reagent.

Answer the following questions when 7.50 grams of oxygen gas react with 5.00 grams of hydrogen gas. What is the limiting reagent? What is the theoretical yield of the water? Calculate the amount of excess reagent left.

Strategy: For finding the Limiting Reagent

1) Write equation and balance it.
2) Find molar masses of the reactants.
3) Find the mols of H_2O formed from each of the reactants.
   DON'T FORGET THE MOL RATIO!!
4) Use the smaller mols of H_2O formed to find grams of H_2O.

Without a balanced equation you cannot solve this problem.

Step 1

$$2H_{2(g)} + O_{2(g)} \rightarrow 2\,H_2O_{(l)}$$

$2H_{2(g)}$ +	$O_{2(g)}$ $\rightarrow$	$2\,H_2O_{(l)}$
5.00 g	7.50 g	**? g**

Step 2

Molar Mass

H_2 2(1.008) = 2.016

O_2 2(15.99) = 31.98

H_2O 2(1.008) + 15.99 = 18.01

Step 3

$$7.50\text{ g }H_2 \times \frac{1\ mol\ H_2}{2.016\ g\ H_2} \times \frac{2\ mol\ H_2O}{2\ mol\ H_2} = 3.72\ mol\ H_2O$$

Excess reagent

$$5.00\text{ g }O_2 \times \frac{1\ mol\ O_2}{31.98\ g\ O_2} \times \frac{2\ mol\ H_2O}{1\ mol\ O_2} = \boxed{0.313\ mol\ H_2O}$$

Limiting reagent

Smaller number of mols of product formed from O_2, so ***O_2 is limiting reagent.***

<u>Strategy: For finding the grams of H_2O formed</u>

Convert the smaller mols of water formed to grams of water.

Step 4 $0.313\ mol\ H_2O \times \frac{18.00\ g\ H_2O}{1\ mol\ H_2O} = \boxed{5.63\ g\ H_2O}$

<u>Strategy: For finding the Excess Reagent</u>

1) Subtract the mols of water formed from the limiting and the excess reagent.
2) Find mol ratio to excess reagent.
3) Convert the mols of excess reagent to grams.

Step 5 (3.72 – 0.313) mol H_2O = 3.407 mol H_2O

Step 6 $3.407\ \text{mol}\ H_2O \times \frac{2\ mol\ H_2}{2\ mol\ H_2O} \times \frac{2.016\ g\ mol\ H_2}{1\ mol\ H_2} = 6.8685 = \boxed{6.87\ g\ H_2}$

Solved Problem: Calculating theoretical yield and excess reagent – 2nd way

Urea, CH_4N_2O, is used as a nitrogen fertilizer. It is manufactured from ammonia and carbon dioxide at high pressure and high temperature:

$2NH_3 + CO_2(g) \rightarrow CH_4N_2O + H_2O$

In a laboratory experiment, 10.0 g NH_3 and 10.0 g CO_2 were added to a reaction vessel. What is the maximum quantity (in grams) of urea that can be obtained? How many grams of the excess reactant are left at the end of the reactions?

Step 1 Equation is given and is balanced.

$$\underset{10.0\text{ g}}{2NH_3} + \underset{10.0\text{ g}}{CO_2(g)} \rightarrow \underset{?\text{ g}}{CH_4N_2O} + H_2O$$

Step 2 Molar masses

NH_3	1(14.01) + 3(1.008) = 17.02 g
CO_2	1(12.01) + 2(16.00) = 44.01 g
CH_4N_2O	1(12.01) + 4(1.008) + 2(14.01) + 1(16.00) = 60.06 g

Step 3

Excess reagent

$$10.0\text{ g NH}_3 \times \frac{1\text{ mol NH}_3}{17.024\text{ g NH}_3} \times \frac{1\text{ mol CH}_4\text{N}_2\text{O}}{2\text{ mol NH}_3} = 0.294\,mol\text{ CH}_4\text{N}_2\text{O}$$

$$= 17.6\text{ g CH}_4\text{N}_2\text{O}$$

Limiting reagent

$$10.0\text{ g CO}_2 \times \frac{1\text{ mol CO}_2}{44.01\text{ g CO}_2} \times \frac{1\text{ mol CH}_4\text{N}_2\text{O}}{1\text{ mol CO}_2} = \boxed{0.227\,mol\text{ CH}_4\text{N}_2\text{O}}$$

$$0.227\text{ mol CH}_4\text{N}_2\text{O}\,\frac{60.06\text{ g CH}_4\text{N}_2\text{O}}{1\text{ mol CH}_4\text{N}_2\text{O}} = \boxed{13.6\text{ g CH}_4\text{N}_2\text{O}}$$

Now convert the smaller mols to give gram of product.

