Calculations from Chemical Equations

Corbis RF/Age Fotostock America, Inc.

Accurate measurement and dosage calculations are critical in dispensing medicine to patients all over the world.

Foundations of College Chemistry, 14th Ed.

Morris Hein and Susan Arena

Chapter Outline

Mole/Molar Mass Review

Molar Mass (MM): sum of the atomic mass of the atoms in an element, compound, or formula unit.

Mole: Avogadro's number (6.022×10^{23}) of units (atoms, molecules, ions etc.)

Useful Conversion Factors

$$\text{Molar mass} = \frac{\text{grams of a substance}}{\text{moles of the substance}}$$

MM allows conversion between g and mol of a substance.

$$\text{Moles of a substance} = \frac{\text{number of units of substance}}{6.022 \times 10^{23}\text{ units of substance}}$$

Introduction to Stoichiometry

Equations must always be balanced before calculation of any mass, moles, or volume of a reactant or product!

Stoichiometry: area of chemistry that deals with quantitative relationships between products and reactants in chemical equations.

Example

$$aA + bB \longrightarrow cC + dD$$

Using X.X g of A, how much C will be formed?

Solving stoichiometry problems always requires the use of:

1. **A balanced chemical equation (coefficients must be known!)**
2. **Conversion factors in units of moles (i.e. mole ratios)**

Mole Ratios

Mole ratio: ratio (conversion factor) between any two species in a chemical reaction.

Example

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

The coefficients of a balanced chemical equation are used to generate mole ratios.

6 possible mole ratios exist:

$$\frac{2\text{ mol }H_2}{1\text{ mol }O_2} \quad \frac{2\text{ mol }H_2}{2\text{ mol }H_2O} \quad \frac{1\text{ mol }O_2}{2\text{ mol }H_2O}$$

$$\frac{1\text{ mol }O_2}{2\text{ mol }H_2} \quad \frac{2\text{ mol }H_2O}{2\text{ mol }H_2} \quad \frac{2\text{ mol }H_2O}{1\text{ mol }O_2}$$

Mole Ratios

The mole ratio can be used as a conversion factor to convert between moles of one substance and another.

Example

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

If 4.0 mol of oxygen are present, how many moles of H_2O could be formed?

$$4.0\text{ mol }O_2 \times \frac{2\text{ mol }H_2O}{1\text{ mol }O_2} = 8.0\text{ mol }H_2O$$

Mole Ratios Practice

Given the following balanced chemical equation, write the mole ratio need to calculate:

a. The moles of H_2O produced from 3 moles of CO_2

b. The moles of H_2 needed to produce 3 moles of H_2O.

$$CO_2\,(g) + 4\,H_2\,(g) \longrightarrow CH_4\,(g) + 2\,H_2O\,(l)$$

a.

$$3.0\ \cancel{mol\ CO_2} \times \frac{2\ mol\ H_2O}{1\ \cancel{mol\ CO_2}} = 6.0\ mol\ H_2O$$

Mole ratio

Desired quantity in the numerator of the mole ratio: known quantity in the denominator

Mole Ratios Practice

Given the following balanced chemical equation, write the mole ratio need to calculate:

a. The moles of H_2O produced from 3 moles of CO_2

b. The moles of H_2 needed to produce 3 moles of H_2O.

$$CO_2\,(g) + 4\,H_2\,(g) \longrightarrow CH_4\,(g) + 2\,H_2O\,(l)$$

b.

$$3.0\ \cancel{mol\ H_2O} \times \frac{4\ mol\ H_2}{2\ \cancel{mol\ H_2O}} = 6.0\ mol\ H_2$$

Mole ratio

Desired quantity in the numerator of the mole ratio: known quantity in the denominator

Mole Ratios Practice

Given the following balanced chemical equation, what is the mole ratio needed to calculate the following: the moles of KCl produced when 4.5 moles of O_2 are formed?

$$2\,KClO_3\,(s) \longrightarrow 2\,KCl\,(s) + 3\,O_2\,(g)$$

$$\frac{2\ mol\ KCl}{3\ mol\ O_2} \qquad \frac{3\ mol\ O_2}{2\ mol\ KCl} \qquad \frac{3\ mol\ KCl}{2\ mol\ O_2} \qquad \frac{2\ mol\ O_2}{3\ mol\ KCl}$$

