11.3: Theoretical Yield, and Percent Yield

Learning Objectives

- Calculate percentage or actual yields from known amounts of reactants.

The world of pharmaceutical production is an expensive one. Many drugs have several steps in their synthesis and use costly chemicals. A great deal of research takes place to develop better ways to make drugs faster and more efficiently. Studying how much of a compound is produced in any given reaction is an important part of cost control.

Percent Yield

Chemical reactions in the real world don't always go exactly as planned on paper. In the course of an experiment, many things will contribute to the formation of less product than predicted. Besides spills and other experimental errors, there are usually losses due to an incomplete reaction, undesirable side reactions, etc. Chemists need a measurement that indicates how successful a reaction has been. This measurement is called the percent yield.

To compute the percent yield, it is first necessary to determine how much of the product should be formed based on stoichiometry. This is called the **theoretical yield**, the maximum amount of product that can be formed from the given amounts of reactants. The **actual yield** is the amount of product that is actually formed when the reaction is carried out in the laboratory. The **percent yield** is the ratio of the actual yield to the theoretical yield, expressed as a percentage.

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

Percent yield is very important in the manufacture of products. Much time and money is spent improving the percent yield for chemical production. When complex chemicals are synthesized by many different reactions, one step with a low percent yield can quickly cause a large waste of reactants and unnecessary expense.

Typically, percent yields are understandably less than 100% because of the reasons indicated earlier. However, percent yields greater than 100% are possible if the measured product of the reaction contains impurities that cause its mass to be greater than it actually would be if the product was pure. When a chemist synthesizes a desired chemical, he or she is always careful to purify the products of the reaction. Example $11.3.1$ illustrates the steps for determining percent yield.

Example $11.3.1$: Decomposition of Potassium Chlorate

Potassium chlorate decomposes upon slight heating in the presence of a catalyst, according to the reaction below:

$$2\text{KClO}_3\,(s) \rightarrow 2\text{KCl}\,(s) + 3\text{O}_2\,(g)$$

In a certain experiment, 40.0 g KClO_3 is heated until it completely decomposes. The experiment is performed and the oxygen gas is collected and its mass is found to be 14.9 g

a. What is the theoretical yield of oxygen gas?
b. What is the percent yield for the reaction?

Solution

a. Calculation of theoretical yield

First, we will calculate the theoretical yield based on the stoichiometry.

Step 1: Identify the "given" information and what the problem is asking you to "find".

Given: Mass of $\text{KClO}_3 = 40.0 \text{ g}$

Mass of O_2 collected = 14.9g

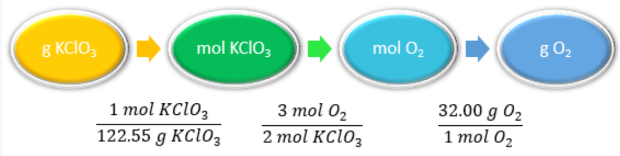
Find: Theoretical yield, g O_2

Step 2: List other known quantities and plan the problem.

1 mol $KClO_3$ = 122.55 g/mol

1 mol O_2 - 32.00 g/mol

Step 3: Apply stoichiometry to convert from the mass of a reactant to the mass of a product:



Step 4: Solve.

$$40.0 \text{ g } \cancel{\text{KClO}_3} \times \frac{1 \text{ mol } \cancel{\text{KClO}_3}}{122.55 \text{ g } \cancel{\text{KClO}_3}} \times \frac{3 \text{ mol } \cancel{\text{O}_2}}{2 \text{ mol } \cancel{\text{KClO}_3}} \times \frac{32.00 \text{ g O}_2}{1 \text{ mol } \cancel{\text{O}_2}} = 15.7 \text{ g O}_2$$

The theoretical yield of O_2 is 15.7 g, $15.\underline{6}7$ g unrounded.

Step 5: Think about your result.

