Chapter 3. Stoichiometry: Calculations with Chemical Formulas and Equations

Common Student Misconceptions

• Students confuse the subscripts in a chemical formula with the coefficients in front of the formula in a balanced reaction equation.
• Students have difficulties grasping the meaning of a mole as a “collective”; a mole of a substance contains a fixed number \((6.022 \times 10^{23})\) of “building blocks” (atoms for most elements, molecules for molecular substances, formula units for ionic substances) in the same fashion as a dozen means 12 (eggs, people, items, etc.).
• Students often do not understand that mass of 1 mole of substance X can be significantly different from the mass of substance Y.
• Some students cannot distinguish between the number of moles actually manipulated in the laboratory versus the number of moles required by stoichiometry.
• Students do not appreciate that the coefficients in an empirical formula are not exact whole numbers because of experimental or round-off errors. In general, students have problems with the existence of experimental error.
• Students do not understand the difference between the amount of material present in the laboratory (or given in the problem) and the number of moles required by stoichiometry.
• Students do not understand that the reagent that gives the smallest amount of product is the limiting reactant.
• Students are often quite happy with a percent yield in excess of 100%.

Teaching Tips

• Students who have good high school backgrounds find this chapter quite easy. Others find this chapter extremely difficult. Very few students have heard the term stoichiometry and can be intimidated by the language of chemistry.
• Balancing equations requires some trial and error. Algorithm-loving students find this uncomfortable. It helps to make some “errors” on purpose when teaching how to balance reaction equations and show some common “tricks” of how to recover from those errors.
• The concept of limiting reactants is one of the most difficult for beginning students. Students need a lot of numerical practice here. The use of analogies is often quite helpful.
• Atomic weights may be obtained with many significant figures. Advise students to use a sufficient number of significant figures such that the number of significant figures in the answer to any calculation is not limited by the number of significant figures in the formula weights they use.

Lecture Outline

3.1 Chemical Equations\(^1,2,3,4,5\)

• The quantitative nature of chemical formulas and reactions is called stoichiometry.
• Lavoisier observed that mass is conserved in a chemical reaction.
  • This observation is known as the law of conservation of mass.

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\(^1\) “More Chemistry in a Soda Bottle: A Conservation of Mass Activity” from Further Readings
\(^2\) “Antoine Lavoisier and The Conservation of Matter” from Further Readings
\(^3\) “Chemical Wastes and the Law of Conservation of Matter” from Further Readings
\(^4\) “Formation of Water” Movie from Instructor’s Resource CD/DVD
\(^5\) Figure 3.3 from Transparency Pack
Chemical equations give a description of a chemical reaction. There are two parts to any equation:

- **reactants** (written to the left of the arrow) and
- **products** (written to the right of the arrow):

\[ 2H_2 + O_2 \rightarrow 2H_2O \]

There are two sets of numbers in a chemical equation:

- numbers in front of the chemical formulas (called stoichiometric coefficients) and
- numbers in the formulas (they appear as subscripts).

Stoichiometric coefficients give the *ratio* in which the reactants and products exist.
The subscripts give the ratio in which the atoms are found in the molecule.

Example:

- \( H_2O \) means there are two \( H \) atoms for each one molecule of water.
- \( 2H_2O \) means that there are two water molecules present.

Note: in \( 2H_2O \) there are *four* hydrogen atoms present (two for each water molecule).

**Balancing Equations**

Matter cannot be lost in any chemical reaction.

Therefore, the products of a chemical reaction have to account for all the atoms present in the reactants—we must *balance* the chemical equation.

When balancing a chemical equation we adjust the stoichiometric coefficients in front of chemical formulas.

- Subscripts in a formula are *never* changed when balancing an equation.
- Example: the reaction of methane with oxygen:

\[ CH_4 + O_2 \rightarrow CO_2 + H_2O \]

- Counting *atoms* in the reactants yields:
  - 1 C;
  - 4 H; and
  - 2 O.
- In the products we see:
  - 1 C;
  - 2 H; and
  - 3 O.
- It appears as though H has been lost and O has been created.
- To balance the equation, we adjust the stoichiometric coefficients:

\[ CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O \]
Indicating the States of Reactants and Products

- The physical state of each reactant and product may be added to the equation:
  \[ \text{CH}_4(g) + 2\text{O}_2(g) \rightarrow \text{CO}_2(g) + 2\text{H}_2\text{O}(g) \]
- Reaction conditions occasionally appear above or below the reaction arrow (e.g., "\(\Delta\)" is often used to indicate the addition of heat).

