Chapter 3 - Moles, Atoms, Mass Percents and Stoichiometry

Section 4 - Stoichiometry – Theoretical Yield and Percent Yields

Dr. Sapna Gupta

Introduction - Stoichiometry

Stoichiometry helps us to find a lot of information about a reaction.

- How much reactant is required to produce a certain amount of product
- The amount of product that can be made from a given amount of reactant.
- Calculating the product if there is more than one starting material. Is there a reactant that will finish sooner (limiting reagent) than the other?
- Will there be any reactant left over if there is more than one reactant?
- We can find out how efficient is the process by calculating percent yield of the product.

A **balanced chemical equation** is required for this process, which we have learned to do in the previous section.

Stoichiometry – Understanding the Chemical Equation

In any balanced chemical equation, there are no loss or gain of atoms after equation is balanced. (Law of conservation of matter).

The coefficients of the balanced chemical equation can be seen as either

(1) numbers of molecules (or ions or formula units) or

(2) numbers of moles, depending on what is being calculated.

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

2 molecules $H_{2(g)}$ + 1 molecule $O_{2(g)}$ $\rightarrow$ 2 molecules $H_2O_{(l)}$

2 moles $H_{2(g)}$ + 1 mole $O_{2(g)}$ $\rightarrow$ 2 moles $H_2O_{(l)}$

The mol relationship is made because of Avogadro's number (N_A)

Stoichiometry – Setting up

$$\textbf{A} \longrightarrow \textbf{B}$$

Let's say you are given the gram amount of A, and you are asked to calculate how much in grams of B will be formed. Follow the steps shown below as a generic setup.

1. Convert grams of A to moles of A - Using the molar mass of A.
2. Find mole ratio of A to B - Using the coefficients in the balanced equation.
3. Convert moles of B to grams of B - Using the molar mass of B.

Grams of A → Mols of A → Mols of B → Grams of B

Find atomic/molar mass of A from periodic table and use it to find mols of A.

Find mol ratio of A to B from balanced chemical equation.

Find atomic/molar mass of B from periodic table and use it to convert mols of B to grams.

Solved Problem: Mol to gram product calculation

Propane, C_3H_8, is normally a gas, but it is sold as a fuel compressed as a liquid in steel cylinders. The gas burns according to the following equation:

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

How many grams of CO_2 are produced when 2.00 mols of propane are burned?

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

1) The equation is balanced.
2) *Optional: write the equation with the numbers below it to see what you have and what you need.*
3) Molar masses:
   C_3H_8: don't need mass for propane because mols are already given.
   CO_2: 1(12.01) + 2(16.00) = 44.01 g
3) Mol ratio needed is of C_3H_8 to CO_2, 1:3.
4) 1 mol of C_3H_8 produces 3 mols of CO_2.
5) Final step will be to covert mols CO_2 of to grams of CO_2.

$$2\ \text{mol}\ C_3H_8 \times \frac{3\ \text{mol}\ CO_2}{1\ \text{mol}\ C_3H_8} \times \frac{44.01\ \text{g}\ CO_2}{1\ \text{mol}\ CO_2} = \boxed{264\ g\ CO_2}$$

Solved Problem: Gram to gram calculation

Propane, C_3H_8, is normally a gas, but it is sold as a fuel compressed as a liquid in steel cylinders. The gas burns according to the following equation:

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

How many grams of O_2 are required to burn 20.0 g of propane?

$$\begin{array}{ccccccc} C_3H_8(g) & + 5O_2(g) & \rightarrow & 3CO_2(g) & + & 4H_2O(g) \\ 20\text{ g} & \textbf{? g} & & & & \end{array}$$

Molar masses:

O_2 $2(16.00) = 32.00$ g/mol

C_3H_8 $3(12.01) + 8(1.008) = 44.094$ g/mol

Strategy:

Grams propane → mols propane → mol ratio propane to oxygen → grams oxygen

$$20.0\text{ g } C_3H_8 \times \frac{1\text{ mol } C_3H_8}{44.094\text{ g } C_3H_8} \times \frac{5\text{ mol } O_2}{1\text{ mol } C_3H_8} \times \frac{32.00\text{ g } O_2}{1\text{ mol } O_2} = 72.57223205\text{ g } O_2$$

$$\boxed{72.6\text{ g } O_2}$$

Solved Problem: gram to gram calculation

A chemist needs 58.75 grams of urea, how many grams of ammonia are needed to produce this amount?

$$2NH_{3(g)} + CO_{2(g)} \rightarrow (NH_2)_2CO_{(aq)} + H_2O_{(l)}$$

$2NH_{3(g)}$	+	$CO_{2(g)}$	$\rightarrow$	$(NH_2)_2CO_{(aq)}$	+ $H_2O_{(l)}$
? g				58.75 g	

Molar masses:

$(NH_2)_2CO$ 4(1.008) + 2(14.00) + 1(12.01) + 1(16.00) = 60.04 g/mol

NH_3 3(1.008) + 1(14.00) = 17.02 g/mol

Strategy:

Gram urea → mol urea → mol ratio urea to ammonia → gram ammonia

$$58.75\text{ g }(NH_2)_2CO \times \frac{1\text{mol }(NH_2)_2CO}{60.04\text{g }(NH_2)_2CO} \times \frac{2\text{mol }NH_3}{1\text{mol }(NH_2)_2CO} \times \frac{17.02\text{g }NH_3}{1\text{mol }NH_3} = \boxed{33.31\text{g }NH_3}$$

Percent Yield

Theoretical Yield (TY)

Theoretical yield is the maximum amount of product that can be obtained by a reaction from given amounts of reactants.

This is a *calculated* amount using stoichiometry. This is also called stoichiometric quantity of product formed.

Actual Yield (AY)

The amount of product that is actually obtained in the lab after carrying out the reaction.

This is a *measured* amount. This quantity has to be given to you in a calculation.

Percentage Yield

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

Solved Problem: Calculating percent yield

When a student reacted 3.75 grams of zinc with excess hydrochloric acid, 1.58 grams of zinc chloride were collected. What is the percent yield for this reaction if the theoretical yield is 2.14 g?

Theoretical yield = 2.14 g $ZnCl_2$
Actual yield = 1.58 g $ZnCl_2$

$$\%\text{yield} = \frac{1.58\text{g}}{2.14\text{g}} \times 100 = \boxed{73.8\%}$$

Solved Problem: Calculating theoretical and percent yield

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

When 12.2 g NH_3 added excess carbon dioxide, 9.3 g of urea was obtained. What is the percent yield of this reaction?

$2NH_{3(g)}$	+ $CO_{2(g)}$	$\rightarrow$	$(NH_2)_2CO_{(aq)}$	+ $H_2O_{(l)}$
12.2 g			AY = 9.3 g	

Step 1

Strategy: First find the **theoretical yield** of urea from the 12.2 g of NH_3, then use the actual yield to find the percent yield.

Molar Masses:

NH_3 1(14.01) + 3(1.008) = 17.02 g

CH_4N_2O 1(12.01) + 4(1.008) + 2(14.01) + 1(16.00) = 60.06 g

Step 2

$$12.2 \text{ g } NH_3 \times \frac{1 \text{ mol } NH_3}{17.024 \text{ g } NH_3} \times \frac{1 \text{ mol } CH_4N_2O}{2 \text{ mol } NH_3} \times \frac{60.06 \text{ g } CH_4N_2O}{1 \text{ mol } CH_4N_2O} = 21.5 \text{ g } CH_4N_2O$$

Step 3

Theoretical yield = 21.5 g

Actual yield = 9.3 g

$$\text{Percent yield} = \frac{9.3 \text{ g}}{21.5 \text{ g}} \times 100\% = \boxed{43.2\% \text{ yield}}$$

Review

- Chemical equations
- Mole concept and conversions
- Stoichiometry
- Theoretical yield
- Actual yield
- Percent yield