Calculate

$$4.5\ \cancel{mol\ O_2} \times \frac{2\ mol\ KCl}{3\ \cancel{mol\ O_2}} = 3.0\ mol\ KCl$$

Mole ratio

Problem Solving for Stoichiometry Problems

1. Make sure the equation is balanced!

2. If needed, convert the quantity of known substance to moles.

$$\text{Moles} = (\text{grams}) \times \frac{1\ \text{mol substance}}{\text{molar mass substance}}$$

3. Convert the moles of known substance to desired substance using a mole ratio.

$$\text{Mole ratio} = \frac{\text{moles of desired substance}}{\text{moles of known substance}}$$

Moles desired substance = Moles of known substance x Mole ratio

From Step 2

Problem Solving for Stoichiometry Problems

4. Convert moles of desired substance to the desired units from the problem.

If answer is in moles, you are finished.

If answer is in grams, multiply by the compound's molar mass.

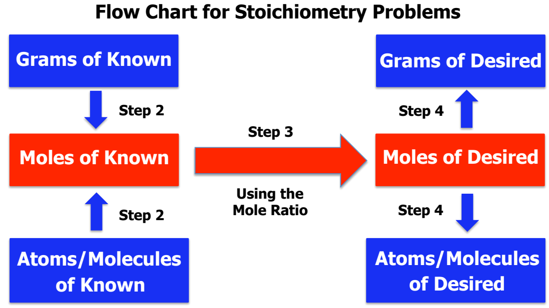
$$\text{grams} = (\text{moles}) \times \frac{\text{Molar mass (in g)}}{1\ \text{mole}}$$

If answer is in atoms/molecules, multiply by Avogadro's number.

$$\text{Atoms/molecules} = (\text{moles}) \times \frac{6.022 \times 10^{23}\ \text{molecules}}{1\ \text{mole}}$$

Problem Solving for Stoichiometry Problems

Flow Chart for Stoichiometry Problems



Mole-Mole Calculations

Known substance is given in moles; desired substance is requested in moles.

How many moles of CO_2 will be produced by reaction of 2.0 mol of glucose, given the following balanced equation?

$$C_6H_{12}O_6 + 6\,O_2 \longrightarrow 6\,CO_2 + 6\,H_2O$$

Solution Map mol $C_6H_{12}O_6$ ⟶ mol CO_2

The mole ratio needed relates mol $C_6H_{12}O_6$ to mol CO_2.

$$\frac{6\text{ mol }CO_2}{1\text{ mol }C_6H_{12}O_6}$$

Calculate

$$2.0\ \text{mol } C_6H_{12}O_6 \times \frac{6\text{ mol }CO_2}{1\text{ mol }C_6H_{12}O_6} = 12\text{ mol }CO_2$$

Mole-Mole Calculations Practice

How many H_2O molecules are produced when 0.010 mol O_2 react, given the following balanced equation?

$$2\,H_2 + O_2 \longrightarrow 2\,H_2O$$

a. 8.3×10^{-27} molecules
b. 3.3×10^{-26} molecules
c. 3.0×10^{21} molecules
d. 1.2×10^{22} molecules

Solution Map

mol O_2 ⟶ mol H_2O ⟶ molecules H_2O

Mole ratio:

$$\frac{2\text{ mol }H_2O}{1\text{ mol }O_2}$$

Calculate

$$0.010\text{ mol }O_2 \times \frac{2\text{ mol }H_2O}{1\text{ mol }O_2} \times \frac{6.022 \times 10^{23}\text{ molecules }H_2O}{1\text{ mole }H_2O} = 1.2 \times 10^{22}\text{ molecules}$$

Mole-Mole Calculations Practice

How many moles of Al are produced when 0.5 mol of O_2 react, given the following balanced equation?