**FORWARD REFERENCES**

- Stoichiometric coefficients will be used to determine molar ratios (stoichiometric factors) in stoichiometric questions later in Chapter 3 as well as in Chapter 4 (section 4.6 on solution stoichiometry), Chapter 5 (stoichiometry of heat and Hess’s Law), Chapter 10 (stoichiometry of gaseous reactions), Chapter 20 (section 20.9 on electrolysis).
- Stoichiometric coefficients will appear as powers to which concentrations and pressures are raised when writing equilibrium constant expressions of reversible reactions in Chapters 15-17, 19-20, and when writing rate law equations for elementary steps in Chapter 14.

3.2 Some Simple Patterns of Chemical Reactivity

**Combination and Decomposition Reactions**

- In **combination reactions** two or more substances react to form one product.
- Combination reactions have more reactants than products.
  - Consider the reaction:
    \[ 2\text{Mg}(s) + \text{O}_2(g) \rightarrow 2\text{MgO}(s) \]
  - Since there are fewer products than reactants, the Mg has combined with \(\text{O}_2\) to form \(\text{MgO}\).
  - Note that the structure of the reactants has changed.
  - Mg consists of closely packed atoms and \(\text{O}_2\) consists of dispersed molecules.
  - \(\text{MgO}\) consists of a lattice of \(\text{Mg}^{2+}\) and \(\text{O}^{2-}\) ions.
- In **decomposition reactions** one substance undergoes a reaction to produce two or more other substances.
  - Decomposition reactions have more products than reactants.
  - Consider the reaction that occurs in an automobile air bag:
    \[ 2\text{NaN}_3(s) \rightarrow 2\text{Na}(s) + 3\text{N}_2(g) \]
  - Since there are more products than reactants, the sodium azide has decomposed into sodium metal and nitrogen gas.

**Combustion Reactions**

- **Combustion reactions** are rapid reactions that produce a flame.
  - Most combustion reactions involve the reaction of \(\text{O}_2(g)\) from air.
  - Example: combustion of a hydrocarbon (propane) to produce carbon dioxide and water.
    \[ \text{C}_3\text{H}_8(g) + 5\text{O}_2(g) \rightarrow 3\text{CO}_2(g) + 4\text{H}_2\text{O}(l) \]

**FORWARD REFERENCES**

- Combustion reactions will be mentioned in Chapter 5 (as exothermic reactions involving fuels) and further discussed in Chapter 24 (as oxidation of organic compounds).
- Additional specific/important types of reactions will be introduced throughout the textbook.

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18 “Lime” from Further Readings
19 Figure 3.6 from Transparency Pack
20 “Reactions with Oxygen” Movie from Instructor’s Resource CD/DVD
21 “Air Bags” Animation from Instructor’s Resource CD/DVD
22 “Nitrogen Triiodide” Movie from Instructor’s Resource CD/DVD
23 “Formation of Aluminum Bromide” Movie from Instructor’s Resource CD/DVD
3.3 Formula Weights

**Formula and Molecular Weights**

- **Formula weight (FW)** is the sum of atomic weights for the atoms shown in the chemical formula.
  - Example: FW (H₂SO₄)
    - \( = 2\text{AW}(H) + \text{AW}(S) + 4\text{AW}(O) \)
    - \( = 2(1.0 \text{ amu}) + 32.1 \text{ amu} + 4(16.0 \text{ amu}) = 98.1 \text{ amu} \).

- **Molecular weight (MW)** is the sum of the atomic weights of the atoms in a molecule as shown in the molecular formula.
  - Example: MW (C₆H₁₂O₆)
    - \( = 6(12.0 \text{ amu}) + 12(1.0 \text{ amu}) + 6(16.0 \text{ amu}) \)
    - \( = 180.0 \text{ amu} \).
  - Formula weight of the repeating unit (formula unit) is used for ionic substances.
    - Example: FW (NaCl)
      - \( = 23.0 \text{ amu} + 35.5 \text{ amu} \)
      - \( = 58.5 \text{ amu} \).

**Percentage Composition from Formulas**

- Percentage composition is obtained by dividing the mass contributed by each element (number of atoms times AW) by the formula weight of the compound and multiplying by 100.

\[
\% \text{ element} = \frac{\text{(number of atoms of that element)(atomic weight of element)(100)}}{\text{formula weight of compound}}
\]

**FORWARD REFERENCES**

- The ability to calculate molecular and formula weights will be an essential skill in finding molar masses throughout the textbook.