Step 4 To find the excess NH_3, we can subtract the two product mols we have calculated to give the mols of the excess reagent.

$$(0.294\text{ mol} - 0.227\text{mol})\ CH_4N_2O = 0.067\text{mol } CH_4N_2O$$

Step 5 Now use the mol of the product to do the mol ratio to excess reagent, NH_3, and convert to it to grams.

$$0.067\ mol\ CH_4N_2O \times \frac{2\text{ mol } NH_3}{1\text{ mol } CH_4N_2O} \times \frac{17.02\text{ g } NH_3}{1\text{ mol } NH_3} = \boxed{2.28\text{ g } NH_3}$$

OLD WAY

$$10.0\text{ g } CO_2 \times \frac{1\text{ mol } CO_2}{44.01\text{ g } CO_2} \times \frac{2\text{ mol } NH_3}{1\text{ mol } CO_2} \times \frac{17.02\text{ g } NH_3}{1\text{ mol } NH_3} = 7.734605771\text{ g } NH_3$$

Now subtract the amount reacted from the starting amount:

10.0	beginning	
<u>–7.73</u>	reacted	$= 7.73\text{ g } NH_3$ reacted
2.27 g	remains	$\boxed{2.27\text{ g } NH_3 \text{ is excess reagent}}$

Solved Problem: Calculating percent yield and excess reagent.

Calculate the percent yield of CH_3CH_2Cl, when 12.4 g of CH_3CH_2Cl is formed from the reaction of 11.3 g C_2H_5OH (alcohol) and 13.48 g PCl_3 given below.

$$3C_2H_5OH + PCl_3 \rightarrow 3CH_3CH_2Cl + H_3PO_3$$

How many grams of the excess reactant are left at the end of the reaction?

Step 1 Equation is given and is balanced.

$3C_2H_5OH$	+	PCl_3	$\rightarrow$	$3CH_3CH_2Cl$	+	H_3PO_3
11.3 g		13.48 g		AY = 12.4 g		

Step 2 Molar masses

C_2H_5OH	2(12.01) + 6(1.008) + 1(16.00) = 46.068 g
PCl_3	1(30.97) + 3(35.45) = 137.32 g
CH_3CH_2Cl	2(12.01) + 5(1.008) + 1(35.45) = 64.5 g

Step 3

$$11.3\ \text{g}\ CH_3CH_2OH \times \frac{1\ \text{mol}\ CH_3CH_2OH}{46.068\ \text{g}\ CH_3CH_2OH} \times \frac{3\ \text{mol}\ CH_3CH_2Cl}{3\ \text{mol}\ CH_3CH_2OH} = \boxed{0.245\ \text{mol}\ CH_3CH_2Cl}$$

Limiting reagent

$$13.48\ \text{g}\ PCl_3 \times \frac{1\ \text{mol}\ PCl_3}{137.32\ \text{g}\ PCl_3} \times \frac{3\ \text{mol}\ CH_3CH_2Cl}{1\ \text{mol}\ PCl_3} = 0.294\ \text{mol}\ CH_3CH_2Cl$$

Excess reagent

$$0.245\ \text{mol}CH_3CH_2Cl\ \text{x}\ \frac{64.5\ \text{g}\ CH_3CH_2Cl}{1\ \text{mol}\ CH_3CH_2Cl} = \boxed{15.8\text{g}\ CH_3CH_2Cl}$$

Step 4 Percent yield

$$\frac{12.4\ \text{g}}{15.8\ \text{g}}\ 100\% = \boxed{78.5\%}$$

Step 5 Now subtract the two product mols and find the g of excess reagent left.

(0.294 – 0.245 mol) CH_3CH_2Cl = 0.049 mol CH_3CH_2Cl

$$0.049\ \text{mol}\ CH_3CH_2Cl \times \frac{1\ \text{mol}\ PCl_5}{3\ \text{mol}CH_3CH_2Cl} \times \frac{137.32\ \text{g}\ PCl_3}{1\ \text{mol}\ PCl_5} = \boxed{2.24\ \text{g}\ PCl_3\ \text{leftover}}$$

Review

- Limiting reactant
- Excess Reagent