$$4\,Al + 3\,O_2 \longrightarrow 2\,Al_2O_3$$

a. 0.38 moles
b. 0.67 moles
c. 1.0 moles
d. 0.25 moles

Solution Map

mol O_2 ⟶ mol Al

Mole ratio:

$$\frac{4\text{ mol Al}}{3\text{ mol }O_2}$$

Calculate

$$0.5\text{ mol }O_2 \times \frac{4\text{ mol Al}}{3\text{ mol }O_2} = 0.67\text{ mol Al}$$

Mole-Mass Calculations

What mass of H_2 can be produced when 6.0 mol of Al reacts with HCl?

$$2\,Al + 6\,HCl \longrightarrow 2\,AlCl_3 + 3\,H_2$$

Solution Map mol Al ⟶ mol H_2 ⟶ g H_2

The mole ratio and molar mass of H_2 are needed:

$$\frac{3\text{ mol }H_2}{2\text{ mol Al}} \qquad \frac{2.016\text{ g }H_2}{1\text{ mol }H_2}$$

Calculate

$$6.0\text{ mol Al} \times \frac{3\text{ mol }H_2}{2\text{ mol Al}} \times \frac{2.016\text{ g }H_2}{1\text{ mol }H_2} = 18\text{ g }H_2$$

Mole-Mass Calculations Practice

How many moles of water are produced when 325 g of octane (C_8H_{18}) are burned?

$$2\,C_8H_{18} + 25\,O_2 \longrightarrow 16\,CO_2 + 18\,H_2O$$

Solution Map g C_8H_{18} ⟶ mol C_8H_{18} ⟶ moles H_2O

The mole ratio and molar mass of C_8H_{18} are needed:

$$\frac{18\text{ mol }H_2O}{2\text{ mol }C_8H_{18}} \qquad \frac{1\text{ mol }C_8H_{18}}{114.2\text{ g }C_8H_{18}}$$

Calculate

$$325.\text{ g }C_8H_{18} \times \frac{1\text{ mol }C_8H_{18}}{114.2\text{ g }C_8H_{18}} \times \frac{18\text{ mol }H_2O}{2\text{ mol }C_8H_{18}} = 25.6\text{ mol }H_2O$$

Mole-Mass Calculations Practice

How many grams of $AgNO_3$ are needed to produce 0.25 mol of Ag_2S?

$$2\,AgNO_3 + H_2S \longrightarrow Ag_2S + 2\,HNO_3$$

a. 42.5 g
b. 57.1 g
c. 2.19×10^{-3} g
d. 85.0 g

Solution Map

mol Ag_2S ⟶ mol $AgNO_3$ ⟶ g $AgNO_3$

The mole ratio and molar mass of $AgNO_3$ are needed:

$$\frac{2\text{ mol }AgNO_3}{1\text{ mol }Ag_2S} \qquad \frac{169.9\text{ g }AgNO_3}{1\text{ mol }AgNO_3}$$

Calculate

$$0.25\text{ mol }Ag_2S \times \frac{2\text{ mol }AgNO_3}{1\text{ mol }Ag_2S} \times \frac{169.9\text{ g }AgNO_3}{1\text{ mol }AgNO_3} = 85.0\text{ g }AgNO_3$$

Mass-Mass Calculations

How many grams of HNO_3 are required to produce 8.75 g of N_2O from the following reaction?

$$4\,Zn + 10\,HNO_3 \longrightarrow 4\,Zn(NO_3)_2 + N_2O + 5\,H_2O$$

Solution Map g N_2O → mol N_2O → mol HNO_3 → g HNO_3

The mole ratio and molar masses of N_2O and HNO_3 are needed:

$$\frac{10\text{ mol }HNO_3}{1\text{ mol }N_2O} \quad \frac{1\text{ mol }N_2O}{44.02\text{ g }N_2O} \quad \frac{63.02\text{ g }HNO_3}{1\text{ mol }HNO_3}$$

Calculate

$$8.75\text{ g }N_2O \times \frac{1\text{ mol }N_2O}{44.02\text{ g }N_2O} \times \frac{10\text{ mol }HNO_3}{1\text{ mol }N_2O} \times \frac{63.02\text{ g }HNO_3}{1\text{ mol }HNO_3} = 125.\text{ g }HNO_3$$