3.4 Avogadro’s Number and The Mole

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24 “Gram Formula Weights and Fruit Salad” from Further Readings
25 “Percentage Composition and Empirical Formula—A New View” from Further Readings
26 “Molecular Weight and Weight Percent” Activity from Instructor’s Resource CD/DVD
27 “Mole, Mole per Liter, and Molar: A Primer on SI and Related Units for Chemistry Students” from Further Readings
28 “Developing an Intuitive Approach to Moles” from Further Readings
29 “The Mole, the Periodic Table, and Quantum Numbers: An Introductory Trio” from Further Readings
30 “The Size of a Mole” from Further Readings
31 “What’s a Mole For?” from Further Readings
32 “The Mole Concept: Developing an Instrument to Assess Conceptual Understanding” from Further Readings
33 “A Mole of M&Ms” from Further Readings
34 “How to Visualize Avogadro’s Number” from Further Readings
35 “Measuring Avogadro’s Number on the Overhead Projector” from Live Demonstrations
36 “Demonstrations for Nonscience Majors: Using Common Objects to Illustrate Abstract Concepts” from Live Demonstrations
37 “Using Monetary Analogies to Teach Average Atomic Mass” from Further Readings
38 “Pictorial Analogies IV: Relative Atomic Weights” from Further Readings
39 “Relative Atomic Mass and the Mole: A Concrete Analogy to Help Students These Abstract Concepts” from Further Readings
• The mole (abbreviated "mol") is a convenient measure of chemical quantities.
• 1 mole of something = \(6.0221421 \times 10^{23}\) of that thing.
  - This number is called Avogadro’s number.
  - Thus, 1 mole of carbon atoms = \(6.0221421 \times 10^{23}\) carbon atoms.
• Experimentally, 1 mole of \(^{12}\text{C}\) has a mass of 12 g.

### Molar Mass

- The mass in grams of 1 mole of substance is said to be the molar mass of that substance. Molar mass has units of \(g/\text{mol}\) (also written \(g\cdot\text{mol}^{-1}\)).
- The mass of 1 mole of \(^{12}\text{C}\) = 12 g. Exactly.
- The molar mass of a molecule is the sum of the molar masses of the atoms:
  - Example: The molar mass of \(\text{N}_2\) = \(2 \times\) (molar mass of N).
- Molar masses for elements are found on the periodic table.
- The formula weight (in amu) is numerically equal to the molar mass (in \(g/\text{mol}\)).

### Interconverting Masses and Moles

- Look at units:
  - Mass: \(g\)
  - Moles: \(\text{mol}\)
  - Molar mass: \(g/\text{mol}\)
- To convert between grams and moles, we use the molar mass.

### Interconverting Masses and Numbers of Particles

- Units:
  - Number of particles: \(6.022 \times 10^{23}\) \(\text{mol}^{-1}\) (Avogadro’s number).
  - Note: \(g/\text{mol} \times \text{mol} = g\) (i.e. molar mass \(\times\) moles = mass), and
  - \(\text{mol} \times \text{mol}^{-1} = \) a number (i.e. moles \(\times\) Avogadro’s number = molecules).
- To convert between moles and molecules we use Avogadro’s number.

### FORWARD REFERENCES

- It may be desirable to calculate molar masses with higher precision in later chapters.
- Avogadro number will be used to calculate the energy of 1 mole of photons in Chapter 6.
- Moles of electrons will be used in Chapter 7 (ionization energy or electron affinity), and in Chapter 20 to balance half-reactions and solve electrolysis problems.
- Bond dissociation energies (Chapter 8) and tabulated thermodynamic data (Appendix C) are mostly expressed per mole of bonds or substance.
- Moles will be used to calculate molar and molal concentrations (Chapters 4 and 11).
- Moles will be used in the Ideal Gas Law in Chapter 10.

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40 “Moles, Pennies, and Nickels” from Further Readings
41 “A Mole Mnemonic” from Further Readings
42 “Analogies to Indicate the Size of Atoms and Molecules and the Magnitude of Avogadro’s Number” from Further Readings
43 Figure 3.8 from Transparency Pack
44 “Demonstrations of the Enormity of Avogadro’s Number” from Further Readings
45 “For Mole Problems, Call Avogadro: 602-1023” from Further Readings
46 Figure 3.12 from Transparency Pack
3.5 Empirical Formulas from Analyses

• Recall that the empirical formula gives the relative number of atoms of each element in the molecule.

• Finding empirical formula from mass percent data:
  • We start with the mass percent of elements (i.e. empirical data) and calculate a formula.
  • Assume we start with 100 g of sample.
  • The mass percent then translates as the number of grams of each element in 100 g of sample.
  • From these masses, the number of moles can be calculated (using the atomic weights from the periodic table).
  • The lowest whole-number ratio of moles is the empirical formula.