The mass of oxygen gas must be less than the 40.0 g of potassium chlorate that was decomposed.

b. Calculation of percent yield

Now we will use the actual yield and the theoretical yield to calculate the percent yield.

Step 1: Identify the "given" information and what the problem is asking you to "find".

Given: Theoretical yield =15.$\underline{6}$7 g, use the un-rounded number for the calculation.

Actual yield = 14.9g

Find: Percent yield, % Yield

Step 2: List other known quantities and plan the problem.

No other quantities needed.

Step 3: Use the percent yield equation below.

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

Step 4: Solve.

$$\text{Percent Yield} = \frac{14.9 \text{ g}}{15.\underline{6}7 \text{ g}} \times 100\% = 94.9\%$$

Step 5: Think about your result.

Since the actual yield is slightly less than the theoretical yield, the percent yield is just under 100%.

Example 11.3.2: Oxidation of Zinc

Upon reaction of 1.274 g of copper sulfate with excess zinc metal, 0.392 g copper metal was obtained according to the equation:

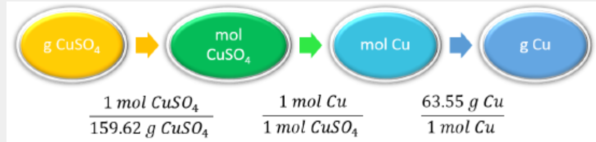
$$\text{CuSO}_4(aq) + \text{Zn}(s) \rightarrow \text{Cu}(s) + \text{ZnSO}_4(aq)$$

What is the percent yield?

Solution

Solutions to Example 8.6.2

Steps for Problem Solving-The Product Method	Example 11.3.1
Identify the "given" information and what the problem is asking you to "find."	Given: 1.274 g CuSO4 Actual yield = 0.392 g Cu Find: Percent yield
List other known quantities.	1 mol CuSO4= 159.62 g/mol 1 mol Cu = 63.55 g/mol Since the amount of product in grams is not required, only the molar mass of the reactants is needed.
Balance the equation.	The chemical equation is already balanced. The balanced equation provides the relationship of 1 mol CuSO4 to 1 mol Zn to 1 mol Cu to 1 mol ZnSO4.

Steps for Problem Solving-The Product Method	Example 11.3.1
Prepare a concept map and use the proper conversion factor.	 The provided information identifies copper sulfate as the limiting reactant, and so the theoretical yield (g Cu) is found by performing **mass-mass** calculation based on the initial amount of $CuSO_4$.
Cancel units and calculate.	$1.274\ \text{g}\ \cancel{\text{CuSO}_4} \times \frac{1\ \text{mol}\ \cancel{\text{CuSO}_4}}{159.62\ \text{g}\ \cancel{\text{CuSO}_4}} \times \frac{1\ \text{mol}\ \cancel{\text{Cu}}}{1\ \text{mol}\ \cancel{\text{CuSO}_4}} \times \frac{63.55\ \text{g Cu}}{1\ \text{mol}\ \cancel{\text{Cu}}} = 0.507$ Using this theoretical yield and the provided value for actual yield, the percent yield is calculated to be: $\text{percent yield} = \left(\frac{\text{actual yield}}{\text{theoretical yield}}\right) \times 100$ $= \left(\frac{0.392\, g\, \text{Cu}}{0.5072\, g\, \text{Cu}}\right) \times 100$ $= 77.3\%$
Think about your result.	Since the actual yield is slightly less than the theoretical yield, the percent yield is just under 100%.

Exercise 11.3.1

What is the percent yield of a reaction that produces 12.5 g of the Freon CF_2Cl_2 from 32.9 g of CCl_4 and excess HF?

$$\text{CCl}_4 + 2\,\text{HF} \rightarrow \text{CF}_2\text{Cl}_2 + 2\,\text{HCl}$$

Answer

48.3%

Summary

Theoretical yield is calculated based on the stoichiometry of the chemical equation. The actual yield is experimentally determined. The percent yield is determined by calculating the ratio of actual yield to theoretical yield.