Mass-Mass Calculations Practice

How many grams of $CrCl_3$ are required to produce 75.0 g of AgCl using the following reaction?

$$CrCl_3 + 3\,AgNO_3 \longrightarrow Cr(NO_3)_3 + 3\,AgCl$$

a. 204 g
b. 249 g
c. 22.6 g
d. 27.6 g

Solution Map

g AgCl → mol AgCl → mol $CrCl_3$ → g $CrCl_3$

Mole ratio/molar masses needed:

$$\frac{1\text{ mol }CrCl_3}{3\text{ mol AgCl}} \quad \frac{1\text{ mol AgCl}}{143.3\text{ g AgCl}} \quad \frac{158.4\text{ g }CrCl_3}{1\text{ mol }CrCl_3}$$

Calculate

$$75.0\text{ g AgCl} \times \frac{1\text{ mol AgCl}}{143.3\text{ g AgCl}} \times \frac{1\text{ mol }CrCl_3}{3\text{ mol AgCl}} \times \frac{158.4\text{ g }CrCl_3}{1\text{ mol }CrCl_3} = 27.6\text{ g }CrCl_3$$

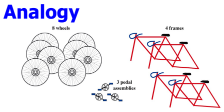
Limiting Reactants

In many chemical reactions, one reactant is used in excess. The maximum amount of product formed depends on the amount of reactant not in excess (the limiting reactant).

A Nonchemical Analogy

To put together a bicycle, you need several parts.

The number of bicycles is limited by the part you have the least of.



Limiting Reactants

Chemical Example

If you started with 5 molecules of H_2 and 3 molecules of Cl_2, how much HCl could you make?

$$H_2 + Cl_2 \longrightarrow 2\,HCl$$

Because you need 1 molecule of H_2 for each molecule of Cl_2, the Cl_2 limits the reaction.

With 3 molecules of Cl_2, you can make a total of 6 molecules of HCl (because of the reaction coefficients).

2 molecules of H_2 remain unused (are in excess).

When the coefficients of the balanced equation are more complex, a general method should be used.

Limiting Reactants

Problem Solving Strategy for Limiting Reactant Problems

1. **Calculate the amount of product formed from each reactant present.**
2. **The reactant that gives the least amount of product is limiting; the other reactant is in excess.**
3. **The amount of product is determined by the calculation from Step 1 with the limiting reactant.**
4. **If the amount of excess reactant is desired, determine the amount of excess reactant needed to consume the limiting reactant and subtract from the initial quantity present.**

Limiting Reactant Problems

How many moles of HCl can be produced from 4.0 mol of H_2 and 3.5 mol of Cl_2? What is the limiting reactant?

$$H_2 + Cl_2 \longrightarrow 2\,HCl$$

Step 1 Calculate the moles of HCl formed from each reactant using the appropriate mole ratios.

$$4.0\text{ mol }H_2 \times \frac{2\text{ mol HCl}}{1\text{ mol }H_2} = 8.0\text{ moles HCl}$$

$$3.5\text{ mol }Cl_2 \times \frac{2\text{ mol HCl}}{1\text{ mol }Cl_2} = 7.0\text{ moles HCl}$$

Step 2 Less HCl is formed with Cl_2, so it is the limiting reactant. The maximum amount of product is 7.0 moles.

Limiting Reactant Problems

How many moles of Fe_3O_4 can be produced from 16.8 g Fe and 10.0 g H_2O? What is the limiting reactant?

$3\ Fe + 4\ H_2O \longrightarrow Fe_3O_4 + 4\ H_2$

Step 1 **Calculate the moles of Fe_3O_4 formed from each reactant using the appropriate molar masses and mole ratios.**

$$16.8\ \text{g Fe} \times \frac{1\ \text{mol Fe}}{55.45\ \text{g Fe}} \times \frac{1\ \text{mol } Fe_3O_4}{3\ \text{mol Fe}} = 0.1001\ \text{mol } Fe_3O_4$$

$$10.0\ \text{g } H_2O \times \frac{1\ \text{mol } H_2O}{18.02\ \text{g } H_2O} \times \frac{1\ \text{mol } Fe_3O_4}{4\ \text{mol } H_2O} = 0.139\ \text{mol } Fe_3O_4$$

Step 2 **Less Fe_3O_4 is formed with Fe, so it is the limiting reactant. The maximum amount of product is 0.1001 moles.**

Limiting Reactant Problems

How many grams of AgBr can be produced from 50.0 g $MgBr_2$ and 100.0 g $AgNO_3$? How much excess reactant remains?