• Finding the empirical mass percent of elements from the empirical formula.
  • If we have the empirical formula, we know how many moles of each element is present in one mole of same.
  • Then we use molar masses (or atomic weights) to convert to grams of each element.
  • We divide the number of grams of each element by the number of grams of 1 mole of sample to get the fraction of each element in 1 mole of sample.
  • Multiply each fraction by 100 to convert to a percent.

Molecular Formulas from Empirical Formulas

• The empirical formula (relative ratio of elements in the molecule) may not be the molecular formula (actual ratio of elements in the molecule).

• Example: ascorbic acid (vitamin C) has the empirical formula C\textsubscript{6}H\textsubscript{8}O\textsubscript{6}.
  • The molecular formula is C\textsubscript{6}H\textsubscript{8}O\textsubscript{6}.
  • To get the molecular formula from the empirical formula, we need to know the molecular weight, MW.
  • The ratio of molecular weight (MW) to formula weight (FW) of the empirical formula must be a whole number.

Combustion Analysis

• Empirical formulas are routinely determined by combustion analysis.
• A sample containing C, H, and O is combusted in excess oxygen to produce CO\textsubscript{2} and H\textsubscript{2}O.
• The amount of CO\textsubscript{2} gives the amount of C originally present in the sample.

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47 “Water” 3-D Model from Instructor’s Resource CD/DVD
48 “Hydrogen Peroxide” 3-D Model from Instructor’s Resource CD/DVD
49 “Sucrose” 3-D Model from Instructor’s Resource CD/DVD
50 “Oxygen” 3-D Model from Instructor’s Resource CD/DVD
51 “Methane” 3-D Model from Instructor’s Resource CD/DVD
52 “Carbon Dioxide” 3-D Model from Instructor’s Resource CD/DVD
53 “Glycine (molecular form)” 3-D Model from Instructor’s Resource CD/DVD
54 “Ethane” 3-D Model from Instructor’s Resource CD/DVD
55 “Methanol” 3-D Model from Instructor’s Resource CD/DVD
56 “A Known-to-Unknown Approach to Teach About Empirical and Molecular Formulas” from Further Readings
58 “A Simple Rhyme for a Simple Formula” from Further Readings
59 Figure 3.13 from Transparency Pack
60 “Empirical Formula Determination: C\textsubscript{6}H\textsubscript{6}O” Activity from Instructor’s Resource CD/DVD
61 “Copper Sulfate: Blue to White” from Live Demonstrations
62 “Combustion of Hydrocarbons: A Stoichiometry Demonstration” from Live Demonstrations

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The amount of H₂O gives the amount of H originally present in the sample.
- Watch the stoichiometry: 1 mol H₂O contains 2 mol H.
- The amount of O originally present in the sample is given by the difference between the amount of sample and the amount of C and H accounted for.
- More complicated methods can be used to quantify the amounts of other elements present, but they rely on analogous methods.

3.6 Quantitative Information from Balanced Equations

- The coefficients in a balanced chemical equation give the relative numbers of molecules (or formula units) involved in the reaction.
- The stoichiometric coefficients in the balanced equation may be interpreted as:
  - the relative numbers of molecules or formula units involved in the reaction or
  - the relative numbers of moles involved in the reaction.
- The molar quantities indicated by the coefficients in a balanced equation are called stoichiometrically equivalent quantities.
- Stoichiometric factors (or molar ratios) may be used to convert between quantities of reactants and products in a reaction.
- It is important to realize that the stoichiometric ratios are the ideal proportions in which reactants are needed to form products.
- A balanced reaction equation often provides more stoichiometric factors (or molar ratios) than needed to solve any particular stoichiometric problem. Often only one or two of them are relevant in a given problem.
- The number of grams of reactant cannot be directly related to the number of grams of product.
  - To get grams of product from grams of reactant:
    - convert grams of reactant to moles of reactant (use molar mass),
    - convert moles of one reactant to moles of other reactants and products (use the stoichiometric ratio from the balanced chemical equation),
    - convert moles back into grams for desired product (use molar mass).

FORWARD REFERENCES

- In Chapter 4 students will learn how to convert solution molarity and volume data into moles.
- In Chapter 10 students will learn how to use P, V and T information to find moles of gas.
- Stoichiometry of reactions will be further exploited when writing rate law expressions for elementary steps (Chapter 14) as well as equilibrium constant and reaction quotient expressions (Chapters 15, 16, 17, 19, and 20).
- Acid-base titrations mentioned in Chapter 4, and further discussed in Chapter 17, are practical applications of stoichiometry of acid-base neutralization reactions.