$MgBr_2 + 2\ AgNO_3 \longrightarrow 2\ AgBr + Mg(NO_3)_2$

Step 1 **Calculate the mass of AgBr formed from each reactant using the appropriate molar masses and mole ratios.**

$$50.0\ \text{g } MgBr_2 \times \frac{1\ \text{mol } MgBr_2}{184.1\ \text{g } MgBr_2} \times \frac{2\ \text{mol AgBr}}{1\ \text{mol } MgBr_2} \times \frac{187.4\ \text{g AgBr}}{1\ \text{mol AgBr}}$$

$$= 102\ \text{g AgBr}$$

Limiting Reactant Problems

How many grams of AgBr can be produced from 50.0 g $MgBr_2$ and 100.0 g $AgNO_3$? How much excess reactant remains?

$MgBr_2 + 2\ AgNO_3 \longrightarrow 2\ AgBr + Mg(NO_3)_2$

Step 1 **Calculate the mass of AgBr formed from each reactant using the appropriate molar masses and mole ratios.**

$$100.0\ \text{g } AgNO_3 \times \frac{1\ \text{mol } AgNO_3}{169.9\ \text{g } AgNO_3} \times \frac{2\ \text{mol AgBr}}{2\ \text{mol } AgNO_3} \times \frac{187.4\ \text{g AgBr}}{1\ \text{mol AgBr}}$$

$$= 110.3\ \text{g AgBr}$$

Step 2 **Less AgBr is formed with $MgBr_2$, so it is the limiting reactant. The maximum amount of product is 102 g.**

Limiting Reactant Problems

From the problem on the previous slide, how much excess reactant remains?

$MgBr_2 + 2\ AgNO_3 \longrightarrow 2\ AgBr + Mg(NO_3)_2$

Step 3 **Calculate how much $AgNO_3$ reacts with the limiting reactant, assuming all $MgBr_2$ reacts.**

$$50.0\ \text{g } MgBr_2 \times \frac{1\ \text{mol } MgBr_2}{184.1\ \text{g } MgBr_2} \times \frac{2\ \text{mol } AgNO_3}{1\ \text{mol } MgBr_2} \times \frac{169.9\ \text{g } AgNO_3}{1\ \text{mol } AgNO_3}$$

$$= 92.3\ \text{g } AgNO_3$$

Unreacted $AgNO_3$ = initial – amount reacted

= 100.0 g – 92.3 g = 7.7 g $AgNO_3$ unused

Limiting Reactant Problems

How many grams of $BaSO_4$ can be produced from 200.0 g of $Ba(NO_3)_2$ and 100.0 g of Na_2SO_4?

$Ba(NO_3)_2 + Na_2SO_4 \longrightarrow BaSO_4 + 2\ NaNO_3$

Step 1 **Calculate the mass of $BaSO_4$ formed from each reactant using the appropriate molar masses and mole ratios.**

$$200.0\ \text{g } Ba(NO_3)_2 \times \frac{1\ \text{mol } Ba(NO_3)_2}{261.4\ \text{g } Ba(NO_3)_2} \times \frac{1\ \text{mol } BaSO_4}{1\ \text{mol } Ba(NO_3)_2} \times \frac{233.4\ \text{g } BaSO_4}{1\ \text{mol } BaSO_4}$$

$$= 178.6\ \text{g } BaSO_4$$

Limiting Reactant Practice

How many grams of $BaSO_4$ can be produced from 200.0 g of $Ba(NO_3)_2$ and 100.0 g of Na_2SO_4?

$Ba(NO_3)_2 + Na_2SO_4 \longrightarrow BaSO_4 + 2\ NaNO_3$

Step 1 **Calculate the mass of $BaSO_4$ formed from each reactant using the appropriate molar masses and mole ratios.**

$$100.0\ \text{g } Na_2SO_4 \times \frac{1\ \text{mol } Na_2SO_4}{142.0\ \text{g } Na_2SO_4} \times \frac{1\ \text{mol } BaSO_4}{1\ \text{mol } Na_2SO_4} \times \frac{233.4\ \text{g } BaSO_4}{1\ \text{mol } BaSO_4}$$

$$= 164.4\ \text{g } BaSO_4$$

Step 2 **Less $BaSO_4$ is formed with Na_2SO_4, so it is the limiting reactant. The maximum amount of product is the smaller amount, 164.4 g.**

Reaction Yield

The amount of products formed calculated by stoichiometry are the maximum yields possible (100%).

Yields are often lower due to side reactions, loss of product while isolating/transferring the material, etc.

Theoretical yield: maximum possible yield for a reaction, calculated based on the balanced chemical equation.

Actual yield: actual yield obtained from the reaction.

Percent yield: ratio of the actual and theoretical yield

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

Calculate % Yield

Calculate the percent yield of AgBr if 375.0 g of the compound are prepared from 200.0 g of $MgBr_2$.

$$MgBr_2 + 2\,AgNO_3 \longrightarrow Mg(NO_3)_2 + 2\,AgBr$$

To calculate the % yield, calculate the theoretical yield.

Solution Map

$$\text{g } MgBr_2 \longrightarrow \text{mol } MgBr_2 \longrightarrow \text{mol AgBr} \longrightarrow \text{g AgBr}$$

$$200.0\ \cancel{\text{g } MgBr_2} \times \frac{1\ \cancel{\text{mol } MgBr_2}}{184.1\ \cancel{\text{g } MgBr_2}} \times \frac{2\ \cancel{\text{mol AgBr}}}{1\ \cancel{\text{mol } MgBr_2}} \times \frac{187.8 \text{ g AgBr}}{1\ \cancel{\text{mol AgBr}}} = 408.0 \text{ g AgBr}$$

With theoretical yield, we can calculate % yield

$$\% \text{ yield} = \frac{\text{Actual yield}}{\text{Theoretical yield}} \times 100 = \frac{375.0 \text{ g}}{408.0 \text{ g}} \times 100 = 91.91\ \%$$

% Yield Practice

Calculate the percent yield of Al_2O_3 if 125.0 g of Al give 100.0 g of Al_2O_3.

$$2\,Al + 3\,CrO \longrightarrow Al_2O_3 + 3\,Cr$$

To calculate the % yield, calculate the theoretical yield.

Solution Map

$$\text{g Al} \longrightarrow \text{mol Al} \longrightarrow \text{mol } Al_2O_3 \longrightarrow \text{g } Al_2O_3$$

$$125.0\ \cancel{\text{g Al}} \times \frac{1\ \cancel{\text{mol Al}}}{26.98\ \cancel{\text{g Al}}} \times \frac{1\ \cancel{\text{mol } Al_2O_3}}{2\ \cancel{\text{mol Al}}} \times \frac{102.0 \text{ g } Al_2O_3}{1\ \cancel{\text{mol } Al_2O_3}} = 236.3 \text{ g } Al_2O_3$$

With theoretical yield, we can calculate % yield

$$\% \text{ yield} = \frac{\text{Actual yield}}{\text{Theoretical yield}} \times 100 = \frac{100.0 \text{ g}}{236.3 \text{ g}} \times 100 = 42.32\ \%$$

Learning Objectives

9.1 Introduction to Stoichiometry

Define stoichiometry and describe the strategy required to solve problems based on chemical equations.

9.2 Mole-Mole Calculations

Solve problems where the reactants and products are both in moles.

9.3 Mole-Mass Calculations

Solve problems where known mass is given and the answer is to be determined in moles or the moles of known are given and mass is determined.

Learning Objectives

9.4 Mass-Mass Calculations

Solve problems where mass is given and the desired unit to be determined is mass.

9.5 Limiting Reactant and Yield Calculations

Solve problems involving limiting reactants and yield.