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63 “How Many Digits Should We Use in Formula or Molar Mass Calculation” from Further Readings
64 “Amounts Tables as a Diagnostic Tool for Flawed Stoichiometric Reasoning” from Further Readings
65 “Stoogiometry: A Cognitive Approach to Teaching Stoichiometry” from Further Readings
66 “Teaching Stoichiometry: A Two-Cycle Approach” from Further Readings
67 “Pictorial Analogies XII: Stoichiometric Calculations” from Further Readings
68 Figure 3.16 from Transparency Pack
69 “Stoichiometry Calculation” Activity from Instructor’s Resource CD/DVD
70 “A Recipe for Teaching Stoichiometry” from Further Readings
3.7 Limiting Reactants

- It is not necessary to have all reactants present in stoichiometric amounts.
- Often, one or more reactants is present in excess.
- Therefore, at the end of reaction those reactants present in excess will still be in the reaction mixture.
- The one or more reactants which are completely consumed are called the limiting reactants.
- Reactants present in excess are called excess reactants.
- Consider 10 H₂ molecules mixed with 7 O₂ molecules to form water.
  - The balanced chemical equation tells us that the stoichiometric ratio of H₂ to O₂ is 2 to 1:
    \[ 2\text{H}_2(g) + \text{O}_2(g) \rightarrow 2\text{H}_2\text{O}(l) \]
  - This means that our 10 H₂ molecules require 5 O₂ molecules (2:1).
  - Since we have 7 O₂ molecules, our reaction is limited by the amount of H₂ we have (the O₂ is present in excess).
  - So, all 10 H₂ molecules can (and do) react with 5 of the O₂ molecules producing 10 H₂O molecules.
  - At the end of the reaction, 2 O₂ molecules remain unreacted.

Theoretical Yields

- The amount of product predicted from stoichiometry, taking into account limiting reactants, is called the theoretical yield.
  - This is often different from the actual yield – the amount of product actually obtained in the reaction.
  - The percent yield relates the actual yield (amount of material recovered in the laboratory) to the theoretical yield:
    \[
    \text{Percent yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100
    \]

FORWARD REFERENCES

- Buffering action calculations in Chapter 17 (section 17.2) and pH calculations in acid-base titrations (section 17.3) can be viewed as stoichiometric problems with a limiting reactant (added strong acid or base).

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71 “Learning Stoichiometry with Hamburger Sandwiches” from Further Readings
72 “Limiting Reagent” Animation from Instructor’s Resource CD/DVD
73 “Limiting and Excess Reagents, Theoretical Yield” from Further Readings
74 “Limiting Reagents” Activity from Instructor’s Resource CD/DVD
75 “Limiting Reactant: An Alternative Analogy” from Further Readings
76 “Limiting Reagent Problems Made Simple for Students” from Further Readings
77 “Election Results and Reaction Yields” from Further Readings
78 Figure 3.17 from Transparency Pack
79 “Interactive Demonstrations for the Mole Ratios and Limiting Reagents” from Live Demonstrations
80 “Coffee, Coins, and Limiting Reagents” from Further Readings
81 “A Dramatic Classroom Demonstration of Limiting Reagent Using the Vinegar and Sodium Hydrogen Carbonate Reaction” from Live Demonstrations

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3-D Models:
- Water
- Hydrogen Peroxide
- Sucrose
- Oxygen
- Methane
- Carbon Dioxide
- Glycine (molecular form)
- Methanol
- Ethane

Other Resources

Further Readings:
- More Chemistry in a Soda Bottle: A Conservation of Mass Activity
- Chemical Wastes and the Law of Conservation of Matter
- Antoine Lavoisier and the Conservation of Matter
- The Fruit Basket Analogy
- Balancing Chemical Equations by Inspection
- A New Inspection Method for Balancing Redox Equations
- On Balancing Chemical Equations: Past and Present (A Critical Review and Annotated Bibliography)
- How to Say How Much: Amounts and Stoichiometry
- Lime
- Gram Formula Weights and Fruit Salad
- Percentage Composition and Empirical Formula—A New View
- Mole, Mole per Liter, and Molar. A Primer on SI and Related Units for Chemistry Students
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Section:
- 3.5 Empirical Formulas from Analyses
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Section:
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Section:
- 3.3 Formula Weights
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Section:
- 3.4 Avogadro’s Number and the Mole
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Further Readings:


**Live Demonstrations:**


